Applications of harmonic analysis to discrete geometry

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Abstract

Fabrício Caluza Machado. **Applications of harmonic analysis to discrete geometry**. Thesis (Doctorate). Institute of Mathematics and Statistics, University of São Paulo, São Paulo, 2021.

Harmonic analysis is the analysis of function spaces under the action of some group. In this project we consider applications of Harmonic analysis on Euclidean space, via the group action of translations, and applications of Harmonic analysis on the sphere, via the orthogonal group action. While the analysis on Euclidean space leads to the classical Fourier analysis and operations such as the Fourier transform, representation theory allows us to see the action of the orthogonal group with the same lens, in such a way that to functions of positive type correspond invariant and positive kernels in the sphere and to the Fourier inversion formula corresponds the decomposition of a spherical function into spherical harmonics. In this thesis we apply these elements to three different geometrical problems. In the first project we use semidefinite programming to bound the maximum number of equiangular lines with a fixed common angle in the Euclidean space and we show how this bound relates to previously known bounds for spherical codes and to independent sets in graphs. In the second project we consider the counting of integer points in dilates of a rational polytope P and use the development of the Fourier transform of a polytope via Stokes formula to determine a formula for the second-order Ehrhart coefficient, namely the coefficient of t^{d-2} in $|tP \cap \mathbb{Z}^d|$. In the third project we consider again the Fourier transform of a polytope and use its development via Brion's theorem to show that it does not contain circles in its null set.

Keywords: Fourier analysis. polytopes. lattice sums. packing. equiangular lines. semidefinite programming bounds. spherical harmonics. Ehrhart quasi-polynomials.

Resumo

Fabrício Caluza Machado. **Aplicações de análise harmônica em geometria discreta**. Tese (Doutorado). Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2021.

Análise harmônica é a análise de espaços de funções sob a ação de algum grupo. Neste projeto consideramos aplicações de análise harmônica no espaço Euclideano, via a ação de translação, e aplicações de análise harmônica na esfera, via a ação do grupo ortogonal. Enquanto a análise no espaço Euclideano leva à análise de Fourier clássica e a operações tais como a transformada de Fourier, a teoria das representações nos permite ver a ação do grupo ortogonal sob um mesmo ponto de vista. Às funções de tipo positivo correspondem os núcleos positivos e invariantes na esfera e à fórmula de inversão de Fourier corresponde a decomposição de uma função esférica em harmônicos esféricos. Nesta tese aplicamos esses elementos em três problemas geométricos distintos. No primeiro projeto, usamos programação semidefinida para limitar o número máximo de retas equiangulares com um ângulo em comum fixo e mostramos como esse limitante se relaciona com limitantes conhecidos para códigos esféricos e para o número de independência de grafos. No segundo projeto consideramos a contagem de pontos inteiros em dilatações de um politopo racional P e usamos o desenvolvimento da transformada de Fourier de um politopo pela fórmula de Stokes para determinar uma fórmula para o coeficiente de Ehrhart de segunda ordem, a saber o coeficiente de t^{d-2} em $|tP \cap \mathbb{Z}^d|$. No terceiro projeto consideramos novamente a transformada de Fourier de um politopo e usamos seu desenvolvimento pelo teorema de Brion para mostrar que ela não possui círculos no seu conjunto nulo.

Palavras-chave: análise de Fourier. politopos. somas em reticulados. empacotamentos. retas equiangulares. limitantes de programação semidefinida. harmônicos esféricos. quasi-polinômios de Ehrhart.

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Chapter 1

Introduction

What is the maximum number of points that can be arranged in a sphere such that their pairwise distances lie in a prescribed set? How well can we estimate the difference between the number of lattice points inside a polytope and its volume, namely $\left||P \cap \frac{1}{t}\mathbb{Z}^d| - t^d \mathrm{vol}(P)\right|$, as t grows and the lattice becomes finer? Does the integral of a continuous function over a polytope and over all of its rigid motions determine the function uniquely? These are some questions considered in this thesis.

Although very different, the first two questions can be seen as problems of discrete geometry and all the three can be solved with similar methods. Matoušek [Mat02] mentions in his preface that "discrete geometry" is admittedly a vague term and presents a selection of topics that these problems may cover. Among them, we mention polyhedral combinatorics; arrangements of convex bodies such as packings, coverings and tilings; problems with lattices; and geometric algorithms. Given the variety of topics, we focus more on the methods and treat these problems as applications for them.

One interesting feature of the problems we consider is that they combine discrete combinatorial properties with the continuous domain on which they are defined: the Euclidean space $\mathbb{R}^d$ and the unit sphere $S^{d-1} := \{x \in \mathbb{R}^d : \|x\| = 1\}$. Furthermore, all problems have symmetries and the analysis of the associated group actions provide a unifying perspective to study them.

A short example that may serve as inspiration for this thesis is the question of whether a measurable set $S \subset \mathbb{R}^d$ tiles $\mathbb{R}^d$ by integer translations, that is, whether the collection $\{S + n : n \in \mathbb{Z}^d\}$ covers $\mathbb{R}^d$ while every two distinct elements have disjoint interior. Defining the *indicator function* $\mathbb{1}_S(x) := 1$ if $x \in S$ and $\mathbb{1}_S(x) := 0$ otherwise, we may express the tiling condition as

$$\sum_{n \in \mathbb{Z}^d} \mathbb{1}_{S+n}(x) = 1 \quad \text{for almost every } x \in \mathbb{R}^d.$$

Since $\mathbb{1}_{S+n}(x) = \mathbb{1}_S(x - n)$, this series defines a periodic function in x. Hence, as we see in Section 2.4.2, it has a Fourier series expansion whose coefficients are given by the Fourier transform of $\mathbb{1}_S$:

$$\sum_{n\in\mathbb{Z}^d} \mathbb{1}_S(x-n) \sim \sum_{n\in\mathbb{Z}^d} \hat{\mathbb{1}}_S(n) e^{2\pi i\langle n,x\rangle},$$

where the symbol ~ stands for an equality in the $L^2([0,1]^d)$-norm, $\langle n, x\rangle$ is the Euclidean inner product between n and x, and $\hat{\mathbb{1}}_S : \mathbb{R}^d \longrightarrow \mathbb{C}$ is defined as

$$\hat{\mathbb{1}}_S(\xi) := \int_S e^{-2\pi i\langle \xi,u\rangle}\,\mathrm{d}u.$$

By the uniqueness of the Fourier series coefficients, the condition that the series has to be equal to 1 almost everywhere is equivalent to $\hat{\mathbb{1}}_S(0) = \mathrm{vol}(S) = 1$ and $\hat{\mathbb{1}}_S(n) = 0$ for all $n \in \mathbb{Z}^d \setminus \{0\}$. Therefore we have an example of a geometrical question that can be answered by the knowledge of $\hat{\mathbb{1}}_S$.

The application $S \mapsto \hat{\mathbb{1}}_S$ extends to a *solid valuation* in the algebra of polyhedra, that is, a linear transformation in the vector space spanned by the indicator functions of all polyhedra which assigns a function to each polyhedra and satisfies relations such as $\hat{\mathbb{1}}_{P\cup S} = \hat{\mathbb{1}}_P + \hat{\mathbb{1}}_S$ whenever $P \cap S$ is not full-dimensional. Similarly, the map

$$S \mapsto \sum_{n\in S\cap\mathbb{Z}^d} e^{-2\pi i\langle \xi,n\rangle}$$

can also be extended to a *valuation* in the algebra of rational polyhedra, that is, a linear transformation ϕ in the vector space spanned by the indicator functions of all rational polyhedra which assigns a function to each polyhedra and satisfies relations such as $\phi(P\cup S) = \phi(P)+\phi(S)-\phi(P\cap S)$. These two valuations can be used to find relations between the volume $\mathrm{vol}(P)$ and the number of integer points $|P\cap\mathbb{Z}^d|$ of a polytope and of its faces. Brion's theorem (Theorems 5.2.6 and 5.2.8) expresses these valuations in terms of the tangent cones at the vertices and this can be used to produce efficient algorithms to count the number of integer points in a polytope when the dimension d is fixed, as done by Barvinok [Bar94] (see also the survey of Barvinok and Pommersheim [BP99]) and more generally, to sum a polynomial in the integer points of a polytope, as done by Berline and Vergne [BV07]. The recent book of Robins [Rob21] provides background for Fourier analysis on polytopes and polyhedral cones.

We use representation theory to study the action of the orthogonal group in the space of spherical functions and this approach allows a comparison with Fourier analysis. To a function of positive type corresponds a positive and invariant kernel and to the Fourier inversion formula corresponds the decomposition of a function into spherical harmonics, which in turn leads to the Gegenbauer polynomials as the building blocks for the positive and invariant kernels in the sphere. In this context the analysis of the Cohn-Elkies bound for the sphere packing density has a special role, since it ties together the Fourier analysis with optimization techniques used in Chapter 4.

Outline of the thesis

Chapter 2. Harmonic Analysis. Here we give a general overview of Harmonic Analysis and present material that will be useful for the rest of the thesis. We consider representation theory to study the action of the orthogonal group and to produce a formula for the invariant and positive kernels in the sphere. We also consider classic Fourier analysis and use the Poisson summation formula to produce formulas for certain lattice sums.

Chapter 3. Packing problems. Here we show how semidefinite programming can be used to produce upper bounds for the independence number of a finite graph and that this method can be adapted to packing problems in geometry. In Section 3.3 we use this viewpoint to present the bound of Cohn and Elkies for the sphere packing density. This chapter serves as an introduction for the ensuing chapters.

Chapter 4. k-point semidefinite programming bounds for equiangular lines. This chapter presents a semidefinite programming bound for the maximum number of equiangular lines in Euclidean space with a fixed common angle. This is an extension of previously known bounds for spherical codes and uses the theory presented in Section 3.2 to strengthen them.

Chapter 5. The Fourier transform of a polytope. Here we discuss the Fourier transform of the indicator function of a polytope. We see how it can be used to count the number of lattice points in a polytope and estimate the difference with its volume. We show two complementary ways to analyze the Fourier transform: via Stokes formula, which produces an expression in terms of the facets and lower dimensional faces of the polytope and via Brion's theorem, which produces an expression in terms of the tangent cones of each vertex of the polytope. This chapter serves as an introduction for Chapters 6 and 7.

Chapter 6. Coefficients of the solid angle and Ehrhart quasi-polynomials. We show an application of the development of the Fourier transform of a polytope via Stokes formula to determine the coefficients of order t^{d-1} and t^{d-2} in $\big||tP \cap \mathbb{Z}^d| - t^d\mathrm{vol}(P)\big|$, also called Ehrhart coefficients. This is done by first considering the solid angle sum, which is defined associating weights to the integer points in the boundary of the polytope. The solid angle sum is a more precise estimate for the volume and it is more amenable to the usage of analytic techniques. It is also interesting in its own right, since for a certain class of polytopes this measure coincides with the volume of the polytope for integer values of t.

Chapter 7. The null set of a body and the Pompeiu property for polytopes. The null set of a polytope is defined as the set of zeros of its Fourier transform. In this chapter we show an application of the development of the Fourier transform of a polytope via Brion's theorem to show that no polytope contains a circle in its null set. Our result regarding the null set implies that every polytope has the Pompeiu property, which means that the integral of a function over the polytope and its rigid motions determines the function uniquely. While this fact was already known (see e.g., Williams [Wil76]), our proof, using Brion's theorem, is simpler.

Chapter 2

Harmonic Analysis

Harmonic Analysis is a term that generally refers to the analysis of function spaces under the action of some *topological group*: a group equipped with a topology in which the group operations, product and inverse, are continuous. When the underlying space is the Euclidean space $\mathbb{R}^d$, the terms "Harmonic Analysis" and "Fourier Analysis" are used interchangeably. Although our main concern are the actions by translation and rotation on functions in $\mathbb{R}^d$, the representation-theoretic approach allows for a more general treatment.

2.1 Basics of representation theory

In this section we see the basic definitions and results from representation theory. As references, we use the beginning of the books of Fulton and Harris [FH91], and Serre [Ser77] for representations of finite groups, the books of Vilenkin [Vil68] and Folland [Fol16] for representations of compact groups and the book of Rudin [Rud62] for the more general representation theory of locally compact abelian groups.

We give special attention to the compact nonabelian case, since in Section 2.3 we will be interested in the orthogonal group and its action on the sphere. We also make considerations about abelian groups and locally compact groups since in Section 2.4 we will see action of translations of the Euclidean space on itself.

One important property of locally compact groups is the existence of the *Haar measure*, which is a measure on the group that is left-invariant and has finite positive values on open subsets with compact closure (see e.g., Section 2.2. of Folland [Fol16]). With this measure we can integrate functions defined in a group G and this integral satisfies

$$\int_G f(x)\,\mathrm{d}x = \int_G f(gx)\,\mathrm{d}x,$$

for all $g \in G$. If the group is compact, the Haar measure is also right-invariant and the measure of the whole group is finite. We may therefore assume that it is normalized so that the measure of the group is 1, and then the Haar measure is unique.

A *representation* of a group G is a continuous function

$$\rho: G \longrightarrow \mathrm{GL}(V)$$

from G to the group of continuous and invertible linear transformations of a vector space V satisfying the equation

$$\rho(gh) = \rho(g)\rho(h) \tag{2.1}$$

for all $g, h \in G$. Here we will not only consider representations on finite dimensional vector spaces but also on infinite dimensional (separable) Hilbert spaces. We assume V is a Hilbert space with inner product $\langle , \rangle$ and say that the representation ρ is *unitary* if

$$\langle \rho(g)x, \rho(g)y \rangle = \langle x, y \rangle ,$$

for all $g \in G$ and $x, y \in V$.

The requirement that a representation is unitary connects the group with the inner product structure of the space. If a group is compact, then every representation in a Hilbert space is unitary for a certain scalar product in that space. Indeed, if a representation $\rho: G \longrightarrow \mathrm{GL}(V)$ is defined on a Hilbert space with inner product $\langle , \rangle_0$, then we may define

$$\langle u, v \rangle := \int_G \langle \rho(g)u, \rho(g)v \rangle_0 \, \mathrm{d}g,$$

where we use the finite measure of the group to guarantee the convergence of the integral and the invariance of the measure to conclude that the representation is unitary.

Two representations $\rho: G \longrightarrow \mathrm{GL}(V)$ and $\tau: G \longrightarrow \mathrm{GL}(W)$ are said to be *equivalent* if there exists an invertible linear operator $A: W \longrightarrow V$ such that

$$\tau(g) = A^{-1}\rho(g)A,$$

for all $g \in G$; one can check that this is indeed an equivalence relation between representations. A subspace U of V is called *invariant* if $\rho(g)x \in U$ for all $g \in G$ and $x \in U$, so that the restriction of ρ to U is a representation in U as well. If a representation only has the null space and the whole space V as invariant subspaces, the representation is said to be *irreducible*.

Lemma 2.1.1 (Schur)**.** *Let $\rho: G \longrightarrow \mathrm{GL}(V)$ and $\tau: G \longrightarrow \mathrm{GL}(W)$ be two finite dimensional irreducible representations of a group G and let $T: V \longrightarrow W$ be a continuous linear transformation that commutes with these representations, that is,*

$$T\rho(g) = \tau(g)T$$

for all $g \in G$. Then either T is the null operator or it is invertible (and consequently ρ and τ are equivalent). Furthermore, if $S: V \longrightarrow W$ is another operator that commutes with these representations, then S is a scalar multiple of T.

Proof. The first part follows easily once we observe that both the kernel and the image of T are invariant subspaces of V and W respectively. Since ρ is a irreducible representation, the kernel of T is either the null space or V and since τ is a irreducible representation, the image of T is either the null space or W. From these constraints, we conclude that T is either null or invertible.

For the second part, since $\det(S - \lambda T)$ is a polynomial in λ, there exists $\lambda \in \mathbb{C}$ such that $S - \lambda T$ is singular. Since $S - \lambda T$ commutes with the representations, by the first part of the lemma $S - \lambda T = 0$. □

Schur's lemma has an important corollary for abelian groups:

Corollary 2.1.2. *If G is abelian, then every finite dimensional irreducible representation of G is one dimensional.*

Proof. If $\rho : G \longrightarrow \mathrm{GL}(V)$ is a finite dimensional irreducible representation of an abelian group G, then for any $h \in G$, $\rho(g)\rho(h) = \rho(h)\rho(g)$ for all $g \in G$. By Lemma 2.1.1, $\rho(h)$ is a multiple of the identity for all $h \in G$. Since ρ is irreducible, V is one dimensional. □

A representation is said to be *completely reducible* if it is the direct sum of irreducible representations. A small example illustrates that not every representation is completely reducible: Consider the representation of $\mathbb{Z}$ in the two dimensional vector space $\mathbb{C}^2$ given by $\rho(n) := \left(\begin{smallmatrix} 1 & n \\ 0 & 1 \end{smallmatrix}\right)$. While $(1\ 0)^{\mathsf{T}}$ spans a one dimensional invariant subspace (so ρ is not irreducible), there is no other complementary invariant subspace.

For unitary representations, the main step for completely reducibility is given by the following lemma.

Lemma 2.1.3. *Let $\rho : G \longrightarrow \mathrm{GL}(V)$ be a unitary representation and U be an invariant subspace of V. Then the orthogonal complement of U is also invariant.*

Proof. For all $u \in U$, $v \in U^{\perp}$ and $g \in G$,

$$\langle \rho(g)v, u \rangle = \left\langle \rho(g)^{-1}\rho(g)v, \rho(g)^{-1}u \right\rangle = \langle v, \rho(g)^{-1}u \rangle = 0,$$

since $\rho(g)^{-1}u \in U$. Therefore $\rho(g)v \in U^{\perp}$ for all $g \in G$ and $U^{\perp}$ is also an invariant subspace. □

Sometimes it is convenient to write a vector space as a direct sum of two invariant subspaces without necessarily having the orthogonality. In these cases the notion of quotient representation is useful. Let $\rho : G \longrightarrow \mathrm{GL}(V)$ be a representation and U be an invariant subspace of V. The *quotient space* V/U is the space formed by the equivalence classes $v + U := \{v + u : u \in U\}$. The *quotient representation* $\tau : G \longrightarrow \mathrm{GL}(V/U)$ is the representation defined by

$$\tau(g)(v + U) := \rho(g)v + U.$$

To see that this representation is well defined, if $v + U = w + U$, then $v - w \in U$ and since U is invariant, $\rho(g)(v - w) \in U$ and thus $\rho(g)v + U = \rho(g)w + U$.

Lemma 2.1.4. *Let $\rho : G \longrightarrow \mathrm{GL}(V)$ be a representation and $V = U \oplus W$ be a decomposition of V as a direct sum of invariant subspaces. Then the restriction of ρ to W is equivalent to the quotient representation on V/U. In particular, if $V = U \oplus W_1$ and $V = U \oplus W_2$ are two* *decompositions of V as direct sum of invariant subspaces, then the restriction of ρ to W_1 is equivalent to the restriction of ρ to W_2.*

Proof. The linear transformation $\phi : W \longrightarrow V/U$ defined by $\phi(w) = w + U$ is an isomorphism between W and V/U that commutes with the representations. Indeed, for any $w \in W$ and $g \in G$,

$$\tau(g)(\phi(w)) = \tau(g)(w + U) = \rho(g)w + U = \phi(\rho(g)w). \qquad \square$$

For finite dimensional representations, a simple induction argument already implies that unitary representations are completely reducible. For infinite dimensional representations the situation is more complicated; however for compact groups it is still true that every representation is completely reducible (recall that every representation of a compact group is unitary for a suitable inner product). Even more is true: for compact groups every irreducible representation is finite dimensional, as shown in Theorem 5.2 from Folland [Fol16]:

Theorem 2.1.5. *If G is compact, then every irreducible representation of G is finite dimensional and every unitary representation of G is a direct sum of irreducible representations.*

We denote by $\hat{G}$ a complete set of non-equivalent irreducible unitary representations of the group G. The decomposition of a representation $\rho : G \longrightarrow \mathrm{GL}(V)$ as a direct sum of irreducible representations is in general not unique, however Theorem 5.3 from Folland [Fol16] says:

Theorem 2.1.6. *Let $\rho : G \longrightarrow \mathrm{GL}(V)$ be a unitary representation of a compact group G and for distinct $\pi, \pi' \in \hat{G}$, let V_π and $V_{\pi'}$ be the closed linear span of all irreducible subspaces of V on which ρ is equivalent to π and π' respectively, Then $V_\pi \perp V_{\pi'}$ and if U is any irreducible subspace of V_π, then the restriction of ρ to U is equivalent to π.*

This shows that if $\rho : G \longrightarrow \mathrm{GL}(V)$ is a unitary representation of a compact group G on a Hilbert space V, then

$$V = \bigoplus_{\pi \in \hat{G}} V_\pi, \qquad V_\pi = \bigoplus_{i=1}^{m_\pi} V_{\pi,i}, \tag{2.2}$$

where V is written uniquely as a orthogonal direct sum, while each V_π is written as a direct sum of equivalent irreducible representations, this latter decomposition being not unique. We call m_π the *multiplicity* of π in ρ even though it might be infinite.

For $\pi \in \hat{G}$, $\pi : G \longrightarrow \mathrm{GL}(H_\pi)$, let $d_\pi := \dim H_\pi$ and $\{e_1, \dots, e_{d_\pi}\}$ be an orthonormal basis for H_π. We call the matrix elements of the representation

$$\pi_{ij}(g) := \left\langle \pi(g)e_j, e_i \right\rangle,$$

special functions of G. Note that (2.1) produces many relations that they must satisfy. Some important problems in representation theory are the description (up to equivalence) of all irreducible unitary representations of a group G (frequently by means of determining its special functions) and to determine how an arbitrary representation can be built from those.

The special functions defined above depend on the basis chosen for H_π, however the linear span of the matrix elements $\pi_{i,j}$ depends only on the equivalence class of π as well the *character* of the representation, defined as $\chi_\pi : G \longrightarrow \mathbb{C}$:

$$\chi_\pi(g) := \sum_{i=1}^{d_\pi} \pi_{ii}(g).$$

For a locally compact group G, let $\mathcal{C}(G)$ be the space of continuous and complex-valued functions on G and $L^2(G)$ be the space of square-integrable and complex-valued functions in G. $L^2(G)$ is a Hilbert space with the inner product

$$\langle \phi, \varphi \rangle := \int_G \phi(g)\overline{\varphi(g)}\, \mathrm{d}g.$$

It has a natural representation called the *left-regular representation*, given by

$$(L(g)\phi)(h) := \phi(g^{-1}h).$$

Any irreducible representation of G is equivalent to the restriction of the left-regular representation on some invariant subspace of $L^2(G)$ (see e.g., Section 1.2.4 in Vilenkin [Vil68]). Even more, when G is compact, $L^2(G)$ can be decomposed as a direct sum of irreducible representations, each of those appearing as many times as its dimension (see e.g., Theorem 5.12 in Folland [Fol16] or Sections 2.3.5 to 2.3.7 in Vilenkin [Vil68]).

Theorem 2.1.7 (Peter-Weyl). *When G is a compact group,*

$$\left\{ \sqrt{d_\pi}\pi_{i,j} \;:\; 1 \leq i, j \leq d_\pi, \pi \in \hat{G} \right\}$$

is a complete orthonormal system for $L^2(G)$ and the space generated by these functions is uniformly dense in $\mathcal{C}(G)$. For each $\pi \in \hat{G}$ and $1 \leq j \leq d_\pi$, the space generated by $\{ \sqrt{d_\pi}\rho_{i,j} : 1 \leq i \leq d_\pi \}$ is invariant under the left-regular representation of G and the restriction of ρ to this space is equivalent to π.

Therefore any function $f \in L^2(G)$ can be written as a "Fourier series"

$$f(g) = \sum_{\pi \in \hat{G}} \sum_{i,j=1}^{d_\pi} \hat{f}^\pi_{i,j} \pi_{i,j}(g),$$

with coefficients

$$\hat{f}^\pi_{i,j} = d_\pi \left\langle f, \pi_{i,j}(g) \right\rangle = d_\pi \int_G f(g)\overline{\pi_{i,j}(g)}\, \mathrm{d}g.$$

2.2 Invariant positive kernels

In this section we assume X is a compact Hausdorff space[1] with a positive Radon measure[2] normalized so that the measure of X is 1. We further assume that G is a compact group that acts continuously on X and that the measure of X is invariant with respect to this action. Next we characterize invariant and positive kernels, following Section 3.3 of Bachoc, Gijswijt, Schrijver, and Vallentin [Bac+12] and Section 3.3 of de Laat [Laa16].

2.2.1 Invariant kernels and positive kernels

Similarly to $L^2(G)$, we consider the Hilbert space $L^2(X)$ of square-integrable and complex-valued functions in X with the inner product

$$\langle \phi, \varphi \rangle := \int_X \phi(x)\overline{\varphi(x)}\,\mathrm{d}x.$$

The action of G in X induces a unitary left-regular representation L in $L^2(X)$ defined by

$$(L(g)\phi)(x) := \phi(g^{-1}x).$$

We call a function $K \in L^2(X \times X)$ a *(Hilbert–Schmidt) kernel*. It defines an integral operator $T_K : L^2(X) \longrightarrow L^2(X)$:

$$(T_K\phi)(x) := \int_X K(x,y)\phi(y)\,\mathrm{d}y. \tag{2.3}$$

We say that a kernel K is *positive* if for all $\phi, \varphi \in L^2(X)$, $\langle T_k\phi, \varphi\rangle = \langle \phi, T_K\varphi\rangle$ and

$$\langle T_k\phi, \phi\rangle \geq 0. \tag{2.4}$$

We say that a kernel K is *continuous* if it is continuous as a function $X \times X \longrightarrow \mathbb{C}$ and we denote it by $K \in \mathcal{C}(X \times X)$. We have the following important characterization of continuous and positive kernels by Bochner [Boc41] (see also Lemma 3.4.2 of de Laat [Laa16]):

Proposition 2.2.1. *A continuous kernel K is positive if and only if for every finite subset $\{x_1, \dots, x_m\} \subset X$, the matrix $\big(K(x_i, x_j)\big)_{i,j=1}^m$ is positive semidefinite.*

Condition (2.4) is satisfied by kernels of the form $K(x,y) = u(x)\overline{u(y)}$ for some $u \in L^2(X)$, as well for positive combinations of kernels of this form. Indeed, for $\phi \in L^2(X)$,

$$\langle T_K\phi, \phi\rangle = \int_X \Big(\int_X u(x)\overline{u(y)}\phi(y)\,\mathrm{d}y \Big)\overline{\phi(x)}\,\mathrm{d}x = \left\| \int_X u(x)\overline{\phi(x)}\,\mathrm{d}x \right\|^2.$$

[1] A *Hausdorff space* is a topological space for which every pair of distinct points have disjoint neighbourhoods.

[2] A *Radon measure* in a topological space is a measure “compatible” with the topology: all open and closed sets are measurable, the measure of any compact set is finite and the measure is *inner regular*, meaning that the measure of any measurable set is the supremum of the measure of its compact subsets.

A kernel $K \in L^2(X \times X)$ is *invariant* if its associated operator T_K commutes with the left-regular representation of G in $L^2(X)$. If $K \in C(X \times X)$, then K is invariant if and only if $K(gx, gy) = K(x, y)$ for all $x, y \in X$ and $g \in G$.

2.2.2 Symmetry adapted systems

The main theorem of this section, Theorem 2.2.2, characterizes the kernels that are both invariant and positive. To state it, we consider a decomposition of $L^2(X)$ as an orthogonal direct sum of irreducible invariant subspaces, as given in (2.2) (recall that m_π is possibly infinite):

$$L^2(X) = \bigoplus_{\pi \in \hat{G}} V_\pi, \qquad V_\pi = \bigoplus_{i=1}^{m_\pi} V_{\pi,i}.$$

Let $C(X)$ be the space of continuous complex-valued functions in X. Since X is compact, it is a dense subset of $L^2(X)$ (Theorem 3.14 from Rudin [Rud87]). We may wonder whether it is possible to make the above decomposition using irreducible invariant subspaces of continuous functions and get uniform convergence in $C(X)$, as stated in the Peter-Weyl theorem for $L^2(G)$. This statement is indeed true and the proof of Peter-Weyl theorem can be adapted to this case, as shown in Section 3.3 of de Laat [Laa16].

For each $\pi \in \hat{G}$, $\pi : G \longrightarrow \mathrm{GL}(H_\pi)$, we use an unitary isomorphism $\phi_{\pi,i} : H_\pi \longrightarrow V_{\pi,i}$ to map a fixed orthonormal basis $\{e_1, \dots, e_{d_\pi}\}$ of H_π to a basis for $V_{\pi,i}$ and let

$$e_{\pi,i,k} := \phi_{\pi,i}(e_k)$$

for $1 \le i \le m_\pi$ and $1 \le k \le d_\pi$.

We call a complete orthonormal system $\{e_{\pi,i,k} : \pi \in \hat{G}, 1 \le i \le m_\pi, 1 \le k \le d_\pi\}$ constructed in this way a *symmetry adapted system*. Besides being a complete orthonormal system for $L^2(X)$, the group acts on each set $\{e_{\pi,i,k} : 1 \le k \le d_\pi\}$ in the same way. That is, for each $\pi \in \hat{G}$, the restrictions of the representation L to each subspace $V_{\pi,i}$ have the same matrix.

The symmetry adapted basis is useful to define invariant kernels. For each $\pi \in \hat{G}$ and $1 \le i, j \le m_\pi$, let $Z^\pi_{i,j}$ be the kernel defined as

$$Z^\pi_{i,j}(x, y) := \sum_{k=1}^{d_\pi} e_{\pi,i,k}(x)\overline{e_{\pi,j,k}(y)}. \tag{2.5}$$

This kernel is invariant, since for $g \in G$:

$$\begin{aligned} Z^\pi_{i,j}(g^{-1}x, g^{-1}y) &= \sum_{k=1}^{d_\pi} e_{\pi,i,k}(g^{-1}x)\overline{e_{\pi,j,k}(g^{-1}y)} \\ &= \sum_{k=1}^{d_\pi} \left(\sum_{s=1}^{d_\pi} \pi_{s,k}(g) e_{\pi,i,s}(x) \right) \left(\sum_{l=1}^{d_\pi} \overline{\pi_{l,k}(g) e_{\pi,j,l}(y)} \right) \\ &= \sum_{s=1}^{d_\pi} \sum_{l=1}^{d_\pi} \left(\sum_{k=1}^{d_\pi} \pi_{s,k}(g)\overline{\pi_{l,k}(g)} \right) e_{\pi,i,s}(x)\overline{e_{\pi,j,l}(y)} \end{aligned}$$

$$= \sum_{s=1}^{d_\pi} e_{\pi,i,s}(x)\overline{e_{\pi,j,s}(y)} = Z^\pi_{i,j}(x,y).$$

Using Definition (2.3), $T_{Z^\pi_{i,j}} f$ is zero for functions orthogonal to $V_{\pi,j}$ and $T_{Z^\pi_{i,j}} f \in V_{\pi,i}$. By Schur's lemma, every transformation from $V_{\pi,j}$ to $V_{\pi,i}$ that commutes with L is a multiple of $T_{Z^\pi_{i,j}}$. It may also be verified that the kernels $Z^\pi_{i,j}$ are orthogonal with respect to the inner product of $L^2(X \times X)$. Therefore the kernels $Z^\pi_{i,j}$ for $\pi \in \hat{G}$, $1 \leq i, j \leq m_\pi$ form a complete orthonormal system for the space of invariant kernels in $L^2(X \times X)$ [Laa16, Proposition 3.4.1]. We define the *zonal matrix* $Z^\pi : X \times X \longrightarrow \mathbb{C}^{m_\pi \times m_\pi}$ as the matrix with entries $Z^\pi_{i,j}$, and use $\langle , \rangle$ to denote the trace product between matrices (also called Frobenius product), which for matrices A, B with the same dimensions is defined as:

$$\langle A, B \rangle := \operatorname{tr}(AB^{\mathsf{T}}) = \sum_{i,j} A_{i,j} B_{i,j}.$$

Next we show that in the basis formed by the kernels $Z^\pi_{i,j}$ the positiveness of a kernel translates into the positivity of its matrix coefficients. When $m_\pi = \infty$, we say that a matrix $A \in \mathbb{C}^{m_\pi \times m_\pi}$ is positive semidefinite if for all $n \in \mathbb{N}$, the matrix $(A_{i,j})_{i,j=1}^n$ is positive semidefinite.

Theorem 2.2.2. *The matrix entries of the zonal matrices Z^π, for $\pi \in \hat{G}$, form a complete orthonormal system for the space of invariant kernels of $L^2(X \times X)$. Given an invariant $K \in L^2(X \times X)$, there exist matrices $\hat{K}_\pi \in \mathbb{C}^{m_\pi \times m_\pi}$ so that*

$$K(x,y) = \sum_{\pi \in \hat{G}} \left\langle \hat{K}_\pi, Z^\pi(x,y) \right\rangle,$$

these coefficients are given by

$$\hat{K}_{\pi,i,j} = \int_X \int_X K(x,y)\overline{Z^\pi_{j,i}(x,y)}\, \mathrm{d}x\, \mathrm{d}y.$$

Furthermore, K is positive if and only if its matrix coefficients $\hat{K}_\pi$ are positive semidefinite.

Proof. Since we already established that the kernels $Z^\pi_{i,j}$ for $\pi \in \hat{G}$, $1 \leq i, j \leq m_\pi$ form a complete orthonormal system for the space of invariant kernels in $L^2(X \times X)$, we prove the statement about the positivity.

Suppose that K is a positive kernel. We shall show that $\hat{K}_\pi$ is positive semidefinite for each $\pi \in \hat{G}$. Let $c_1, \ldots, c_{m_\pi} \in \mathbb{C}$ and $\phi_k(x) := \sum_{i=1}^{m_\pi} c_i e_{\pi,i,k}(x)$. We have:

$$\begin{aligned}
\sum_{i,j=1}^{m_\pi} c_i \overline{c_j} \hat{K}_{\pi,i,j} &= \sum_{i,j=1}^{m_\pi} c_i \overline{c_j} \int_X \int_X K(x,y)\overline{Z^\pi_{j,i}(x,y)}\, \mathrm{d}x\, \mathrm{d}y \\
&= \sum_{i,j=1}^{m_\pi} c_i \overline{c_j} \int_X \int_X K(x,y)\Big(\sum_{k=1}^{d_\pi} \overline{e_{\pi,j,k}(x)} e_{\pi,i,k}(y) \Big)\, \mathrm{d}x\, \mathrm{d}y \\
&= \sum_{k=1}^{d_\pi} \int_X \int_X K(x,y)\phi_k(y)\overline{\phi_k(x)}\, \mathrm{d}x\, \mathrm{d}y = \sum_{k=1}^{d_\pi} \langle T_k \phi_k, \phi_k \rangle \geq 0.
\end{aligned}$$

Therefore $\hat{K}_\pi$ is positive semidefinite.

For the other direction, we assume that for each $\pi \in \hat{G}$, $\hat{K}_\pi$ is positive semidefinite and let $\phi \in L^2(X)$. Then

$$\begin{aligned}\langle T_k\phi, \phi\rangle &= \int_X \int_X K(x,y)\phi(y)\overline{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_X \int_X \sum_{\pi\in\hat{G}} \big\langle \hat{K}_\pi, Z^\pi(x,y)\big\rangle \phi(y)\overline{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y \\ &= \sum_{\pi\in\hat{G}} \Big\langle \hat{K}_\pi, \int_X \int_X Z^\pi(x,y)\phi(y)\overline{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y \Big\rangle,\end{aligned}$$

where the integral in the matrix is entrywise. Denoting $\hat{\phi}_{\pi,j,k} := \int_X \overline{e_{\pi,j,k}(x)}\phi(x)\,\mathrm{d}x$, its entries are:

$$\begin{aligned}\int_X \int_X Z^\pi_{i,j}(x,y)\phi(y)\overline{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y &= \int_X \int_X \sum_{k=1}^{d_\pi} e_{\pi,i,k}(x)\overline{e_{\pi,j,k}(y)}\phi(y)\overline{\phi(x)}\,\mathrm{d}x\,\mathrm{d}y \\ &= \sum_{k=1}^{d_\pi} \int_X e_{\pi,i,k}(x)\overline{\phi(x)}\,\mathrm{d}x \int_X \overline{e_{\pi,j,k}(y)}\phi(y)\,\mathrm{d}y \\ &= \sum_{k=1}^{d_\pi} \overline{\hat{\phi}_{\pi,i,k}}\hat{\phi}_{\pi,j,k}.\end{aligned}$$

The matrices $\left(\overline{\hat{\phi}_{\pi,i,k}}\hat{\phi}_{\pi,j,k}\right)_{i,j=1}^{m_\pi}$ are positive semidefinite, hence

$$\langle T_k\phi, \phi\rangle = \sum_{\pi\in\hat{G}} \sum_{k=1}^{d_\pi} \Big\langle \hat{K}_\pi, \left(\overline{\hat{\phi}_{\pi,i,k}}\hat{\phi}_{\pi,j,k}\right)_{i,j=1}^{m_\pi} \Big\rangle \geq 0,$$

and therefore the kernel K is positive. □

Remark 2.2.3. The orthogonality between the subspaces $V_{\pi,i}$ is used only to derive the formula for the coefficients $\hat{K}_{\pi,i,j}$, not to relate the positivity of K with the positive semidefinite matrices $\hat{K}_\pi$. Another way to observe this is taking an invertible matrix $A \in \mathbb{C}^{m_\pi \times m_\pi}$ and replacing $\hat{K}_\pi$ by $AA^{-1}\hat{K}_\pi A^{-*}A^*$, then:

$$K(x,y) = \sum_{\pi\in\hat{G}} \big\langle \hat{K}_\pi, Z^\pi(x,y)\big\rangle = \sum_{\pi\in\hat{G}} \big\langle A^{-1}\hat{K}_\pi A^{-*}, A^* Z^\pi(x,y)A\big\rangle.$$

Observe that $\hat{K}_\pi$ is positive semidefinite if and only if $A^{-1}\hat{K}_\pi A^{-*}$ is as well. Moreover $A^*Z^\pi(x,y)A$ corresponds to the zonal matrix associated to another decomposition of V_π into invariant irreducible subspaces. A similar remark is made in Bachoc and Vallentin [BV08].

Theorem 2.2.2 guarantees convergence for the series of a kernel $K \in L^2(X \times X)$. Regarding whether a kernel $K \in C^2(X \times X)$ can be uniformly approximated by the above series, this is not true in general, but does hold in certain cases. When the action of G in X is transitive, this is the content of Bochner theorem [Boc41] and when the the action of

G in X has finitely many orbits, the uniform convergence is proved in Theorem 3.4.4 of de Laat [Laa16].

2.3 Harmonic analysis on the sphere

In this section we consider the *orthogonal group*

$$\mathrm{O}(d) := \{A \in \mathbb{R}^{d\times d} : A^{\mathsf{T}}A = I\},$$

and for each $m \leq d-2$ we consider the subgroup of $\mathrm{O}(d)$ that fixes the last m coordinates of $\mathbb{R}^d$, which is isomorphic to $\mathrm{O}(d-m)$ and is also denoted by $\mathrm{O}(d-m)$. Next we describe how $L^2(S^{d-1})$ decomposes into irreducible invariant subspaces and the zonal matrices associated to these decompositions. In this section we always denote $x := (x_1, \dots, x_d) \in \mathbb{R}^d$, $x' := (x_1, \dots, x_{d-1})$, and similarly, $y := (y_1, \dots, y_d) \in \mathbb{R}^d$, $y' := (y_1, \dots, y_{d-1})$.

2.3.1 The zonal functions from the representation of $\mathrm{O}(d)$ in $L^2(S^{d-1})$

Let Hom_k^d be the space of *homogeneous polynomials* of degree k in d variables. Since for $r \geq 0$, $\xi \in S^{d-1}$, and $p \in \mathrm{Hom}_k^d$, we have $p(r\xi) = r^k p(\xi)$, the application that sends a polynomial $p \in \mathrm{Hom}_k^d$ to its restriction to the sphere $p \mapsto p|_{S^{d-1}}$ is injective. Hence Hom_k^d is isomorphic to its image in $L^2(S^{d-1})$, which we denote by $\mathrm{Hom}_k^d(S^{d-1})$ and call the space of *spherical homogeneous polynomials* of degree k in d variables. Note that while the sum $\mathrm{Hom}_k^d + \mathrm{Hom}_l^d$ for $k \neq l$ is direct, the same in general is not true for $\mathrm{Hom}_k^d(S^{d-1}) + \mathrm{Hom}_l^d(S^{d-1})$.

We say that a polynomial f is *harmonic* if $\Delta f = 0$, where $\Delta := \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}$ is the *Laplace operator*. Let Har_k^d be the space of *homogeneous harmonic polynomials* of degree k in d variables and, as above, let $\mathrm{Har}_k^d(S^{d-1})$ be the space of *spherical homogeneous harmonic polynomials* of degree k in d variables.

The next theorem states the decomposition of $L^2(S^{d-1})$ under the action of $\mathrm{O}(d)$ (see Section IX.2.7 in Vilenkin [Vil68]):

Theorem 2.3.1. *For $d \geq 3$, the space $L^2(S^{d-1})$ under the action of $\mathrm{O}(d)$ decomposes as the following orthogonal direct sum of nonequivalent irreducible subspaces:*

$$L^2(S^{d-1}) = \bigoplus_{k=0}^{\infty} \mathrm{Har}_k^d(S^{d-1}).$$

First we observe that by Stone-Weierstrass theorem (see e.g., Theorem IV.10 in Reed and Simon [RS72]), every continuous function in S^{d-1} can be uniformly approximated by polynomials and hence every function in $L^2(S^{d-1})$ can be approximated in the L^2-norm by polynomials as well. Let $\mathrm{Pol}(S^{d-1})_{\leq k}$ be the space of *spherical polynomials* of degree at most k. This is an invariant and finite dimensional subspace of $L^2(S^{d-1})$ and by letting $k \longrightarrow \infty$ we get the whole space $L^2(S^{d-1})$. While we may write $\mathrm{Pol}(S^{d-1})_{\leq k} = \sum_{l=0}^{k} \mathrm{Hom}_l^d(S^{d-1})$, as spherical polynomials this sum is not direct. The following theorem shows that the harmonic property produces a orthogonal direct sum decomposition:

Theorem 2.3.2. *For $d \geq 3$, the space* $\mathrm{Pol}(S^{d-1})_{\leq k}$ *under the action of* $\mathrm{O}(d)$ *decomposes as the following orthogonal direct sum of invariant and nonequivalent irreducible subspaces:*

$$\mathrm{Pol}(S^{d-1})_{\leq k} = \mathrm{Har}_0^d(S^{d-1}) \oplus \cdots \oplus \mathrm{Har}_k^d(S^{d-1}).$$

The main step necessary for the proof of this theorem is called *harmonic projection*, from which we may conclude that every spherical polynomial of degree at most k is equal to a spherical harmonic polynomial of degree at most k (see Section IX.2.5 of Vilenkin [Vil68]):

Proposition 2.3.3. *The space* Hom_k^d *can be written as the direct sum between the subspace* Har_k^d *and* $\|x\|^2\mathrm{Hom}_{k-2}^d$, *of polynomials of the form* $\|x\|^2 g$ *with* $g \in \mathrm{Hom}_{k-2}^d$, *namely*

$$\mathrm{Hom}_k^d = \mathrm{Har}_k^d \oplus \|x\|^2\mathrm{Hom}_{k-2}^d.$$

Therefore,

$$\mathrm{Hom}_k^d = \bigoplus_{l=0}^{\lfloor d/2 \rfloor} \|x\|^{2l}\mathrm{Har}_{k-2l}^d.$$

Proof. First we proof that $\mathrm{Har}_k^d \cap \|x\|^2\mathrm{Hom}_{k-2}^d = \emptyset$. Next we show that $\dim(\mathrm{Har}_k^d) \geq \dim(\mathrm{Hom}_k^d) - \dim(\|x\|^2\mathrm{Hom}_{k-2}^d)$, which together shows that their sum is direct and spans the whole space.

To show that $\mathrm{Har}_k^d \cap \|x\|^2\mathrm{Hom}_{k-2}^d = \emptyset$, we take $f \in \|x\|^2\mathrm{Hom}_{k-2}^d$ and show that $\Delta f \neq 0$. We may write $f(x) = \|x\|^{2m}g(x)$, with $g \in \mathrm{Hom}_{k-2m}$, $1 \leq m \leq k/2$ and g not divisible by $\|x\|^2$. We have:

$$\begin{aligned}
\Delta f(x) &= \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}\Big(\|x\|^{2m}g(x)\Big) = \sum_{i=1}^d \frac{\partial}{\partial x_i}\Big(2m\|x\|^{2(m-1)}x_i g(x) + \|x\|^{2m}\frac{\partial}{\partial x_i}g(x)\Big) \\
&= \sum_{i=1}^d \Big(4m(m-1)\|x\|^{2(m-2)}x_i^2 g(x) + 2m\|x\|^{2(m-1)}g(x) \\
&\qquad\qquad + 4m\|x\|^{2(m-1)}x_i\frac{\partial}{\partial x_i}g(x) + \|x\|^{2m}\frac{\partial^2}{\partial x_i^2}g(x)\Big) \\
&= 4m(m-1)\|x\|^{2(m-1)}g(x) + 2md\|x\|^{2(m-1)}g(x) \\
&\qquad\qquad + 4m\|x\|^{2(m-1)}\Big(\sum_{i=1}^d x_i\frac{\partial}{\partial x_i}g(x)\Big) + \|x\|^{2m}\Delta g(x) \\
&= 2m\big(2(m-1) + d + 2(k-2m)\big)\|x\|^{2(m-1)}g(x) + \|x\|^{2m}\Delta g(x) \\
&= 2m(d + 2k - 2m - 2)\|x\|^{2(m-1)}g(x) + \|x\|^{2m}\Delta g(x).
\end{aligned}$$

Suppose that $\Delta f(x) = 0$. From $1 \leq m \leq k/2$, we get $(d + 2k - 2m - 2) > 0$. Canceling $\|x\|^{2(m-1)}$, we see that g is divisible by $\|x\|^2$, a contradiction. Therefore $\Delta f(x) \neq 0$.

To show that $\dim(\mathrm{Har}_k^d) \geq \dim(\mathrm{Hom}_k^d) - \dim(\|x\|^2\mathrm{Hom}_{k-2}^d)$, note that if $f \in \mathrm{Hom}_k^d$, the equation $\Delta f = 0$ imposes no more than $\dim(\mathrm{Hom}_{k-2}^d) = \dim(\|x\|^2\mathrm{Hom}_{k-2}^d)$ linear conditions on the coefficients of f. □

Using the previous theorem we may compute the dimension of Har_k^d. The dimension of Hom_k^d is equal to the number of d-uples of nonnegative integers that sum to k, which is $\binom{d+k-1}{k}$. Similarly, the dimension of $\|x\|^2\mathrm{Hom}_{k-2}^d$ is $\binom{d+k-3}{k-2}$. Hence,

$$h_k^d := \dim(\mathrm{Har}_k^d) = \dim(\mathrm{Hom}_k^d) - \dim(\mathrm{Hom}_{k-2}^d) = \binom{d+k-1}{k} - \binom{d+k-3}{k-2}. \tag{2.6}$$

Restricting these polynomials to the sphere, we have $\|x\|^2 = 1$ and Proposition 2.3.3 shows that $\mathrm{Hom}_k^d(S^{d-1})$ can be written as a sum of spaces $\mathrm{Har}_l^d(S^{d-1})$ and the same can be said for $\mathrm{Pol}(S^{d-1})_{\leq k}$. Next we prove that this sum is direct by showing that the spaces $\mathrm{Har}_k^d(S^{d-1})$ are orthogonal with respect to the inner product of $L^2(S^{d-1})$. This proof uses the divergence theorem (see e.g., Theorem 5.8 in Spivak [Spi65]), which relates the integral of the *divergence* of a vector field $\Phi : \mathbb{R}^d \longrightarrow \mathbb{C}^d$,

$$\operatorname{div}\Phi(x) := \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\Phi_j(x),$$

inside a domain with a surface integral over its boundary:

Theorem 2.3.4. *Let $V \subset \mathbb{R}^d$ be a compact set with a piecewise smooth boundary ∂V and Φ be a continuously differentiable vector field. Then*

$$\int_V \operatorname{div}\Phi(x)\,\mathrm{d}x = \int_{\partial V} \langle \Phi(x), n(x)\rangle\,\mathrm{d}\sigma(x),$$

where $n(x)$ is the outer unit normal vector of ∂V at x and $\mathrm{d}\sigma$ is the surface measure of ∂V.

Lemma 2.3.5. *The spaces $\mathrm{Har}_k^d(S^{d-1})$ and $\mathrm{Har}_l^d(S^{d-1})$ with $k \neq l$ are orthogonal to each other.*

Proof. Define the *gradient* of a continuously differentiable scalar field $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ as the vector field $\operatorname{grad}(f) := \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_d}\right)$. Note that $\operatorname{div}\operatorname{grad}(f) = \Delta f$.

Let $f_k \in H_k^d$, $f_l \in \mathrm{Har}_l^d$ and define the vector field $\Phi(x) := f_k(x)\overline{\operatorname{grad}(f_l)(x)} - \overline{f_l(x)}\operatorname{grad}(f_k)(x)$. Applying Theorem 2.3.4 to Φ we get

$$\int_{\|x\|\leq 1} \operatorname{div}\Phi(x)\,\mathrm{d}x = \int_{S^{d-1}} \langle \Phi(x), x\rangle\,\mathrm{d}\sigma(x).$$

Since f_k and f_l are harmonic,

$$\operatorname{div}\Phi(x) = \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left(f_k(x)\frac{\partial}{\partial x_j}\overline{f_l(x)} - \overline{f_l(x)}\frac{\partial}{\partial x_j}f_k(x)\right) = f_k(x)\overline{\Delta f_l(x)} - \overline{f_l(x)}\Delta f_k(x) = 0.$$

On the other hand, since f_k and f_l are homogeneous of degree k and l respectively,

$$\langle \Phi(x), x\rangle = \sum_{j=1}^{d} \left(f_k(x)\frac{\partial}{\partial x_j}\overline{f_l(x)} - \overline{f_l(x)}\frac{\partial}{\partial x_j} f_k(x)\right) x_j = l f_k(x)\overline{f_l(x)} - k\overline{f_l(x)}f_k(x).$$

Since $k - l \neq 0$, we get $\int_{S^{d-1}} f_k(x)\overline{f_l(x)}\,\mathrm{d}\sigma(x) = 0$ and therefore the restrictions of f_k and f_l to S^{d-1} are orthogonal in $L^2(S^{d-1})$. □

To prove Theorems 2.3.1 and 2.3.2, we still have to show that the spaces $\mathrm{Har}_k^d(S^{d-1})$ are invariant and irreducible for the representation of $\mathrm{O}(d)$.

Proposition 2.3.6. *The spaces* $\mathrm{Har}_k^d(S^{d-1})$ *are invariant for the representation of* $\mathrm{O}(d)$.

Proof. The invariance of the spaces of spherical homogeneous harmonic polynomials follows from the fact that the composition with a linear transformation preserves homogeneity and that orthogonal transformations commute with the Laplace operator. Indeed, for $f \in \mathrm{Har}_k^d$ and $T \in \mathrm{O}(d)$, $T = (t_{ij})_{i,j=1}^d$, we have $\sum_{l=1}^d t_{li}t_{lj} = 1$ if $i = j$ and 0 otherwise, hence:

$$\begin{aligned}\Delta\big(L(T)f(x)\big) &= \sum_{l=1}^{d} \frac{\partial^2}{\partial x_l^2}\big(f(T^{-1}x)\big) = \sum_{l=1}^{d} \frac{\partial}{\partial x_l}\left(\sum_{i=1}^{d} t_{li}\frac{\partial}{\partial x_i} f(T^{-1}x)\right) \\ &= \sum_{l=1}^{d}\sum_{i=1}^{d} t_{li}\sum_{j=1}^{n} t_{lj}\frac{\partial^2}{\partial x_j \partial x_i} f(T^{-1}x) = \sum_{i=1}^{d}\sum_{j=1}^{d}\left(\sum_{l=1}^{d} t_{li}t_{lj}\right)\frac{\partial^2}{\partial x_j\partial x_i} f(T^{-1}x) \\ &= \sum_{i=1}^{d}\frac{\partial^2}{\partial x_i^2} f(T^{-1}x) = \Delta f(T^{-1}x) = L(T)\big(\Delta f(x)\big).\end{aligned}$$

□

The next proposition is the main step to show that the spaces $\mathrm{Har}_k^d(S^{d-1})$ are irreducible (see Theorem IV.2.12 of Stein and Weiss [SW71]):

Proposition 2.3.7. *For each integer $k \geq 0$ and $d \geq 3$, the* $\mathrm{O}(d-1)$*-invariant subspace of* Har_k^d *is one dimensional. Furthermore, the* $\mathrm{O}(d-1)$*-invariant subspace of* $\mathrm{Har}_k^d(S^{d-1})$ *is generated by a polynomial of degree k in x_d.*

Proof. Let $f \in \mathrm{Har}_k^d$ be an $\mathrm{O}(d-1)$-invariant function and $x' := (x_1, \dots, x_{d-1})$. If we write

$$f(x) = \sum_{j=0}^{k} x_d^{k-j} f_j(x'),$$

we have that each f_j is a homogeneous polynomial of degree j in $d-1$ variables and $\mathrm{O}(d-1)$-invariant. Since $\|x'\|^{-j} f_j(x')$ is invariant under rotations and 0-homogeneous, it is constant. Therefore $f_j(x') = c_j\|x'\|^j$ and since f_j is a polynomial, $f_j = 0$ when j is odd. Hence,

$$f(x) = \sum_{j=0}^{\lfloor k/2\rfloor} c_j x_d^{k-2j}(x_1^2 + \cdots + x_{d-1}^2)^j. \tag{2.7}$$

Since $\Delta f = 0$, we have:

$$
\begin{aligned}
0 = \Delta f(x) &= \sum_{j=0}^{\lfloor k/2 \rfloor} \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} \Big(c_j x_d^{k-2j} (x_1^2 + \cdots + x_{d-1}^2)^j \Big) \\
&= \sum_{j=0}^{\lfloor k/2 \rfloor - 1} (k-2j)(k-2j-1) c_j x_d^{k-2j-2} (x_1^2 + \cdots + x_{d-1}^2)^j \\
&\quad + \sum_{j=1}^{\lfloor k/2 \rfloor} \sum_{i=2}^{d} \Big(2jc_j x_1^{k-2j} (x_1^2 + \cdots + x_{d-1}^2)^{j-1} + 4j(j-1) c_j x_d^{k-2j} x_i^2 (x_1^2 + \cdots + x_{d-1}^2)^{j-2} \Big) \\
&= \sum_{j=1}^{\lfloor k/2 \rfloor} (k-2j+2)(k-2j+1) c_{j-1} x_d^{k-2j} (x_1^2 + \cdots + x_{d-1}^2)^{j-1} \\
&\quad + \sum_{j=1}^{\lfloor k/2 \rfloor} 2j(d+2j-3) c_j x_d^{k-2j} (x_1^2 + \cdots + x_{d-1}^2)^{j-1} \\
&= \sum_{j=1}^{\lfloor k/2 \rfloor} \Big((k-2j+2)(k-2j+1) c_{j-1} + 2j(d+2j-3) c_j \Big) x_d^{k-2j} (x_1^2 + \cdots + x_{d-1}^2)^{j-1}.
\end{aligned}
$$

Hence

$$
c_j = -\frac{(k-2j+2)(k-2j+1)}{2j(d+2j-3)} c_{j-1}
$$

for each $1 \le j \le \lfloor k/2 \rfloor$ and c_0 determines f. Therefore the $\mathrm{O}(d-1)$-invariant functions in Har_k^d are scalar multiples of each other.

If $x \in S^{d-1}$, we have $x_1^2 + \cdots + x_{d-1}^2 = 1 - x_d^2$ and from (2.7) we get that a $\mathrm{O}(d-1)$-invariant function in $\mathrm{Har}_k^d(S^{d-1})$ is a polynomial of degree k in x_d. □

Proposition 2.3.8. *The spaces $\mathrm{Har}_k^d(S^{d-1})$ are irreducible for the representation of $\mathrm{O}(d)$ and for $k \neq l$, $\mathrm{Har}_k^d(S^{d-1})$ and $\mathrm{Har}_l^d(S^{d-1})$ are not equivalent.*

Proof. To prove that the spaces $\mathrm{Har}_k^d(S^{d-1})$ are irreducible, we fix an orthonormal basis $\{Y_{k,1}, \ldots, Y_{k,h_k^d}\}$ for $\mathrm{Har}_k^d(S^{d-1})$ and as in (2.5), define an $\mathrm{O}(d)$-invariant kernel:

$$
Z(x, y) := \sum_{l=1}^{h_k^d} Y_{k,l}(x) \overline{Y_{k,l}(y)}.
$$

This kernel satisfies $Z(Tx, Ty) = Z(x, y)$ for all $T \in \mathrm{O}(d)$, $x, y \in S^{d-1}$. Fixing $e = (0, \ldots, 0, 1)$ and letting $P(x) := Z(x, e)$, we have that $P \in \mathrm{Har}_k^d$ and is invariant with respect to $\mathrm{O}(d-1)$, the subgroup of $\mathrm{O}(d)$ that fixes the last coordinate. If Har_k^d was not irreducible, the same construction could be used on its proper invariant subspaces and produce other $\mathrm{O}(d-1)$-invariant functions in Har_k^d. Proposition 2.3.7 shows that this is not the case.

The statement about the nonequivalence between the representations of different degree follows simply from the dimension of these spaces, computed in (2.6). □

Proposition 2.3.7 shows that the zonal function associated to $\mathrm{Har}_k^d(S^{d-1})$ is a polynomial of degree k in $\langle x, y\rangle$. Fixing an orthonormal basis $\{Y_{k,1}, \ldots, Y_{k,h_k^d}\}$ for $\mathrm{Har}_k^d(S^{d-1})$, we define the *Gegenbauer polynomials* P_k^d by

$$P_k^d(\langle x, y\rangle) := \frac{1}{h_k^d} \sum_{l=1}^{h_k^d} Y_{k,l}(x) Y_{k,l}(y). \tag{2.8}$$

They do not depend on the choice of the orthonormal basis. Using Lemma 2.3.5, one may show (see e.g., Theorem IV.2.14 in Stein and Weiss [SW71]) that for $k \neq l$,

$$\int_{-1}^{1} P_k^d(t) P_l^d(t)(1 - t^2)^{\frac{d-3}{2}}\, \mathrm{d}t = 0,$$

which allows the identification of the Gegenbauer polynomials with scalar multiples of the Jacobi polynomials with parameters $(\frac{d-3}{2}, \frac{d-3}{2})$ (see Chapter 4 of Szegö [Sze39]), but normalized so that $P_k^d(1) = 1$. The theory of orthogonal polynomials gives many properties, including a recurrence formula [Sze39, Formula (4.5.1)] that makes them easy to compute.

Finally, note that since the spaces $\mathrm{Har}_k^d(S^{d-1})$ are nonequivalent and irreducible, the multiplicities m_π in the notation of Theorem 2.2.2 are all 1 and a $\mathrm{O}(d)$-invariant and positive kernel $K \in L^2(S^{d-1} \times S^{d-1})$ is given by a series

$$K(x, y) = \sum_{k=0}^{\infty} f_k P_k^d(\langle x, y\rangle),$$

with $f_k \geq 0$ for all k and such that $\sum_{k=0}^{\infty} f_k^2$ converges. The similar statement with a condition for uniform convergence in $C(S^{d-1} \times S^{d-1})$ is known as Schoenberg's theorem [Sch42]:

Theorem 2.3.9 (Schoenberg). *A kernel $K : S^{d-1} \times S^{d-1} \longrightarrow \mathbb{R}$ is continuous, positive, and $\mathrm{O}(d)$-invariant if, and only if,*

$$K(x, y) = \sum_{k=0}^{\infty} f_k P_k^d(\langle x, y\rangle), \tag{2.9}$$

with $f_k \geq 0$ for all k and such that $\sum_{k=0}^{\infty} f_k$ converges, in which case the series (2.9) converges absolutely and uniformly over $S^{d-1} \times S^{d-1}$.

2.3.2 The zonal functions from the representation of $\mathrm{O}(d - m)$ in $L^2(S^{d-1})$

For a positive integer $m \leq d - 2$, $\mathrm{O}(d - m)$ is a subgroup of $\mathrm{O}(d)$ and the representations $\mathrm{Har}_k^d(S^{d-1})$ break into smaller pieces. We first consider the case $m = 1$ and later we will be able to iterate the procudere and also cover the other $m \leq d - 2$. To describe the decomposition of $\mathrm{Har}_k^d(S^{d-1})$ under the action of $\mathrm{O}(d - 1)$ we follow Section IX.2.8 from Vilenkin [Vil68] and to describe the zonal functions that define the invariant and positive kernels we follow Bachoc and Vallentin [BV08]. The general case $m \leq d - 2$ is described by Musin [Mus14].

Proposition 2.3.10. *Let $x' := (x_1, \dots, x_{d-1})$. The space Hom_k^d can be written as the direct sum between the subspaces $x_d^{k-l}\mathrm{Har}_l^{d-1}$ for $0 \leq l \leq k$, of polynomials of the form $x_d^{k-l}g(x')$ with $g \in \mathrm{Har}_l^{d-1}$, and the subspace $\|x\|^2\mathrm{Hom}_{k-2}^d$, of polynomials of the form $\|x\|^2 g(x)$ with $g \in \mathrm{Hom}_{k-2}^d$,*

$$\mathrm{Hom}_k^d = \bigoplus_{l=0}^{k} x_d^{k-l}\mathrm{Har}_l^{d-1} \oplus \|x\|^2\mathrm{Hom}_{k-2}^d.$$

Proof. First we show that every $f \in \mathrm{Hom}_k^d$ can be written in the format above. Substituting x_d^2 by $\|x\|^2 - \|x'\|^2$ and putting x_d in evidence, we may write f as

$$f(x) = \|x\|^2 F(x) + x_d\varphi_1(x') + \varphi_2(x'),$$

with $F \in \mathrm{Hom}_{k-2}^d$, $\varphi_1 \in \mathrm{Hom}_{k-1}^{d-1}$ and $\varphi_2 \in \mathrm{Hom}_k^{d-1}$. Applying the decomposition from Proposition 2.3.3 to φ_1 and φ_2, we get

$$f(x) = \|x\|^2 F(x) + \sum_{l=0}^{\lfloor (k-1)/2 \rfloor} x_d\|x'\|^{2l} g_{k-2l-1}(x') + \sum_{l=0}^{\lfloor k/2 \rfloor} \|x'\|^{2l} g_{k-2l}(x'),$$

with $g_s \in \mathrm{Har}_s^{d-1}$. Substituting $\|x'\|^{2l} = (\|x\|^2 - x_d^2)^l = \sum_{j=0}^{l} \binom{l}{j}(-1)^j x_d^{2j}\|x\|^{2(l-j)}$ and grouping together the terms with $\|x\|^2$, we get

$$f(x) = \|x\|^2 f_1(x) + \sum_{l=0}^{k} x_d^{k-l} h_l(x'),$$

with $f_1 \in \mathrm{Hom}_{k-2}^d$ and $h_l \in \mathrm{Har}_l^{d-1}$.

To show that the sum is direct we simply compute the dimension of the subspaces. Since $\dim(\mathrm{Hom}_k^d) = \binom{d+k-1}{d-1}$ and $\dim(\mathrm{Har}_k^d) = \binom{d+k-1}{d-1} - \binom{d+k-3}{d-1}$, we have

$$\begin{aligned}
\sum_{l=0}^{k} \dim(\mathrm{Har}_l^{d-1}) + \dim(\mathrm{Hom}_{k-2}^d) &= \sum_{l=0}^{k}\left(\binom{d+l-2}{d-2} - \binom{d+l-4}{d-2}\right) + \binom{d+k-3}{d-1} \\
&= \binom{d+k-2}{d-2} + \binom{d+k-3}{d-2} + \binom{d+k-3}{d-1} \\
&= \binom{d+k-1}{d-1} = \dim(\mathrm{Hom}_k^d).
\end{aligned}$$

□

Theorem 2.3.11. *The space $\mathrm{Har}_k^d(S^{d-1})$ under the action of $\mathrm{O}(d-1)$ decomposes as the following orthogonal direct sum of invariant and nonequivalent irreducible subspaces:*

$$\mathrm{Har}_k^d(S^{d-1}) = \mathrm{Har}_{k,0}^d(S^{d-1}) \oplus \cdots \oplus \mathrm{Har}_{k,k}^d(S^{d-1}),$$

where the representation of $\mathrm{O}(d-1)$ on each subspace $\mathrm{Har}_{k,l}^d(S^{d-1})$ is equivalent to Har_l^{d-1}.

Proof. Since the action of $\mathrm{O}(d-1)$ in $\mathbb{R}^d$ fixes the last coordinate, the subspaces in the decompositions from Propositions 2.3.3 and 2.3.10 are all invariant and therefore by Lemma 2.1.4, the representation of $\mathrm{O}(d-1)$ in Har_k^d is equivalent to the representation of $\mathrm{O}(d-1)$ in $x_d^k\mathrm{Har}_0^{d-1} \oplus x_d^{k-1}\mathrm{Har}_1^{d-1} \oplus \cdots \oplus \mathrm{Har}_k^{d-1}$. Next we note that the restriction map $\mathrm{Har}_k^d \longrightarrow \mathrm{Har}_k^d(S^{d-1})$ commutes with $\mathrm{O}(d-1)$ and hence the representations on these spaces are equivalent. Furthermore, for each $0 \leq l \leq k$, the maps $x_d^l\mathrm{Har}_{k-l}^{d-1} \longrightarrow \mathrm{Har}_{k-l}^{d-1}$ also commute with $\mathrm{O}(d-1)$ and hence the representations on these spaces are also equivalent. Therefore $\mathrm{Har}_k^d(S^{d-1})$ has a decomposition as in the statement. □

Next we follow Bachoc and Vallentin [BV08] and use Section 2.2.2 to define the zonal functions that describe a positive and invariant kernel. Since the representations of $\mathrm{O}(d-1)$ in the spaces Har_l^{d-1} are irreducible, composing Theorems 2.3.2 and 2.3.11, we get a decomposition of $\mathrm{Pol}(S^{d-1})_{\leq k}$ into invariant irreducible subspaces under the action of $\mathrm{O}(d-1)$:

$$\begin{array}{rclclclcl} \mathrm{Pol}(S^{d-1})_{\leq k} & = & \mathrm{Har}_0^d(S^{d-1}) & \oplus & \mathrm{Har}_1^d(S^{d-1}) & \oplus & \cdots & \oplus & \mathrm{Har}_k^d(S^{d-1}) \\ & = & \mathrm{Har}_{0,0}^d(S^{d-1}) & \oplus & \mathrm{Har}_{1,0}^d(S^{d-1}) & \oplus & \cdots & \oplus & \mathrm{Har}_{k,0}^d(S^{d-1}) \\ & & & \oplus & \mathrm{Har}_{1,1}^d(S^{d-1}) & \oplus & \cdots & \oplus & \mathrm{Har}_{k,1}^d(S^{d-1}) \\ & & & & & & & & \cdots\cdots\cdots \\ & & & & & & & \oplus & \mathrm{Har}_{k,k}^d(S^{d-1}). \end{array}$$

Putting together the equivalent irreducible subspaces:

$$\begin{aligned} \mathrm{Pol}(S^{d-1})_{\leq k} &= I_0 \oplus \cdots \oplus I_k, \\ I_l &:= \mathrm{Har}_{l,l}^d(S^{d-1}) \oplus \cdots \oplus \mathrm{Har}_{k,l}^d(S^{d-1}) \simeq (k-l+1)\mathrm{Har}_l^{d-1}. \end{aligned} \tag{2.10}$$

The proof of Theorem 2.3.11 does not give an explicit description of the subspaces $\mathrm{Har}_{k,l}^d(S^{d-1})$ since it uses the quotient $\mathrm{Hom}_k^d/(\|x\|^2\mathrm{Hom}_{k-2}^d)$ to establish the equivalence. Recall that the decomposition of a representation into equivalent irreducible subspaces is not unique, next we will find a simpler decomposition giving up of finding $\mathrm{Har}_{j,l}^d(S^{d-1})$ as a subspace of $\mathrm{Har}_j^d(S^{d-1})$ for $l \leq j \leq k$.

For a univariate polynomial p of degree at most $k-l$, let $p(x_d)\mathrm{Har}_l^{d-1}(S^{d-1}) \subset \mathrm{Pol}(S^{d-1})_{\leq k}$ be the subspace of spherical polynomials of the form $p(x_d)g(x')$, with $g \in \mathrm{Har}_l^{d-1}$. We rewrite $p(x_d)g(x')$ in terms of the spherical polynomial in $\mathrm{Har}_l^{d-1}(S^{d-2})$ that g also induces, for this we use that if $x \in S^{d-1}$ and $x' \neq 0$, then $(1-x_d^2)^{-1/2}x' \in S^{d-2}$ and since g is homogeneous of degree l, then

$$p(x_d)g(x') = p(x_d)(1-x_d^2)^{l/2}g\big((1-x_d^2)^{-1/2}x'\big). \tag{2.11}$$

Since the action of $\mathrm{O}(d-1)$ fixes x_d, the representation of $\mathrm{O}(d-1)$ in $p(x_d)\mathrm{Har}_l^{d-1}(S^{d-1})$ is equivalent to Har_l^{d-1} and since this holds for any polynomial p, for a basis $p_0, \ldots, p_{k-l}$ of univariate polynomials of degree at most $k-l$ (e.g. the monomial basis), we have the following decomposition of I_l as a direct sum of equivalent irreducible subspaces:

$$I_l = p_0(x_d)\mathrm{Har}_l^{d-1}(S^{d-1}) \oplus \cdots \oplus p_{k-l}(x_d)\mathrm{Har}_l^{d-1}(S^{d-1}).$$

Choosing the basis appropriately one can make the direct sum orthogonal, as done in the proof of Theorem 3.2 of Bachoc and Vallentin [BV08]. Given Remark 2.2.3, the monomial basis is enough to produce zonal functions that can be used to define positive and invariant kernels.

For $0 \le l \le k$, we fix an orthonormal basis $\{Y_{l,1}, \dots, Y_{l,h_l^{d-1}}\}$ of real-valued functions for $\mathrm{Har}_l^{d-1}(S^{d-2})$ and for $0 \le i \le k-l$, we use (2.11) to turn it into a basis for $p_i(x_d)\mathrm{Har}_l^{d-1}(S^{d-1})$. For each $0 \le i, j \le k-l$, the zonal functions (as defined in (2.5)) for the representations of $\mathrm{O}(d-1)$ equivalent to Har_l^{d-1} in $\mathrm{Pol}(S^{d-1})_{\le k}$ are:

$$\begin{aligned} Z_{i,j}^l(x,y) &:= \frac{1}{h_l^{d-1}} \sum_{s=1}^{h_l^{d-1}} p_i(x_d)(1-x_d^2)^{l/2} Y_{l,s}\big((1-x_d^2)^{-1/2}x'\big) p_j(y_d)(1-y_d^2)^{l/2} Y_{l,s}\big((1-y_d^2)^{-1/2}y'\big) \\ &= p_i(x_d)p_j(y_d)\big((1-x_d^2)(1-y_d^2)\big)^{l/2} P_l^{d-1}\left(\frac{\langle x,y\rangle - x_d y_d}{\sqrt{(1-x_d^2)(1-y_d^2)}}\right), \end{aligned}$$

where we have used (2.8) and $\langle x', y'\rangle = \langle x, y\rangle - x_d y_d$.

Since $\mathrm{Pol}(S^{d-1})_{\ge k}$ approximates $L^2(S^{d-1})$ as $k \longrightarrow \infty$, using Theorem 2.2.2 and the formula above, we have a description for the $\mathrm{O}(d-1)$-invariant and positive kernels of $L^2(S^{d-1} \times S^{d-1})$.

The case for $1 \le m \le d-2$ and the action of $\mathrm{O}(d-m)$ is very similar. We iterate Theorem 2.3.11 with $\mathrm{O}(d-2)$ in place of $\mathrm{O}(d-1)$ and decompose each $\mathrm{Har}_{k,l}^d(S^{d-1})$ into a direct sum of irreducible subspaces

$$\mathrm{Har}_{k,l}^d(S^{d-1}) = \mathrm{Har}_{k,l,0}^d(S^{d-1}) \oplus \cdots \oplus \mathrm{Har}_{k,l,l}^d(S^{d-1}),$$

where the representation of $\mathrm{O}(d-2)$ in each $\mathrm{Har}_{k,l,i}^d(S^{d-1})$ is equivalent to Har_i^{d-2}. Repeating this process until $\mathrm{O}(d-m)$, we conclude that $\mathrm{Pol}(S^{d-1})_{\le k}$ decomposes into irreducible subspaces equivalent to Har_l^{d-m} for $0 \le l \le k$, with each representation Har_l^{d-m} appearing $\binom{k-l+m}{m}$ times (the number of ways that m nonnegative integers can add up to $k-l$). Using an orthonormal basis of real-valued functions for $\mathrm{Har}_l^{d-m}(S^{d-m-1})$ and a polynomial of degree at most $k-l$ in m variables p, we may procede similarly to (2.11) and transform it into a basis for $p(u)\mathrm{Har}_l^{d-m}(S^{d-1}) \subset \mathrm{Pol}(S^{d-1})_{\le k}$, where we use u to denote the last m coordinates of x.

For $0 \le m \le d-2$, $t \in \mathbb{R}$, and $u, v \in \mathbb{R}^m$, we define the *Multivariate Gegenbauer polynomial* $P_l^{d,m}$ as the $(2m+1)$-variable polynomial

$$P_l^{d,m}(t,u,v) := \big((1-\|u\|^2)(1-\|v\|^2)\big)^{l/2} P_l^{d-m}\left(\frac{t - \langle u, v\rangle}{\sqrt{(1-\|u\|^2)(1-\|v\|^2)}}\right). \tag{2.12}$$

If we use the convention $\mathbb{R}^0 = \{0\}$, then $P_l^d(t) = P_l^{d,0}(t,0,0)$. Fix $k \ge 0$, let $\mathcal{B}_l$ be a basis of the space of m-variable polynomials of degree at most l (e.g. the monomial basis), and write $z_l(u)$ for the column vector containing the polynomials of $\mathcal{B}_l$ evaluated at $u \in \mathbb{R}^m$. The matrix $Y_l^{d,m}$ is the matrix of polynomials

$$Y_l^{d,m}(t,u,v) = P_l^{d,m}(t,u,v) z_{k-l}(u) z_{k-l}(v)^{\mathsf{T}}.$$

Theorem 2.3.12 (Musin [Mus14]). *Let $0 \le m \le d-2$ and for $x \in \mathbb{R}^d$, let $Ex := (x_{d-m+1}, \dots, x_d)$ be the projection of x onto the last m coordinates. Let $k \ge 0$ and, for* *each* $0 \leq l \leq k$, *let* $\hat{K}_l$ *be a positive semidefinite matrix of size* $\binom{k-l+m}{m} \times \binom{k-l+m}{m}$. *Then* $K : S^{d-1} \times S^{d-1} \longrightarrow \mathbb{R}$ *given by*

$$K(x, y) = \sum_{l=0}^{k} \left\langle \hat{K}_l, Y_l^{d,m}(\langle x, y\rangle, Ex, Ey)\right\rangle$$

is a positive, continuous, and $\mathrm{O}(d-m)$*-invariant kernel.*

This theorem follows from Theorem 2.2.2, nevertheless we repeat the proof explicitly. First we prove that the polynomials $P_l^{d,m}$ satisfy the following positivity property [Mus14, Theorem 3.1].

Proposition 2.3.13 (Musin [Mus14]). *Let* $0 \leq m \leq d-2$ *and for* $x \in \mathbb{R}^d$, *let* $Ex := (x_{d-m+1}, \ldots, x_d)$ *be the projection of* x *onto the last* m *coordinates. Let* C *be a finite subset of* S^{d-1}. *Then, for every nonnegative integer* l, *the matrix* $\left(P_l^{d,m}(\langle x, y\rangle, Ex, Ey)\right)_{x,y\in C}$ *is positive semidefinite.*

Proof. If $l = 0$ then all polynomials evaluate to 1 and the proposition holds, so we assume $l \neq 0$. Let L be the subspace spanned by the last m coordinates of $\mathbb{R}^d$ and z be a unit vector in $L^\perp$. For each $x \in C$, write $x = x' + Ex$ with $x' := (x_1, \ldots, x_{d-m}) \in L^\perp$ and $Ex \in L$. If $\|x'\| > 0$, then let $\bar{x} := x'/\|x'\|$, otherwise write $\bar{x} = z$. If $\|x'\|, \|y'\| \neq 0$, then

$$\langle \bar{x}, \bar{y}\rangle = \frac{\langle x', y'\rangle}{\|x'\|\|y'\|} = \frac{\langle x, y\rangle - \langle Ex, Ey\rangle}{\sqrt{(1-\|Ex\|^2)(1-\|Ey\|^2)}}.$$

From Definition (2.12), we have $\|x'\|^l\|y'\|^l P_l^{d-m}(\langle \bar{x}, \bar{y}\rangle) = P_l^{d,m}(\langle x, y\rangle, Ex, Ey)$.

If, say, $\|x'\| = 0$, then $\|x'\|^l\|y'\|^l P_l^{d-m}(\langle \bar{x}, \bar{y}\rangle) = 0$, while $P_l^{d,m}(\langle x, y\rangle, Ex, Ey)$ is also 0 as can be seen from (2.12), since $\langle x, y\rangle - \langle Ex, Ey\rangle = \langle x', y'\rangle = 0$.

Now $\{\bar{x} : x \in C\}$ is contained in S^{d-m-1} and by (2.8) we have that $\left(P_l^{d-m}(\langle \bar{x}, \bar{y}\rangle)\right)_{x,y\in C}$ is positive semidefinite. Since $\left(\|x'\|^l\|y'\|^l\right)_{x,y\in C}$ is positive semidefinite, so is $\left(\|x'\|^l\|y'\|^l P_l^{d-m}(\langle \bar{x}, \bar{y}\rangle)\right)_{x,y\in C}$, and we are done. ☐

Proof of Theorem 2.3.12. Since all entries of $Y_l^{d,m}$ are polynomials, K is continuous, and since $\langle x, y\rangle$, Ex, and Ey are invariant under the action of $\mathrm{O}(d-m)$ on (x, y), K is invariant. To prove positivity, let C be a finite subset of S^{d-1} and $w : C \longrightarrow \mathbb{R}$ be a function. We have

$$\sum_{x,y\in C} w(x)w(y)K(x, y) = \sum_{l=0}^{k} \left\langle F_l, \sum_{x,y\in C} w(x)w(y)Y_l^{d,m}(\langle x, y\rangle, Ex, Ey)\right\rangle.$$

To show this quantity is nonnegative, we will show that for all $l = 0, \ldots, k$ the matrix $\sum_{x,y\in C} w(x)w(y)Y_l^{d,m}\left(\langle x, y\rangle, Ex, Ey\right)$ is positive semidefinite writing it as a product of matrices: if B is the matrix whose columns are given by $z_{k-l}(Ex)$ for $x \in C$, then

$$\begin{aligned}\sum_{x,y\in C} w(x)w(y)Y_l^{d,m}(\langle x, y\rangle, Ex, Ey) &= \sum_{x,y\in C} w(x)w(y)z_{k-l}(Ex)z_{k-l}(Ey)^\mathsf{T} P_l^{d,m}(\langle x, y\rangle, Ex, Ey)\\ &= B\left(P_l^{d,m}(\langle x, y\rangle, Ex, Ey)\right)_{x,y\in C} B^\mathsf{T},\end{aligned}$$

and, since the matrix $\left(P_l^{d,m}(\langle x, y\rangle, Ex, Ey)\right)_{x,y\in C}$ is positive semidefinite by Proposition 2.3.13, we are done. $\square$

2.4 Fourier Analysis

We consider the Euclidean space $\mathbb{R}^d$ and its action on itself by translations. It is a locally compact Hausdorff space with an invariant measure known as the Lebesgue measure. We consider two kinds of functions defined in $\mathbb{R}^d$: periodic functions, which for some lattice L satisfy $f(x+m) = f(x)$ for all $x \in \mathbb{R}^d$, $m \in L$ and functions with some decay condition, namely absolutely integrable or square-integrable functions. First we present some basic definitions and facts about lattices.

2.4.1 Lattices

A *k-dimensional lattice* L in $\mathbb{R}^d$ is a discrete additive subgroup generated by k linearly independent vectors $w_1, \dots, w_k \in \mathbb{R}^d$:

$$L := \{n_1 w_1 + \cdots + n_k w_k \,:\, n_1, \dots, n_k \in \mathbb{Z}\}.$$

When the dimension is not specified, we assume that the lattice is full-dimensional. Let $B \in \mathbb{R}^{d\times k}$ be a matrix with $w_1, \dots, w_k$ as columns. The *fundamental parallelepiped* of L with respect to this basis is the set

$$B[0,1]^k := \{Bx \,:\, x \in [0,1]^k\} = \{x_1 w_1 + \cdots + x_k w_k \,:\, x_1, \dots, x_k \in [0,1]\}.$$

Any set of k vectors that generates L is called a *lattice basis*. The columns of a matrix $Z \in \mathbb{R}^{d\times k}$ form another basis for L if and only if $Z = BU$ for some unimodular matrix $U \in \mathbb{Z}^{k\times k}$. The *determinant* $\det(L)$ of L is the k-dimensional volume of a fundamental parallelepiped for L, it can be computed as

$$\det(L) = \det(B^{\mathsf{T}} B)^{1/2}. \tag{2.13}$$

Since any two bases for a lattice are related by a unimodular transformation, the determinant does not depend on the choice of the basis. Due to this relation, we also use the notation $|\det(B)| := \det(B^{\mathsf{T}} B)^{1/2}$.

The *dual lattice* L^* is defined as

$$L^* := \{y \in \operatorname{span}(L) \,:\, \langle x, y\rangle \in \mathbb{Z} \text{ for all } x \in L\}.$$

The columns of $B(B^{\mathsf{T}} B)^{-1}$ form a lattice basis for Λ^*. Thus, $\det(L)\det(L^*) = 1$.

Next we assume that L is a subset of another lattice $\Lambda \subseteq \mathbb{R}^d$ and define

$$L^{\perp} := \{v \in \Lambda^* \,:\, \langle v, x\rangle = 0 \text{ for all } x \in L\},$$

note that $L^\perp \subseteq \Lambda^*$. The lattice L is called a *primitive lattice* with respect to Λ, when

$$\operatorname{span}(L) \cap \Lambda = L.$$

The following two lemmas are very useful for Chapter 6, moreover they give some elementary but extremely useful facts about lattices, especially in the case that they are not full-dimensional.

Lemma 2.4.1. *Let $\Lambda \subseteq \mathbb{R}^d$ be a d-dimensional lattice and let $L \subseteq \Lambda$ be a primitive lattice with respect to Λ. Then*

$$\det(L^\perp) = \frac{\det(L)}{\det(\Lambda)}.$$

Proof. Through this proof, for any set $v_1, \dots, v_s$ of vectors in $\mathbb{R}^d$, we use the notation $\det(v_1, \dots, v_s) := \det(V^\top V)^{1/2}$, where V is the matrix with $v_1, \dots, v_s$ as columns.

Let $a_1, \dots, a_k$ be a basis for L and $a_{k+1}, \dots, a_d$ be a completion to a basis for Λ (that is possible since L is primitive), so $\det(a_1, \dots, a_k) = \det(L)$ and $\det(a_1, \dots, a_d) = \det(\Lambda)$. Let $f_1, \dots, f_d$ be the dual basis for Λ^*, that is, $f_1, \dots, f_d$ are defined such that $\left\langle f_i, a_j \right\rangle = \delta_{i,j}$ for all $i, j = 1, \dots, d$. Note that $f_{k+1}, \dots, f_d$ is a basis for $L^\perp$, so $\det(f_{k+1}, \dots, f_d) = \det(L^\perp)$.

Now, for $i = 1, \dots, k$, let $\tilde{f}_i := f_i - \operatorname{Proj}_{\operatorname{span}(L)^\perp}(f_i)$, so that $\tilde{f}_i \in \operatorname{span}(L)$ and $f_i - \tilde{f}_i \in \operatorname{span}(L)^\perp = \operatorname{span}(f_{k+1}, \dots, f_d)$. Since, for $i = 1, \dots, k$, the difference between f_i and $\tilde{f}_i$ is a linear combination of $f_{k+1}, \dots, f_d$, we have that $\det(f_1, \dots, f_d) = \det(\tilde{f}_1, \dots, \tilde{f}_k, f_{k+1}, \dots, f_d)$ and since $\tilde{f}_1, \dots, \tilde{f}_k \in \operatorname{span}(L)$ and $f_{k+1}, \dots, f_d \in \operatorname{span}(L)^\perp$, we also have that

$$\det(\tilde{f}_1, \dots, \tilde{f}_k, f_{k+1}, \dots, f_d) = \det(\tilde{f}_1, \dots, \tilde{f}_k) \det(f_{k+1}, \dots, f_d). \tag{2.14}$$

Furthermore, since for all $i, j = 1, \dots, k$, $\langle \tilde{f}_i, a_j \rangle = \left\langle f_i, a_j \right\rangle = \delta_{i,j}$ and $\tilde{f}_1, \dots, \tilde{f}_k \in \operatorname{span}(L)$, they form a basis for L^* and so $\det(\tilde{f}_1, \dots, \tilde{f}_k) = 1/\det(L)$.

Thus, from (2.14), we see that $1/\det(\Lambda) = \det(L^\perp)/\det(L)$, as desired. □

We note that Lemma 2.4.1 is non-trivial even in the case that $\Lambda := \mathbb{Z}^d$ and L is a $(d-1)$-dimensional sublattice.

Example 2.4.2. *Let $\Lambda = \mathbb{Z}^3$ and $A \subset \mathbb{R}^3$ be a rational plane, so that $L := A \cap \mathbb{Z}^3$ is a 2-dimensional lattice. Then according to Lemma 2.4.1, the area of a fundamental parallelepiped of L is equal to the length of the shortest integer vector orthogonal to A (see Figure 2.1).*

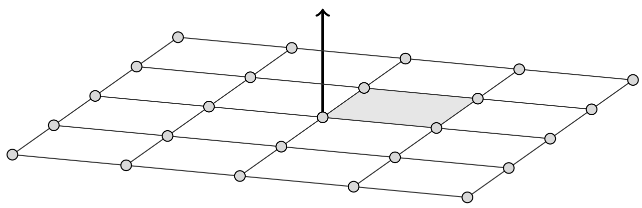

Figure 2.1: *A lattice with its fundamental domain in a plane and a vector orthogonal to the plane.*

Lemma 2.4.3. *Let $\Lambda \subseteq \mathbb{R}^d$ be a d-dimensional lattice and $L \subseteq \Lambda$ be a primitive lattice with respect to Λ. Then*

$$L^* = \mathrm{Proj}_{\mathrm{span}(L)}(\Lambda^*).$$

Proof. As in the proof of the previous lemma, let $a_1, \dots, a_k$ be a basis for L, $a_{k+1}, \dots, a_d$ be a completion to a basis for Λ, and let $f_1, \dots, f_d$ be the dual basis for Λ^*, that is, $f_1, \dots, f_d$ are defined such that $\left\langle f_i, a_j \right\rangle = \delta_{i,j}$ for all $i, j = 1, \dots, d$. Denoting by A_k the matrix with $a_1, \dots, a_k$ as columns, we have that $P = A_k(A_k^\top A_k)^{-1} A_k^\top$ is the orthogonal projection onto $\mathrm{span}(L)$, indeed, $PA_k = A_k$ and $Pv = 0$ for $v \in \mathrm{span}(L)^\perp$. Denoting by F the matrix with $f_1, \dots, f_d$ as columns, we get that $\mathrm{Pr}_{\mathrm{span}(L)}(\Lambda^*)$ is spanned by the columns of $PF = A_k(A_k^\top A_k)^{-1} A_k^\top F = \left(A_k(A_k^\top A_k)^{-1} \mid 0\right)$. We finish the proof noting that the columns of $A_k(A_k^\top A_k)^{-1}$ are indeed a lattice basis for L^*, to see this simply note that $A_k^\top \left(A_k(A_k^\top A_k)^{-1}\right) = I$. □

2.4.2 Harmonic analysis on the torus

Let $\Lambda \subset \mathbb{R}^d$ be a d-dimensional lattice. Functions $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ periodic by lattice translations can be seen as functions defined in the *torus* $\mathbb{T}^d := \mathbb{R}^d/\Lambda$. For the integration of a function over $\mathbb{T}^d$ we may fix a lattice basis for Λ and take $\mathbb{T}^d \simeq B[0,1]^d$, where B is a matrix with the basis in its columns. However to say that a function over $\mathbb{T}^d$ is continuous we must consider the sides of $B[0,1]^d$ "glued". For instance, when $d = 1$ a function $f \in C(\mathbb{T})$ must satisfy $f(0) = f(1)$ besides being continuous in $[0,1]$.

The torus is a compact abelian group, so as shown in Corollary 2.1.2 and Theorem 2.1.7, $L^2(\mathbb{T}^d)$ has a complete orthonormal system of functions for which the left-regular representation $(L(y)f)(x) := f(x-y)$ becomes a scalar multiplication. These functions are the exponentials

$$\phi_m(x) := \det(\Lambda)^{-1/2} e^{2\pi i \langle m, x\rangle},$$

for $m \in \Lambda^*$. The expression of a function $f \in L^2(\mathbb{T}^d)$ in terms of this basis is the *Fourier series* of f and the coefficients of this series can be computed using the orthonormality of this basis (see e.g., Theorem 3.54 in Einsiedler and Ward [EW17]):

Theorem 2.4.4 (Fourier series)**.** *The functions $\{\phi_m : m \in \Lambda^*\}$ form a complete orthonormal system for $L^2(\mathbb{T}^d)$, so that every $f \in L^2(\mathbb{T}^d)$ can be written as*

$$f(x) \sim \frac{1}{\det(\Lambda)} \sum_{m \in \Lambda^*} \hat{f}_m e^{2\pi i \langle m, x\rangle}, \tag{2.15}$$

where the symbol $\sim$ stands for an equality in the $L^2(\mathbb{T}^d)$-norm, not necessarily for all $x \in \mathbb{T}^d$. The coefficients $\hat{f}_m$ can be computed using:

$$\hat{f}_m = \det(\Lambda)^{1/2} \langle f, \phi_m\rangle = \int_{\mathbb{T}^d} f(x) e^{-2\pi i \langle m, x\rangle}\, \mathrm{d}x, \tag{2.16}$$

and moreover,

$$\|f\|_2^2 := \int_{\mathbb{T}^d} |f(x)|^2\, \mathrm{d}x = \frac{1}{\det(\Lambda)} \sum_{m \in \Lambda^*} |\hat{f}_m|^2.$$

The harmonic analysis perspective appears when we note that for a function $f \in L^2(\mathbb{T}^d)$

and $y \in \mathbb{T}^d$, the coefficients of $L(y)f$ have a nice form in terms of the coefficients of f, namely the coefficients are multiplied by a factor:

$$(\widehat{L(y)f})_m = e^{-2\pi i \langle m,y \rangle} \hat{f}_m.$$

In order to obtain pointwise or uniform convergence in the Fourier series (2.15) for a continuous function $f \in C(\mathbb{T}^d)$, other hypothesis are necessary. Indeed, there are examples of continuous functions for which the Fourier series diverges at a given point (see e.g., Theorem 4.9 in Einsiedler and Ward [EW17] or Theorem 4.19 in Travaglini [Tra14]). Let $C^k(\mathbb{T}^d)$ be the class of functions for which all the partial derivatives up to order k exist and are continuous. For $d = 1$, $f \in C^1(\mathbb{T})$ implies uniform convergence of its Fourier series, and more generally, Theorem 3.57 of Einsiedler and Ward [EW17] says:

Theorem 2.4.5. *Suppose that $f \in C^k(\mathbb{T}^d)$ for some $k \geq 1$ and let $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq k$. Then the Fourier coefficient $(\widehat{\partial_\alpha f})_m$ of $\partial_\alpha f$ is given by*

$$(\widehat{\partial_\alpha f})_m = (2\pi i n_1)^{\alpha_1} \dots (2\pi i n_d)^{\alpha_d} \hat{f}_m.$$

If $k > d/2$, then the Fourier series converges absolutely and uniformly to f.

When $d = 1$ and continuity of f and its derivative are relaxed to piecewise continuity, the Fourier series converges pointwise to the mean on every $x \in \mathbb{T}$ (e.g., Theorem 4.18 in Travaglini [Tra14]):

$$\sum_{m \in \mathbb{Z}^d} \hat{f}_m e^{2\pi i \langle m, x_0 \rangle} = \frac{1}{2}\left(\lim_{x \to x_0^+} f(x) + \lim_{x \to x_0^-} f(x) \right).$$

The lack of uniform convergence of the Fourier series for continuous functions should not be confused with the statement of Theorem 2.1.7, which says that any continuous function can be uniformly approximated by a sequence of trigonometric polynomials. The next theorem (see e.g., Proposition 3.65 in Einsiedler and Ward [EW17]) shows how a function in $C(\mathbb{T})$ can be uniformly approximated by a sequence of trigonometric polynomials, however note that it does not use a trigonometric series for this approximation since the coefficients are functions of N:

Theorem 2.4.6 (Fejér)**.** *If $f \in C(\mathbb{T})$, then the sequence*

$$\frac{1}{N} \sum_{n=0}^{N-1} \left(\sum_{m=-n}^{n} \hat{f}_m e^{2\pi i m x} \right) = \sum_{m=-N+1}^{N-1} \left(1 - \frac{|m|}{N} \right) \hat{f}_m e^{2\pi i m x}$$

converges uniformly to $f(x)$ as $N \longrightarrow \infty$.

2.4.3 Harmonic analysis on the Euclidean space

We review some facts from the Fourier transform, the proofs for all of them can be found e.g. in Chapter I of Stein and Weiss [SW71].

For a measurable function $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ and $1 \leq p < \infty$, the *p-norm* of f is $\|f\|_p :=$

$\left(\int_{\mathbb{R}^d} |f(x)|^p \, dx\right)^{1/p}$ and

$$L^p(\mathbb{R}^d) := \{f : \mathbb{R}^d \longrightarrow \mathbb{C} : \|f\|_p < \infty\}.$$

Identifying functions with norm 0, these are complete normed vector spaces (i.e., Banach spaces).

The *Fourier transform* of a function $f \in L^1(\mathbb{R}^d)$ is the function $\hat{f} : \mathbb{R}^d \longrightarrow \mathbb{C}$ defined by

$$\hat{f}(\xi) := \mathcal{F}(f)(\xi) := \int_{\mathbb{R}^d} f(x) e^{-2\pi i \langle x, \xi \rangle} \, dx. \tag{2.17}$$

The main advantage in working with $L^1(\mathbb{R}^d)$ is the Dominated Convergence Theorem (see e.g., Theorem 1.34 in Rudin [Rud87]), which gives conditions to exchange a limit with an integral. This leads to many properties, next we list a few (see Chapter 1 of Stein and Weiss [SW71] or Chapter 9 of Rudin [Rud87]):

Theorem 2.4.7. *If $f \in L^1(\mathbb{R}^d)$, then:*

(a) $\hat{f}$ is uniformly continuous.

(b) $\hat{f}(\xi) \longrightarrow 0$ as $\|\xi\| \longrightarrow \infty$.

(c) $\sup_{\xi \in \mathbb{R}^d} |\hat{f}(\xi)| \leq \|f\|_1$.

(d) Let $g(x) := x_k f(x)$, where x_k is the k-th coordinate of x. If $g \in L^1(\mathbb{R}^d)$, then $\hat{f}$ is differentiable with respect to x_k and

$$\frac{\partial \hat{f}}{\partial x_k}(\xi) = -2\pi i \hat{g}(\xi).$$

The definition of the Fourier transform can be extended to square-integrable functions $f \in L^2(\mathbb{R}^d)$ with the limit

$$\lim_{n \longrightarrow \infty} \int_{\|x\| \leq n} f(x) e^{-2\pi i \langle x, \xi \rangle} \, dx, \tag{2.18}$$

using the fact that $L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$. The space $L^2(\mathbb{R}^d)$ is more suitable for our considerations, since it is an Hilbert space with an inner product structure. For $f, g \in L^2(\mathbb{R}^d)$,

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

It is also the space of the left-regular representation of $\mathbb{R}^d$. For $f \in L^2(\mathbb{R}^d)$ and $y \in \mathbb{R}^d$,

$$(L(y)f)(x) := f(x - y).$$

It will be convenient to denote the *translation by y* as $T_y(x) := x - y$, so that $(L(y)f)(x) = (f \circ T_y)(x)$. One important property of the Fourier transform in $L^2(\mathbb{R}^d)$ is that $\hat{f}$ also lies in $L^2(\mathbb{R}^d)$ and it is an isometry:

Theorem 2.4.8. *If $f \in L^2(\mathbb{R}^d)$, then $\hat{f} \in L^2(\mathbb{R}^d)$ and furthermore $\|f\|_2 = \|\hat{f}\|_2$. More generally, for all $f, g \in L^2(\mathbb{R}^d)$, $\langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle$.*

For a function in $L^1(\mathbb{R}^d)$, the analogue statement is not necessarily true: a counter-example is $\mathbb{1}_{[-\frac{1}{2},\frac{1}{2}]} \in L^1(\mathbb{R})$, whose Fourier transform $\hat{\mathbb{1}}_{[-\frac{1}{2},\frac{1}{2}]}(\xi) = \frac{\sin(\pi\xi)}{\pi\xi} \notin L^1(\mathbb{R})$.

The Fourier transform is invertible in $L^2(\mathbb{R}^d)$ (Theorem I.2.4 in Stein and Weiss [SW71]):

Theorem 2.4.9. *For any function $f \in L^2(\mathbb{R}^d)$,*

$$f(x) = \int_{\mathbb{R}^d} \hat{f}(\xi) e^{2\pi i\langle x,\xi\rangle} d\xi = (\mathcal{F}\circ\mathcal{F})f(-x), \tag{2.19}$$

where the equality holds in the $L^2(\mathbb{R}^d)$-norm, not necessarily for all $x \in \mathbb{R}^d$.

A similar statement holds pointwise for $f \in L^1(\mathbb{R}^d)$ continuous, but then it is also necessary to assume that $\hat{f} \in L^1(\mathbb{R}^d)$ (Corollary I.1.21 in Stein and Weiss [SW71]):

Theorem 2.4.10. *If f is a continuous function in $L^1(\mathbb{R}^d)$ such that $\hat{f} \in L^1(\mathbb{R}^d)$, then*

$$f(x) = \int_{\mathbb{R}^d} \hat{f}(\xi) e^{2\pi i\langle x,\xi\rangle} d\xi = (\mathcal{F}\circ\mathcal{F})f(-x), \tag{2.20}$$

for all $x \in \mathbb{R}^d$.

The harmonic analysis perspective appears when we note that the exponentials $e^{2\pi i\langle x,\xi\rangle}$ for $\xi \in \mathbb{R}^d$ span the one dimensional irreducible representations of $\mathbb{R}^d$ in $L^2(\mathbb{R}^d)$ and (2.19) reconstructs $f \in L^2(\mathbb{R}^d)$ in terms of its projection on these subspaces. Since $\mathbb{R}^d$ is not a compact group, the decomposition comes in the form of an integral instead of a direct sum, like we had with the Fourier series (2.15).

Similarly to the Fourier series, the Fourier transform changes nicely when composed with the left-regular representation, namely:

$$\mathcal{F}(L(y)f)(\xi) = \mathcal{F}(f\circ T_y)(\xi) = e^{-2\pi i\langle y,\xi\rangle}\hat{f}(\xi). \tag{2.21}$$

With another change of variables, we also have the following useful identity. For an invertible matrix $M \in \mathbb{R}^{d\times d}$:

$$(\hat{f}\circ M^\top)(\xi) = \frac{1}{|\det(M)|}\mathcal{F}(f\circ M^{-1})(\xi). \tag{2.22}$$

An operation commonly used together with the Fourier transform is the *convolution* between two functions, which is defined for $f, g \in L^1(\mathbb{R}^d)$ as

$$(f * g)(x) := \int_{\mathbb{R}^d} f(y)g(x-y)\,\mathrm{d}y.$$

Using Fubini's theorem and exchanging the integration order, the convolution satisfies the following properties (see e.g., Stein and Weiss [SW71] and Rudin [Rud62]):

Proposition 2.4.11. *For $f, g, h \in L^1(\mathbb{R}^d)$,*

(a) $f * g \in L^1(\mathbb{R}^d)$ and $\|f * g\|_1 \leq \|f\|_1\|g\|_1$,

(b) $f * g = g * f$,

(c) $f * (g * h) = (f * g) * h$.

More generally, using Minkowski's integral inequality, if $f \in L^p(\mathbb{R}^d)$, $1 \leq p < \infty$, *and* $g \in L^1(\mathbb{R}^d)$,

(d) $f * g \in L^p(\mathbb{R}^d)$ *and* $\|f * g\|_p \leq \|f\|_p \|g\|_1$.

And for $1 < p, q < \infty$ *such that* $\frac{1}{p} + \frac{1}{q} = 1$, *if* $f \in L^p(\mathbb{R}^d)$ *and* $g \in L^q(\mathbb{R}^d)$, *then*

(e) $f * g \in C_0(\mathbb{R}^d)$, *the space of continuous functions in* $\mathbb{R}^d$ *that vanish at infinity.*

Convolutions behave nicely with the Fourier transform. For $f, g \in L^1(\mathbb{R}^d)$ and again using Fubini's theorem to exchange the integration order,

$$\mathcal{F}(f * g)(\xi) = \hat{f}(\xi)\hat{g}(\xi). \tag{2.23}$$

Convolutions are useful to approximate functions by "nicer" functions. As Theorem I.1.18 from Stein and Weiss [SW71] shows:

Theorem 2.4.12. *Suppose* $\phi \in L^1(\mathbb{R}^d)$ *with* $\int_{\mathbb{R}^d} \phi(x)\,\mathrm{d}x = 1$ *and for* $\epsilon > 0$ *let* $\phi_\epsilon(x) := \epsilon^{-d}(x/\epsilon)$. *If* $f \in L^p(\mathbb{R}^d)$, $1 \leq p < \infty$, *then* $\|\phi_\epsilon * f - f\|_p \longrightarrow 0$ *as* $\epsilon \longrightarrow 0$. *If* f *is continuous and goes to* 0 *at* ∞, *then* $\phi_\epsilon * f \longrightarrow f$ *uniformly.*

The Schwartz space

The space $\mathcal{S}^d$ of *Schwartz functions* is the space of functions $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ infinitely differentiable and such that for all $\alpha, \beta \in \mathbb{N}_0^d$, $x^\alpha D^\beta f$ is a bounded function.

Despite being a very restrictive condition, functions in this space can approximate well other functions and the Fourier transform behaves very nicely in this space. In particular, $\mathcal{F}$ is a bijection in $\mathcal{S}^d$ and the Schwartz space is also closed under convolutions, products, differentiation and products with polynomials. Furthermore $\mathcal{S}^d \subset L^p(\mathbb{R}^d)$ and is dense in $L^p(\mathbb{R}^d)$ for all $1 \leq p < \infty$. See Chapter IX of Reed and Simon [RS72] or Chapter 2 of Woolf [Wol03] for the proofs of the main facts about this space.

Any infinitely differentiable function with compact support is a Schwartz function. Another important example is the *Gaussian*, $\phi_{d,\epsilon} : \mathbb{R}^d \longrightarrow \mathbb{C}$, for $\epsilon > 0$, defined as

$$\phi_{d,\epsilon}(x) := \epsilon^{-d/2} e^{-\pi\|x\|^2/\epsilon}. \tag{2.24}$$

As suggested by the notation, it satisfies the assumptions from Theorem 2.4.12. Its Fourier transform is (see e.g., [SW71, Chapter I, Theorem 1.13])

$$\hat{\phi}_{d,\epsilon}(\xi) = e^{-\epsilon\pi\|\xi\|^2}.$$

Note that $\hat{\phi}_{d,\epsilon}$ doesn't explicitly depend on d (except for the 2-norm in $\mathbb{R}^d$) so we also denote it by $\hat{\phi}_\epsilon$.

Functions of positive type

A function $f \in \mathbb{R}^d \longrightarrow \mathbb{C}$ is of *positive type* (also called positive-definite) if for all $N \geq 1$, $x_1, \ldots, x_N \in \mathbb{R}^d$, and $c_1, \ldots, c_N \in \mathbb{C}$,

$$\sum_{n,m=1}^{N} c_n \overline{c_m} f(x_n - x_m) \geq 0.$$

From this definition it follows that for any $x \in \mathbb{R}^d$, $f(-x) = \overline{f(x)}$ and $|f(x)| \leq f(0)$. If f is a function for which the inverse Fourier transform (2.19) holds pointwise and $\hat{f}$ is nonnegative, then it is of positive type:

$$\sum_{n,m=1}^{N} c_n \overline{c_m} f(x_n - x_m) = \sum_{n,m=1}^{N} c_n \overline{c_m} \int_{\mathbb{R}^d} \hat{f}(\xi) e^{2\pi i \langle x_n - x_m, \xi \rangle} d\xi = \int_{\mathbb{R}^d} \hat{f}(\xi) \left| \sum_{n=1}^{N} c_n e^{2\pi i \langle x_n, \xi \rangle} \right|^2 d\xi \geq 0.$$

Bochner's theorem (see Theorem IX.9 of Reed and Simon [RS72] and Section 1.4.3 of Rudin [Rud62]) characterizes the positive type continuous functions in $\mathbb{R}^d$. They are essentially the functions of the form above, with the integration with $\hat{f}(\xi)\, \mathrm{d}\xi$ being replaced by a nonnegative measure $\mathrm{d}\mu(\xi)$ in $\mathbb{R}^d$:

Theorem 2.4.13 (Bochner)**.** *A continuous function $f \in \mathbb{R}^d \longrightarrow \mathbb{C}$ is of positive type if and only if there is a finite, regular, and nonnegative measure μ such that*

$$f(x) = \int_{\mathbb{R}^d} e^{2\pi i \langle x, \xi \rangle}\, \mathrm{d}\mu(\xi).$$

The notion of a function of positive type in $\mathbb{R}^d$ is very similar to the invariant and positive kernels in a compact space defined in Section 2.2. In this case we have the locally compact and abelian group $\mathbb{R}^d$ acting in itself and to an invariant "kernel" $K : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{C}$ corresponds the function $f \in \mathbb{R}^d \longrightarrow \mathbb{C}$ such that $K(x, y) = f(x - y)$. Theorem 2.4.13 corresponds to Theorem 2.2.2, with the difference that since $\mathbb{R}^d$ is abelian, its irreducible representations are one-dimensional and given by the characters $e^{2\pi i \langle x, \xi \rangle}$ for $\xi \in \mathbb{R}^d$. The direct sum decomposition (2.2) is replaced by an integral on the group of characters, which is isomorphic to $\mathbb{R}^d$ itself (Theorem 2.19). To the positive semidefinite matrix coefficients from Theorem 2.2.2 corresponds the finite, regular, and nonnegative measure from Theorem 2.4.13.

Bessel functions

Now we consider briefly the action of $\mathrm{O}(d)$ on $L^2(\mathbb{R}^d)$. According to (2.22), the Fourier transform commutes with this action and therefore it will leave invariant each of the nonequivalent subspaces.

Recall from Section 2.3.1 that Har_k^d is the space of homogeneous harmonic polynomials of degree k in d variables and $\mathrm{Har}_k^d(S^{d-1})$ is the isomorphic space defined by the restriction of these functions to the sphere. Let $\mathfrak{H}_k^d$ be the subspace of $L^2(\mathbb{R}^d)$ spanned by functions of the form $f(x) = f_0(\|x\|)p(x)$, where $p \in \mathrm{Har}_k^d$ and $f_0 \in [0, \infty) \longrightarrow \mathbb{C}$ is such that $f \in L^2(\mathbb{R}^d)$.

The next proposition is Lemma IV.2.18 from Stein and Weiss [SW71]:

Proposition 2.4.14. *The spaces $\mathfrak{H}_k^d$ are closed subspaces of $L^2(\mathbb{R}^d)$. For $k \neq l$, $\mathfrak{H}_k^d$ and $\mathfrak{H}_l^d$ are orthogonal to each other and*

$$L^2(\mathbb{R}^d) = \bigoplus_{k=0}^{\infty} \mathfrak{H}_k^d.$$

Moreover, the Fourier transform maps each $\mathfrak{H}_k^d$ into itself.

To show that the Fourier transform maps $\mathfrak{H}_k^d$ into itself, we need two auxiliary statements: If $p \in \mathrm{Har}_k^d(S^{d-1})$, it follows from (2.8) that

$$p(\xi) = h_k^d \int_{S^{d-1}} p(\eta) P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\eta. \tag{2.25}$$

Next, for given $u \in S^{d-1}$ and $r \in [0, \infty)$, we consider the function in $\eta \in S^{d-1}$:

$$\Phi_k(u, r; \eta) := \int_{S^{d-1}} e^{-2\pi i r \langle \xi, u \rangle} P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\xi.$$

To show that $\Phi_k(u, r; \cdot) \in \mathrm{Har}_k^d(S^{d-1})$, let $h \in \mathrm{Har}_l^d(S^{d-1})$ with $l \neq k$,

$$\begin{aligned} \langle \Phi_k(u, r; \cdot), h \rangle &= \int_{S^{d-1}} \left(\int_{S^{d-1}} e^{-2\pi i r \langle \xi, u \rangle} P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\xi \right) \overline{h(\eta)} \,\mathrm{d}\eta \\ &= \int_{S^{d-1}} \left(\int_{S^{d-1}} P_k^d(\langle \xi, \eta \rangle) \overline{h(\eta)} \,\mathrm{d}\eta \right) e^{-2\pi i r \langle \xi, u \rangle} \,\mathrm{d}\xi = 0, \end{aligned}$$

since $P_k^d(\langle \xi, \eta \rangle) \in \mathrm{Har}_k^d(S^{d-1})$ as a function of η and the spaces $\mathrm{Har}_k^d(S^{d-1})$ and $\mathrm{Har}_l^d(S^{d-1})$ are orthogonal to each other according to Lemma 2.3.5. Furthermore, it is straightforward to check that for $A \in \mathrm{O}(d)$ that fixes u, $\Phi_k(u, r; A\eta) = \Phi_k(u, r; \eta)$ and hence by Proposition 2.3.7, $\Phi_k(u, r; \eta)$ is a multiple of $P_k^d(\langle \eta, u \rangle)$. So there is a function φ_k such that

$$\int_{S^{d-1}} e^{-2\pi i r \langle \xi, u \rangle} P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\xi = \varphi_k(r) P_k^d(\langle \eta, u \rangle). \tag{2.26}$$

In the following we use $\omega_d := \frac{2\pi^{d/2}}{\Gamma(d/2)}$ to denote the surface measure of S^{d-1} and note that when integrating in $\mathbb{R}^d$ with polar coordinates, we have $\mathrm{d}x = \omega_d \,\mathrm{d}s \,\mathrm{d}\xi$ for $x \in \mathbb{R}^d$, $s \in [0, \infty)$ and $\xi \in S^{d-1}$, since to integrate in S^{d-1} we are using the Haar measure of S^{d-1} normalized such that $\int_{S^{d-1}} \mathrm{d}\xi = 1$. To show that the Fourier transform maps $\mathfrak{H}_k^d$ into itself is enough to consider $f \in \mathfrak{H}_k^d \cap L^1(\mathbb{R}^d)$ since this subspace is dense in $\mathfrak{H}_k^d$ and then we may exchange integration order in the following expressions. For $f \in \mathfrak{H}_k^d \cap L^1(\mathbb{R}^d)$, we have that $f(x) = f_0(\|x\|) p(x)$ for some $f_0 : [0, \infty) \longrightarrow \mathbb{C}$ and $p \in \mathrm{Har}_k^d$. For $r \in [0, \infty)$ and $u \in S^{d-1}$:

$$\begin{aligned} \hat{f}(ru) &= \int_{\mathbb{R}^d} e^{-2\pi i \langle x, ru \rangle} f(x) \,\mathrm{d}x \\ &= \omega_d \int_0^{\infty} f_0(s) \int_{S^{d-1}} e^{-2\pi i r s \langle \xi, u \rangle} p(\xi) \,\mathrm{d}\xi \; s^{k+d-1} \,\mathrm{d}s \end{aligned}$$

$$
\begin{aligned}
&= h_k^d \omega_d \int_0^\infty f_0(s) \int_{S^{d-1}} e^{-2\pi i r s \langle \xi, u \rangle} \Big(\int_{S^{d-1}} p(\eta) P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\eta \Big) \,\mathrm{d}\xi \, s^{k+d-1} \,\mathrm{d}s \\
&= h_k^d \omega_d \int_0^\infty f_0(s) \int_{S^{d-1}} p(\eta) \Big(\int_{S^{d-1}} e^{-2\pi i r s \langle \xi, u \rangle} P_k^d(\langle \xi, \eta \rangle) \,\mathrm{d}\xi \Big) \,\mathrm{d}\eta \, s^{k+d-1} \,\mathrm{d}s \\
&= h_k^d \omega_d \int_0^\infty f_0(s) \varphi_k(rs) r^{k+d-1} \,\mathrm{d}s \Big(\int_{S^{d-1}} p(\eta) P_k^d(\langle \eta, u \rangle) \,\mathrm{d}\eta \Big) \\
&= \omega_d \int_0^\infty f_0(r) \varphi_k(rs) s^{k+d-1} \,\mathrm{d}s \, p(u),
\end{aligned}
$$

and hence $\hat{f} \in \mathfrak{H}_k^d$.

The computation above gives a formula for the Fourier transform of a function in $\mathfrak{H}_k^d$ in terms of φ_k implicitly defined in (2.26). Next we state Theorem IV.3.10 from Stein and Weiss [SW71], which gives an explicit formula in terms of Bessel functions.

The *Bessel function* J_p of order $p > -\frac{1}{2}$ is defined as

$$
J_p(x) := \frac{(x/2)^p}{\Gamma\left(p + \frac{1}{2}\right) \Gamma(\frac{1}{2})} \int_{-1}^1 e^{ixs} (1 - s^2)^{(2p-1)/2} \,\mathrm{d}s. \tag{2.27}
$$

For integer n, it can be shown (Lemma IV.3.1 in Stein and Weiss [SW71]) that this definition simplifies to

$$
J_n(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix \sin t} e^{-int} \,\mathrm{d}t,
$$

so that the Bessel functions of integer order can be seen as the Fourier coefficients of $e^{ix \sin t}$.

Theorem 2.4.15. *Let $f \in \mathfrak{H}_k^d \cap L^1(\mathbb{R}^d)$ have the form $f(x) = f_0(\|x\|) p(x)$ with $f_0 : [0, \infty) \longrightarrow \mathbb{C}$ and $p \in \mathrm{Har}_k^d$. Then for $r \in [0, \infty)$ and $u \in S^{d-1}$,*

$$
\hat{f}(ru) = 2\pi i^{-k} r^{-(d-2)/2} \int_0^\infty f_0(s) J_{(d+2k-2)/2}(2\pi r s) s^{(d+2k)/2} \,\mathrm{d}s \, p(u).
$$

In particular, if $f(x) = f_0(\|x\|)$ is radial, then

$$
\hat{f}(\xi) = 2\pi r^{-(d-2)/2} \int_0^\infty f_0(s) J_{(d-2)/2}(2\pi \|\xi\| s) s^{d/2} \,\mathrm{d}s.
$$

2.4.4 The Poisson summation formula

The Fourier series and the Fourier transform have an important relationship. Given a d-dimensional lattice $\Lambda \subset \mathbb{R}^d$, the torus $\mathbb{T}^d := \mathbb{R}^d / \Lambda$ and a function $f \in L^1(\mathbb{R}^d)$, we may define the periodic function $g \in L^1(\mathbb{T}^d)$:

$$
g(x) := \sum_{m \in \Lambda} f(x + m).
$$

A remarkable fact is that the coefficients of the Fourier series of g are the Fourier transform of f (Theorem VII.2.4 of Stein and Weiss [SW71]):

$$\sum_{m\in\Lambda} f(x+m) \sim \frac{1}{\det(\Lambda)} \sum_{\xi\in\Lambda^*} \hat{f}(\xi) e^{2\pi i\langle \xi, x\rangle}, \tag{2.28}$$

where the relation $\sim$ means that equality holds in the $L^1(\mathbb{R}^d)$-norm, not necessarily for all $x \in \mathbb{R}^d$.

Under some additional conditions, satisfied for instance by functions in the Schwartz space, we have pointwise equality, a result known as the *Poisson summation formula* (see e.g., Corollary VII.2.6 in Stein and Weiss [SW71]):

Theorem 2.4.16 (Poisson summation)**.** *Let $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ be a function that enjoys the following two decay conditions. Suppose there exist positive constants δ, C such that for all $x \in \mathbb{R}^d$:*

(a) $|f(x)| < C(1+|x|)^{-d-\delta}$,

(b) $|\hat{f}(x)| < C(1+|x|)^{-d-\delta}$.

Then both f and $\hat{f}$ are continuous and for any $x \in \mathbb{R}^d$,

$$\sum_{m\in\Lambda} f(x+m) = \frac{1}{\det(\Lambda)} \sum_{\xi\in\Lambda^*} \hat{f}(\xi) e^{2\pi i\langle \xi, x\rangle}, \tag{2.29}$$

and both sides of (2.29) *converge absolutely. In particular,*

$$\sum_{m\in\Lambda} f(m) = \frac{1}{\det(\Lambda)} \sum_{\xi\in\Lambda^*} \hat{f}(\xi). \tag{2.30}$$

2.5 Lattice sums

The Poisson summation formula is a very useful tool to find formulas for certain sums over lattices. One general approach involves using some function with a desired form and whose Fourier transform has compact support, in such a way that the lattice sum over this function is mapped to a finite sum. In this section we will derive a formula that will be useful for Chapter 6 using this idea and the Bernoulli polynomials. This section is based on Section 4 from Machado and Robins [MR19].

Let Λ be a k-dimensional lattice in $\mathbb{R}^d$, $w_1, \ldots, w_k$ be linearly independent vectors from Λ^* and $W \in \mathbb{R}^{d\times k}$ be a matrix with them as columns. For a k-uple $e = (e_1, \ldots, e_k)$ of positive integers, let $|e| := \sum_{j=1}^k e_j$. For all $x \in \mathbb{R}^d$, our goal in this section is to evaluate the following limit of lattice sums:

$$L_\Lambda(W, e; x) := \lim_{\epsilon\longrightarrow 0^+} \frac{1}{(2\pi i)^{|e|}} \sum_{\substack{\xi\in\Lambda: \\ \langle w_j, \xi\rangle \neq 0,\, \forall j}} \frac{e^{-2\pi i\langle x, \xi\rangle}}{\prod_{j=1}^k \langle w_j, \xi\rangle^{e_j}} e^{-\epsilon\pi\|\xi\|^2}. \tag{2.31}$$

These expressions come up in the development of Chapter 6, they also appear in the work of Witten, on 2-dimensional gauge theory [Wit92, pp. 363], and a similar expression with a different limit process is called a "Dedekind sum" by Gunnels and Sczech [GS03]. This name is justified since the expression obtained in Theorem 2.5.4 can be written as a Dedekind-Rademacher sum when $k = 2$ and $e = (1,1)$ (Dedekind-Rademacher sums are defined in Section 6.2 and this relation is seem in Section 6.4.1).

The limit in (2.31) is necessary since in general the series does not converge absolutely when $\epsilon = 0$. Only when all $e_j > 1$ the sum with $\epsilon = 0$ is absolutely convergent and we may interchange the limit with the sum and remove both the limit and the exponential $e^{-\epsilon\pi\|\xi\|^2}$ from the formula. Recall the Gaussian function, which for $\epsilon > 0$ is denoted as

$$\phi_{d,\epsilon}(x) := \epsilon^{-d/2} e^{-\pi\|x\|^2/\epsilon},$$

and its Fourier transform:

$$\hat{\phi}_{d,\epsilon}(\xi) = e^{-\epsilon\pi\|\xi\|^2}.$$

To evaluate the lattice sum we will identify the summands as the Fourier transform of certain functions and them apply the Poisson summation formula, Theorem 2.4.16, leading to a simpler expression. These functions are the Bernoulli polynomials, which we define now. The *Bernoulli polynomial* of order r is defined by the generating function

$$\frac{ze^{xz}}{e^z - 1} = \sum_{r=0}^{\infty} \frac{B_r(x)}{r!} z^r, \tag{2.32}$$

so that the first couple are given by $B_1(x) = x - 1/2$ and $B_2(x) = x^2 - x + 1/6$. Here we truncate them, so that they are supported in the unit interval:

$$B_r(x) := 0, \quad \text{for } x \notin [0,1].$$

Now we may define the *periodized Bernoulli polynomials* as:

$$\overline{B}_1(x) := \begin{cases} B_1(x - \lfloor x \rfloor) & \text{when } x \notin \mathbb{Z}, \\ 0 & \text{when } x \in \mathbb{Z}, \end{cases} \tag{2.33}$$

and

$$\overline{B}_r(x) := B_r(x - \lfloor x \rfloor)$$

for all $r > 1$.

For any k-uple $e = (e_1, \dots, e_k)$ of positive integers we define the *k-dimensional Bernoulli polynomial* $\mathcal{B}_e : \mathbb{R}^k \longrightarrow \mathbb{R}$ as

$$\mathcal{B}_e(x) := B_{e_1}(x_1) \cdots B_{e_k}(x_k).$$

Note that $\mathcal{B}_e$ is supported in $[0,1]^k$. The reason for defining these polynomials is that their Fourier transforms evaluated at integer inputs are the inverse of products of linear forms, as stated in the lemma below (see e.g. Apostol [Apo76, Theorem 12.19]):

Lemma 2.5.1. *For all $r \geq 1$, the Fourier transform of the Bernoulli polynomial $B_r(x)$ satisfies:*

$$\hat{B}_r(n) = \begin{cases} 0 & \text{if } n = 0, \\ -\frac{r!}{(2\pi i)^r n^r} & \text{if } n \in \mathbb{Z} \setminus \{0\}. \end{cases}$$

Thus for any k-uple $e = (e_1, \ldots, e_k)$ of positive integers,

$$\hat{\mathcal{B}}_e(m) = \begin{cases} 0 & \text{if } m_j = 0 \text{ for some } j, \\ \frac{(-1)^k e_1! \cdots e_k!}{(2\pi i)^{|e|} m_1^{e_1} \cdots m_k^{e_k}} & \text{if } m \in (\mathbb{Z} \setminus \{0\})^k. \end{cases}$$

Proof. First we use the generating function (2.32) to prove three auxiliary results. Integrating it term-by-term, we get:

$$1 = \frac{e^z - 1}{e^z - 1} = \int_0^1 \frac{z e^{xz}}{e^z - 1} dx = \sum_{r=0}^{\infty} \int_0^1 B_r(x)\, \mathrm{d}x \frac{z^r}{r!},$$

and therefore

$$\hat{B}_r(0) = \int_0^1 B_r(x)\, \mathrm{d}x = \begin{cases} 1 & \text{if } r = 0, \\ 0 & \text{for } r \geq 1. \end{cases}$$

Differentiating (2.32) term-by-term, we get

$$\sum_{r=1}^{\infty} B_r'(x) \frac{z^r}{r!} = \frac{z^2 e^{xz}}{e^z - 1} = \sum_{r=0}^{\infty} B_r(x) \frac{z^{r+1}}{r!} = \sum_{r=1}^{\infty} r B_{r-1}(x) \frac{z^r}{r!},$$

and therefore for $r \geq 1$,

$$B_r'(x) = r B_{r-1}(x). \tag{2.34}$$

Last, we use (2.32) to compute the difference $B_r(x+1) - B_r(x)$:

$$\sum_{r=0}^{\infty} \frac{B_r(x+1) - B_r(x)}{r!} z^r = \frac{z e^{(x+1)z}}{e^z - 1} - \frac{z e^{xz}}{e^z - 1} = \frac{z e^{xz}}{e^z - 1}(e^z - 1) = \sum_{r=0}^{\infty} \frac{x^r z^{r+1}}{r!} = \sum_{r=1}^{\infty} \frac{x^{r-1} z^r}{(r-1)!},$$

and therefore for $r \geq 1$,

$$B_r(x+1) - B_r(x) = r x^{r-1}. \tag{2.35}$$

We proof the lemma using induction in r. For $r = 1$ and $n \neq 0$, we have $B_1(x) = x - 1/2$ for $0 < x < 1$, hence

$$\begin{aligned} \int_0^1 B_1(x) e^{-2\pi i n x}\, \mathrm{d}x &= \int_0^1 \left(x - \frac{1}{2}\right) e^{-2\pi i n x}\, \mathrm{d}x = \int_{-\frac{1}{2}}^{\frac{1}{2}} x e^{-2\pi i n x} e^{-\pi i n}\, \mathrm{d}x \\ &= e^{-\pi i n} \frac{x e^{-2\pi i n x}}{(-2\pi i n)} \Big|_{x=-\frac{1}{2}}^{\frac{1}{2}} + \frac{e^{-\pi i n}}{2\pi i n} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-2\pi i n x}\, \mathrm{d}x = e^{-\pi i n} \frac{e^{\pi i n}}{(-2\pi i n)} = -\frac{1}{2\pi i n}. \end{aligned}$$

For $r \geq 2$ and $n \neq 0$, we integrate by parts and use (2.34). We also use that by (2.35),

$B_r(1) = B_r(0)$ for $r \geq 2$:

$$\begin{aligned}\hat{B}_r(n) &= \int_0^1 B_r(x)e^{-2\pi inx}\,\mathrm{d}x = B_r(x)\frac{e^{-2\pi inx}}{(-2\pi in)}\Big|_{x=0}^1 + \int_0^1 B_r'(x)\frac{e^{-2\pi inx}}{2\pi in}\,\mathrm{d}x \\ &= \frac{r}{2\pi in}\int_0^1 B_{r-1}(x)e^{-2\pi inx}\,\mathrm{d}x = \frac{r}{2\pi in}\frac{-(r-1)!}{(2\pi i)^{r-1}n^{r-1}} = \frac{-r!}{(2\pi i)^r n^r}.\end{aligned}$$

The formula for $\hat{\mathcal{B}}_e(m)$ follows from $\hat{B}_r(n)$ since $\mathcal{B}_e$ is separable. □

The next piece necessary to evaluate $L_\Lambda(W, e; x)$ is a method to handle the limit in ϵ. We use Lemma 3 and Theorem 5 from Diaz, Le and Robins [DLR16]. To state it, let P be a full-dimensional polytope in $\mathbb{R}^d$ and at each point $x \in \mathbb{R}^d$, define the *solid angle* with respect to P:

$$\omega_P(x) := \lim_{\epsilon \longrightarrow 0^+} \frac{\mathrm{vol}(S^{d-1}(x,\epsilon) \cap P)}{\mathrm{vol}(S^{d-1}(x,\epsilon))},$$

where $S^{d-1}(x, \epsilon)$ denotes the $(d-1)$-dimensional sphere centered at x with radius ϵ.

Lemma 2.5.2. *Let P be a full-dimensional polytope in $\mathbb{R}^d$ and f be a continuous function in P and zero outside P. For points in the boundary of P we assume that f is continuous from the inside of P only. Then for all $x \in \mathbb{R}^d$,*

$$\lim_{\epsilon \longrightarrow 0^+} (f * \phi_{d,\epsilon})(x) = f(x)\omega_P(x).$$

Moreover,

$$\lim_{\epsilon \longrightarrow 0^+} \sum_{x \in \mathbb{Z}^d} (f * \phi_{d,\epsilon})(x) = \sum_{x \in \mathbb{Z}^d} f(x)\omega_P(x). \tag{2.36}$$

Proof. Using that the support of f is contained in P, the change of variables $y = \frac{u-x}{\sqrt{\epsilon}}$ and that $\phi_{d,\epsilon}(-\sqrt{\epsilon}y) = \epsilon^{-d/2}\phi_{d,1}(y)$, we have:

$$\begin{aligned}\lim_{\epsilon \longrightarrow 0^+} (f * \phi_{d,\epsilon})(x) &= \lim_{\epsilon \longrightarrow 0^+} \int_P f(u)\phi_{d,\epsilon}(x-u)\,\mathrm{d}u \\ &= \lim_{\epsilon \longrightarrow 0^+} \int_{\frac{1}{\sqrt{\epsilon}}(P-x)} f(x+\sqrt{\epsilon}y)\phi_{d,1}(y)\,\mathrm{d}y \\ &= f(x)\lim_{\epsilon \longrightarrow 0^+} \int_{\frac{1}{\sqrt{\epsilon}}(P-x)} \phi_{d,1}(y)\,\mathrm{d}y + \lim_{\epsilon \longrightarrow 0^+} \int_{\frac{1}{\sqrt{\epsilon}}(P-x)} (f(x+\sqrt{\epsilon}y) - f(x))\phi_{d,1}(y)\,\mathrm{d}y.\end{aligned}$$

To compute the limit of the first integral, we use that as $\epsilon \longrightarrow 0^+$, $\frac{1}{\sqrt{\epsilon}}(P-x)$ tends to the cone of feasible directions of P at x. Since $\phi_{d,1}$ is a radial function and $\int_{\mathbb{R}^d} \phi_{d,1}(y)\,\mathrm{d}y = 1$, the integral gives the fraction of the space subtended by the cone, which is $\omega_P(x)$. For the second integral, we use the estimate

$$\begin{aligned}\lim_{\epsilon \longrightarrow 0^+} \left| \int_{\frac{1}{\sqrt{\epsilon}}(P-x)} (f(x+\sqrt{\epsilon}y) - f(x))\phi_{d,1}(y)\,\mathrm{d}y \right| &\leq \lim_{\epsilon \longrightarrow 0^+} \int_{\mathrm{fcone}(P,\,x)} \left|(f(x+\sqrt{\epsilon}y) - f(x))\right|\phi_{d,1}(y)\,\mathrm{d}y \\ &= \int_{\mathrm{fcone}(P,\,x)} \lim_{\epsilon \longrightarrow 0^+} \left|(f(x+\sqrt{\epsilon}y) - f(x))\right|\phi_{d,1}(y)\,\mathrm{d}y = 0,\end{aligned}$$

the interchange between the limit and the integral is justified by Lebesgue's Dominated Convergence Theorem (see e.g., Theorem 1.34 in Rudin [Rud87]).

To prove (2.36), we must interchange the limit with the series. This is again justified by Lebesgue's Dominated Convergence Theorem, this time applied to $\mathbb{Z}^d$ with the counting measure. To apply it we note that for $\|x\|^2 > \frac{d}{2\pi}$, $\phi_{d,\epsilon}(x) < \phi_{d,1}(x)$ and hence for x large,

$$|(f * \phi_{d,\epsilon})(x)| = \left| \int_P f(u)\phi_{d,\epsilon}(x-u)\,\mathrm{d}u \right| \le \mathrm{vol}(P) \sup_{u\in P} |f(u)\phi_{d,1}(x-u)|$$

and since f is bounded and $\phi_{d,1}$ is summable, the hypothesis of the theorem is satisfied. □

Note that the right-hand side of (2.36) is a finite sum since P is compact and $\omega_P(x) = 0$ for $x \notin P$, while the left-hand side is the limit of an infinite series.

Returning to the evaluation of $L_\Lambda(W, e; x)$, we assume first that Λ is the full-dimensional integer lattice $\mathbb{Z}^d$; in this case W is invertible. Let $P_{W,x}$ be the parallelepiped

$$P_{W,x} := \{n \in \mathbb{R}^d \; : \; W^{-1}(n-x) \in [0,1]^d\} = x + W[0,1]^d.$$

We prove the following theorem, which gives a finite form for (2.31), in terms of a sum over the integer points in $P_{W,x}$ and the d-dimensional Bernoulli polynomial times a local solid angle.

Theorem 2.5.3. *If $W \in \mathbb{Z}^{d\times d}$ is an invertible matrix with columns $w_1, \dots, w_d$, $e = (e_1, \dots, e_d)$ is a d-uple of positive integers and $x \in \mathbb{R}^d$, then:*

$$L_{\mathbb{Z}^d}(W, e; x) = \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \sum_{n \in \mathbb{Z}^d \cap P_{W,x}} \mathcal{B}_e\big(W^{-1}(n-x)\big)\,\omega_{P_{W,x}}(n).$$

Proof. We recognize each term inside sum (2.31) as the Fourier transform of a function, apply Poisson summation and then use Lemma 2.5.2 to compute the limit.

Using Lemma 2.5.1 and identity (2.22) with $\mathcal{B}_e$ and W, for any $\xi \in \mathbb{Z}^d$ such that $\langle w_j, \xi \rangle \neq 0$ for all j, we have:

$$\frac{1}{(2\pi i)^{|e|} \prod_{j=1}^d \langle w_j, \xi \rangle^{e_j}} = \frac{(-1)^d}{e_1! \cdots e_d!} (\hat{\mathcal{B}}_e \circ W^\top)(\xi) = \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \mathcal{F}(\mathcal{B}_e \circ W^{-1})(\xi).$$

To obtain the same term that appears in (2.31), we make use of identity (2.21) and recall that $\hat{\phi}_\epsilon(\xi) = e^{-\pi\epsilon\|\xi\|^2}$. Further noticing that $(\hat{\mathcal{B}}_e \circ W^\top)(\xi) = 0$ when $\langle w_j, \xi \rangle = 0$ for some j, we have:

$$L_{\mathbb{Z}^d}(W, e; x) = \lim_{\epsilon \to 0^+} \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \sum_{\xi \in \mathbb{Z}^d} \mathcal{F}(\mathcal{B}_e \circ W^{-1} \circ T_x)(\xi) \hat{\phi}_\epsilon(\xi).$$

Using identity (2.23) and Poisson summation (Theorem 2.4.16),

$$L_{\mathbb{Z}^d}(W, e; x) = \lim_{\epsilon \to 0^+} \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \sum_{n \in \mathbb{Z}^d} \big((\mathcal{B}_e \circ W^{-1} \circ T_x) * \phi_{d,\epsilon}\big)(n).$$

Note that the support of $\mathcal{B}_e \circ W^{-1} \circ T_x$ is exactly $P_{W,x}$ and $(\mathcal{B}_e \circ W^{-1} \circ T_x)(n) = \mathcal{B}_e\big(W^{-1}(n-x)\big)$. This enables us to use Lemma 2.5.2 and obtain

$$L_{\mathbb{Z}^d}(W, e; x) = \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \sum_{n \in \mathbb{Z}^d \cap P_{W,x}} \mathcal{B}_e\big(W^{-1}(n-x)\big) \omega_{P_{W,x}}(n). \qquad \square$$

The situation is almost the same for the general case where Λ is a k-dimensional lattice in $\mathbb{R}^d$, however in this case we must restrict attention to the subspace spanned by Λ. Note that $W \in \mathbb{R}^{d \times k}$ is not invertible but when we see it as a linear transformation $W : \mathbb{R}^k \longrightarrow \operatorname{span}(\Lambda)$ it is, such inverse is called the *pseudoinverse* and can be computed as

$$W^+ = (W^\top W)^{-1} W^\top.$$

Furthermore, it follows that WW^+ is the orthogonal projection $\operatorname{Proj}_{\operatorname{span}(\Lambda)}$ from $\mathbb{R}^d$ to $\operatorname{span}(\Lambda)$. The parallelepiped $P_{W,x}$ becomes a k-dimensional parallelepiped in $\operatorname{span}(\Lambda)$:

$$P_{W,x} := \{n \in \operatorname{span}(\Lambda) \,:\, W^+(n-x) \in [0,1]^k\} = \operatorname{Proj}_{\operatorname{span}(\Lambda)}(x) + W[0,1]^k.$$

Identity (2.22) also has to be adapted, since we are dealing with a k-dimensional subspace embedded in $\mathbb{R}^d$. More specifically, for $f : \mathbb{R}^k \longrightarrow \mathbb{C}$ and $\xi \in \operatorname{span}(\Lambda)$, in place of (2.22) we use:

$$\det(W^\top W)^{1/2} \int_{\mathbb{R}^k} f(y) e^{-2\pi i \langle y, W^\top \xi \rangle} \, dy = \int_{\operatorname{span}(\Lambda)} f(W^+ x) e^{-2\pi i \langle x, \xi \rangle} \, dx.$$

With these remarks, the same proof of the previous theorem gives:

Theorem 2.5.4. *If $W \in \mathbb{R}^{d \times k}$ is a matrix with linearly independent columns $w_1, \dots, w_k \in \Lambda^*$, $e = (e_1, \dots, e_k)$ is a k-uple of positive integers and $x \in \mathbb{R}^d$, then:*

$$L_\Lambda(W, e; x) = \frac{(-1)^k}{e_1! \cdots e_k! \det(W^\top W)^{1/2} \det(\Lambda)} \sum_{n \in \Lambda^* \cap P_{W,x}} \mathcal{B}_e\big(W^+(n-x)\big) \omega_{P_{W,x}}(n).$$

Comments about the Dedekind sums of Gunnels and Sczech

We remark here that we may compare Theorem 2.5.3 with Proposition 2.7 of Gunnels and Sczech [GS03]. The main difference between these two results is that Theorem 2.5.3 above uses solid angle weights. But when all $e_j > 1$, the sum in (2.31) is absolutely convergent for $\epsilon = 0$ and we may interchange the limit with the lattice sum. The resulting sum is then equal to the Dedekind sum considered by Gunnels and Sczech, and Theorem 2.5.3 can be compared with their Proposition 2.7.

The result for $L_{\mathbb{Z}^d}(W, e; x)$ given in Proposition 2.7 of Gunnels and Sczech [GS03] is:

$$L_{\mathbb{Z}^d}(W, e; x) = \frac{(-1)^d}{e_1! \cdots e_d! |\det(W)|} \sum_{n \in \mathbb{Z}^d / W\mathbb{Z}^d} \mathcal{B}_e\big(W^{-1}(n-x)\big),$$

which is almost the same, but without the solid angle weights, and with the sum over the half-open parallelepiped

$$\mathbb{Z}^d/W\mathbb{Z}^d := \{a_1 w_1 + \cdots + a_d w_d : 0 \le a_j < 1\} \cap \mathbb{Z}^d.$$

To understand why this formula follows from Theorem 2.5.3, for $n \in P_{W,x}$, let $n = x + \sum_{j=1}^d a_j w_j$ with $a_j \in [0,1]$, and let $J := \{j \in \{1,\dots,d\} : a_j \in \{0,1\}\}$. Consider the $2^{|J|}$ vectors $n(S) := x + \sum_{j=1}^d a_j(S) w_j$, for all $S \subseteq J$, where $a_j(S) := 1 - a_j$ if $j \in S$ and $a_j(S) := a_j$ otherwise.

To see that

$$\sum_{S \subseteq J} \omega_{P_{W,x}}(n(S)) = 1,$$

we observe that when we translate the parallelepiped $P_{W,x}$ and form a tiling of $\mathbb{R}^d$, some of its boundary points $n(S)$ meet several copies of its translates; for these boundary points, their relevant solid angles add up perfectly to give a weight of 1.

Also, since W is an integer matrix, if $n \in \mathbb{Z}^d \cap \partial P_{W,x}$, all $n(S)$ are also in $\mathbb{Z}^d \cap \partial P_{W,x}$ and $\mathcal{B}_e(n(S)) = \mathcal{B}_e(n)$ because $B_s(0) = B_s(1)$ for all $s > 1$. In other words, if we were to periodize the Bernoulli polynomials, their periodizations would all be continuous on $\mathbb{R}$, except for $B_1(x)$.

When $e_j = 1$ for some j, the sum for $\epsilon = 0$ is just conditionally convergent and our limit differs from the definition in Gunnels and Sczech [GS03]. In this case the solid angles do appear, since $B_1(1) = 1/2$ and $B_1(0) = -1/2$. Note that if $\omega_{P_{W,x}}(n) = 1/2$, then $|J| = 1$ and n has only one neighbor, whose contribution to the sum cancels the contribution of n. This observation is used in the proof of Theorem 3 in Diaz, Le, and Robins [DLR16] and justifies the definition of $\overline{B}_1(x) = 0$ for $x \in \mathbb{Z}$.

Chapter 3

Packing problems

In this chapter we discuss methods to upper bound the size of diverse geometrical packing problems. We begin listing three problems that illustrates the differences in the domains: finite, infinite but compact, and infinite but locally compact. Our goal is to highlight the similarities between these problems and study the limits of these similarities. See the expository paper from Oliveira and Vallentin [OV15] and the book chapter from Bachoc, Gijswijt, Schrijver, and Vallentin [Bac+12] for a further discussion.

The first example we consider has the Euclidean space $\mathbb{R}^n$ as domain. Given a convex body $K \subset \mathbb{R}^n$ (i.e. a compact and convex set), a *packing* of K is a subset $\mathcal{P} \subseteq \mathbb{R}^n$ formed by a union of copies of K with disjoint interior. When the copies of K consist of rotations followed by translations we say $\mathcal{P}$ is a *congruent packing*, when only translations of K are allowed we say $\mathcal{P}$ is a *translational packing* and when we only have translations and the set of translations form a lattice we say $\mathcal{P}$ is a *lattice packing*. The *density* of $\mathcal{P}$ is defined as the limit

$$\delta(\mathcal{P}) := \limsup_{r \to \infty} \sup_{c \in \mathbb{R}^n} \frac{\operatorname{vol}(B(c,r) \cap \mathcal{P})}{\operatorname{vol}(B(c,r))}, \tag{3.1}$$

where $B(c,r) := \{x \in \mathbb{R}^n : \|x - c\| \leq r\}$.

To determine the maximum packing density of a given type we must find lower bounds via explicit constructions and find upper bounds via techniques that we discuss next. The case when K is a ball is simpler and has the strongest results, note that in this case the notions of congruent packing and translative packing are equivalent. In general, congruent packings are much harder to study (see Oliveira and Vallentin [OV18]). See also the dissertation of Dostert [Dos17] about translative packings of non-spherical shapes.

The second example we mention has the sphere S^{n-1} as domain. The *spherical cap* $\operatorname{Cap}(e, \phi) \subseteq S^{n-1}$ of center $e \in S^{n-1}$ and radius $0 < \phi \leq \pi$ is defined as

$$\operatorname{Cap}(e, \phi) := \{x \in S^{n-1} : \langle e, x \rangle \geq \cos(\phi)\}.$$

A *packing of spherical caps* is a subset of the sphere formed by a union of spherical caps with a given radius and disjoint interior. Since the sphere is compact, such a packing must have a finite number of caps and, instead of using the density as done in (3.1), we may simply count the number of caps in the packing. We equivalently define the packing in terms of the centers of the caps, with the constraint that two centers $x, y \in S^{n-1}$ can be in the same packing only if $\langle x, y \rangle \leq \cos(\phi)$. More generally, given a closed set $D \subseteq [-1, 1)$, a subset C of the unit sphere is a *spherical D-code* if $\langle x, y \rangle \in D$ for all distinct x, $y \in C$. The maximum cardinality of a spherical D-code in S^{n-1} is denoted by $A(n, D)$. Different sets D describe different problems that can be treated with similar techniques. The most important cases are when D is an interval and when D is a finite set. We will return to this example in Chapter 4.

The third example we consider has the discrete set $\{0, 1\}^n$ of binary words of length n as domain. It is not geometrical, in the sense that it is not contained in the Euclidean space, but it is a metric space with the *Hamming distance*, defined as the number of positions at which two words differ. A subset of $\{0, 1\}^n$ is said a *$(d - 1)$-error detecting code* if the minimum Hamming distance between two words is d. The maximum cardinality of a $(d - 1)$-error detecting code is denoted by $A_2(n, d)$. Comparing with the previous problems, not only the number of words in a code is finite, but the universe of all possible words, $\{0, 1\}^n$, is also finite. This gives a simple way to compute $A_2(n, d)$, namely verifying all the 2^n possible subsets. However such strategy is not viable in practice for moderate values of n, hence the question is how $A_2(n, d)$ can be computed efficiently.

3.1 Modeling packing problems with graphs

Let $G = (V, E)$ be a graph. A subset $S \subseteq V$ is *independent* if no two elements from S are connected by an edge. The *independence number* $\alpha(G)$ is the maximal size of an independent set in G. We can model a packing problem as the independence number of the graph with vertex set representing all possible positions of the body being packed and edges between any pair of positions that intersect. This model works with binary codes and also with spherical codes, despite $V = S^{d-1}$ being infinite. For the packing in $\mathbb{R}^n$ the independence number must be replaced with the packing density, but the analogy is still useful. Next we consider two special structures that a graph may have and that helps us to deal with these infinite graphs used to model geometric packing problems.

The first structure is topological. A *topological packing graph* is a graph whose vertex set is a Hausdorff space and in which every finite clique is contained in an open clique. When the vertex set is also compact, we say it is a compact topological packing graph. Such graphs model geometrical packing problems since, intuitively, every small perturbation of a convex body has an intersection with itself. This constraint enables the extension made in Section 4.2.2 of the semidefinite programming bounds for finite graphs to infinite graphs.

For an integer $k \geq 0$, let I_k be the set of independent sets in G of size at most k and $I_{=k}$ be the set of independent sets in G of size exactly k. The main consequences of the definition of a compact topological packing graph is that the independence number is finite and I_k, considered with the topology inherited from V, is the disjoint union of the compact and open sets $I_{=s}$ for $s \in \{0, \dots, k\}$ (see Section 2 in de Laat [LV15]).

The second structure we consider is the symmetry. The graphs associated to the problems above are highly symmetrical and this is a key feature to efficiently search for solutions to them. The *automorphism group* $\mathrm{Aut}(G)$ of a graph $G = (V, E)$ is the group of permutations $\sigma : V \longrightarrow V$ that respect the adjacency relation; that is, $\sigma(x)$ and $\sigma(y)$ are adjacent if and only if x and $y \in V$ are adjacent. When the vertex set has a topology, we further assume that the action of $\mathrm{Aut}(G)$ is continuous.

A *Cayley graph* is a graph $G = (V, E)$ whose vertex set is a group with identity e and there is a subset $X \subset V$ such that $e \notin X$, $X = X^{-1}$, and $g, h \in V$ are adjacent if and only if $g^{-1}h \in X$. This kind of graph is highly symmetrical, with $V \subset \mathrm{Aut}(G)$ and it appears naturally in the context of packing problems. When the set of motions of the body K being packed form a group V, then letting $X := \{g \in V \setminus \{e\} : \mathrm{int}(K) \cap \mathrm{int}(gK) \neq \emptyset\}$, we have $\mathrm{int}(gK) \cap \mathrm{int}(hK) \neq \emptyset$ if and only if $g^{-1}h \in X$.

3.2 Semidefinite programming bounds for the independence number of a finite graph

Before considering geometrical packing problems, in this section we consider the combinatorial counterpart of finding an independent set in a finite graph. The methods discussed here will serve as a model that later will be adapted to the geometrical problems.

Throughout this section we assume $G = (V, E)$ is a finite graph, for instance the graph modeling the $(d-1)$-error detecting codes in $\{0,1\}^n$. Determining the independence number of a graph is NP-hard in general, thus we should not expect an efficient (polynomial time) method for it, even less when considering graphs that are themselves large, such as in the example with vertex set $\{0,1\}^n$. This motivates the consideration of semidefinite programming methods to upper bound the size of the independent sets.

We start defining some notation for semidefinite programs. See e.g. the lecture notes from Laurent and Vallentin [LV12] or the monograph from Tunçel [Tun10] for more information and proofs of the main facts about positive semidefinite matrices.

For a finite set U, we consider a function $f : U \longrightarrow \mathbb{R}$ as a column vector, so that for $f, g : U \longrightarrow \mathbb{R}$, $f^{\mathsf{T}}g = \langle f, g\rangle = \sum_{u\in U} f(u)g(u)$ is a real number and fg^{T} is the matrix $(fg^{\mathsf{T}})(u,v) = f(u)g(v)$, for $u, v \in U$. Let $\mathcal{S}^U$ denote the set of real symmetric matrices indexed by U. A matrix $X \in \mathcal{S}^U$ is *positive semidefinite* if for all $f : U \longrightarrow \mathbb{R}$,

$$f^{\mathsf{T}}Xf = \sum_{u,v\in U} X(u,v)f(u)f(v) \geq 0.$$

We denote the set of positive semidefinite matrices by $\mathcal{S}^U_{\succeq 0}$ and use $X \succeq 0$ for $X \in \mathcal{S}^U_{\succeq 0}$.

Let I be the identity matrix and J be the all-ones matrix (we keep the domain U implicit whenever possible). We use $\langle , \rangle$ to denote the trace product:

$$\langle A, B\rangle := \mathrm{tr}(A^{\mathsf{T}}B) = \sum_{u,v\in U} A(u,v)B(u,v).$$

We will often use the fact that for $A, B \succeq 0$, we have $\langle A, B\rangle \geq 0$.

Given matrices $C, A_1, \dots, A_k \in \mathcal{S}^U$ and numbers $b_1, \dots, b_m$, a *semidefinite program* is an optimization problem of the form

$$\begin{aligned} \max\ & \langle C, X \rangle, \\ & X \succeq 0, \\ & \langle A_j, X \rangle = b_j, \quad \text{for } j \in \{1, \dots, m\}. \end{aligned} \tag{3.2}$$

A matrix $X \in \mathcal{S}^U_{\succeq 0}$ which satisfies all constraints is said a *feasible solution*. The *optimal value* of the program is the supremmum

$$\sup\{\langle C, X \rangle : X \succeq 0,\ \langle A_j, X \rangle = b_j,\ \text{for } j \in \{1, \dots, m\}\}.$$

We also call "semidefinite program" any optimization problem that can be put in the form above with some transformation such as a change of variables. For instance, problems with several positive semidefinite matrices or with the maximization replaced by a minimization objective.

To problem (3.2) is associated a *dual program*, given by

$$\begin{aligned} \min\ & \sum_{j=1}^{m} b_j y_j, \\ & y_1, \dots, y_m \in \mathbb{R}, \\ & \sum_{j=1}^{m} y_j A_j - C \succeq 0. \end{aligned} \tag{3.3}$$

If X and $(y_1, \dots, y_m)$ are feasible solutions for (3.2) and (3.3) then

$$\left\langle \sum_{j=1}^{m} y_j A_j - C, X \right\rangle \geq 0 \implies \langle C, X \rangle \leq \left\langle \sum_{j=1}^{m} y_j A_j, X \right\rangle = \sum_{j=1}^{m} y_j \langle A_j, X \rangle = \sum_{j=1}^{m} b_j y_j.$$

Therefore any feasible solution for (3.3) upper bounds the optimal value of (3.2) and any feasible solution for (3.2) lower bounds the optimal value of (3.3). Furthermore if X and $(y_1, \dots, y_m)$ are feasible solutions such that $\langle C, X \rangle = \sum_{j=1}^{m} b_j y_j$, then both are optimal and $\left\langle \sum_{j=1}^{m} y_j A_j - C, X \right\rangle = 0$.

The facts mentioned above are called *weak duality*. Stronger assumptions imply the existence of optimal solutions with the same value for both problems, a fact called *strong duality*. One such set of assumptions is the following (see e.g., Section 3.4 in Laurent and Vallentin [LV12]), to state it we say that a feasible solution X for (3.2) is *strictly feasible* if it is positive definite, which means that for all nonzero $f : U \longrightarrow \mathbb{R}$, $f^{\mathsf{T}} X f = \sum_{u,v \in U} X(u,v) f(u) f(v) > 0$.

Proposition 3.2.1. *If program (3.2) has a strictly feasible solution and its optimal value is bounded, then program (3.3) has an optimal solution with the same value.*

3.2.1 The Lovász theta number

Given a graph $G = (V, E)$, the Lovász theta number $\theta(G)$ is a parameter defined as the optimal value of a semidefinite program. It can be numerically approximated in polynomial time [GLS81] and upper bounds the independence number $\alpha(G)$.

The intuition behind its definition comes from representing an independent set $S \subset V$ with its indicator function $\mathbb{1}_S : V \longrightarrow \{0, 1\}$ and "lift" it to the positive semidefinite matrix $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^{\mathsf{T}}$, which will be a feasible solution to the following semidefinite program:

$$\begin{aligned} \max\ & \langle J, X\rangle, \\ & X \in \mathcal{S}^V_{\succeq 0}, \\ & \langle I, X\rangle = 1, \\ & X(u, v) = 0,\ \text{if } uv \in E. \end{aligned} \tag{3.4}$$

It is a direct verification that for any independent set $S \subset V$, $X = \frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^{\mathsf{T}}$ is feasible for (3.4) and that $\langle J, X\rangle = |S|$. Therefore $\theta(G)$, the optimal value of (3.4), upper bounds $\alpha(G)$.

The dual of (3.4) is very useful since by weak duality any feasible solution for it gives an upper bound for $\alpha(G)$:

$$\begin{aligned} \min\ & \lambda, \\ & \lambda \in \mathbb{R},\ Z \in \mathcal{S}^V, \\ & Z - J \succeq 0, \\ & Z(u, u) = \lambda,\ \text{for all } u \in V, \\ & Z(u, v) = 0,\ \text{if } u \neq v,\ uv \notin E. \end{aligned} \tag{3.5}$$

Since $X = \frac{1}{|V|}I$ is strictly feasible for (3.4) and $Z = |V|I$, $\lambda = |V|$ is feasible for (3.5), Proposition 3.2.1 holds and by strong duality the optimal value of (3.5) is also equal to $\theta(G)$.

The Lovász theta number has other applications, it bounds the Shannon capacity of a graph [Lov79] and also lower bounds the chromatique number of its complement [Knu94]. When the goal is to upper bound the independence number, it is possible to make a simple improvement, which we call $\theta'(G)$, the modified Lovász theta number [Sch79], next we present it both in primal and dual form:

$$\begin{aligned} \max\ & \langle J, X\rangle, \\ & X \in \mathcal{S}^V_{\succeq 0}, \\ & X(u, v) \geq 0,\ \text{for all } u, v \in V, \\ & \langle I, X\rangle = 1, \\ & X(u, v) = 0,\ \text{if } uv \in E. \end{aligned} \tag{3.6}$$

$$\begin{aligned} \min\ & \lambda, \\ & \lambda \in \mathbb{R},\ Z \in \mathcal{S}^V, \\ & Z - J \succeq 0, \\ & Z(u, u) \leq \lambda,\ \text{for all } u \in V, \\ & Z(u, v) \leq 0,\ \text{if } u \neq v,\ uv \notin E. \end{aligned} \tag{3.7}$$

The Lovász theta number and its modified version are not sharp in general. For the pentagon C_5, one may show that $\theta(C_5) = \theta'(C_5) = \sqrt{5}$ while $\alpha(C_5) = 2$.

3.2.2 The Lasserre hierarchy

Lasserre [Las02] showed that every nonlinear optimization problem formulated with polynomials and a variable $x \in \{0,1\}^n$ is equivalent to a semidefinite program with $2^n - 1$ variables. The optimal value of both problems are the same and from every optimal solution of one, one may find an optimal solution of the other. This formulation leads to a sequence of semidefinite relaxations whose first steps have moderate size and that are guaranteed to converge to the original 0-1 program in finitely many steps.

Here we follow Laurent [Lau03] and Section 5.2 from Laurent and Vallentin [LV12] and present this method in terms of moment matrices and harmonic analysis in the boolean lattice, an approach very similar to the one we presented in Chapter 2. Applied to the independence number of a graph, the first step corresponds to the Lovász theta number and the following steps will give stronger bounds for the independence number.

By "boolean lattice" we mean the family $\mathcal{P}(V)$ of all subsets of V together with the partial order of inclusion. We consider the space $\mathbb{R}^{\mathcal{P}(V)}$ of real valued functions $\mathcal{P}(V) \longrightarrow \mathbb{R}$ with the inner product $\langle , \rangle$:

$$\langle f, g\rangle := \sum_{A\subseteq V} f(A)g(A).$$

For each subset $B \subseteq V$, let $\chi_B : \mathcal{P}(V) \longrightarrow \mathbb{R}$ be

$$\chi_B(A) := \begin{cases} 1 & \text{if } A \subseteq B, \\ 0 & \text{otherwise.} \end{cases}$$

The functions χ_B for $B \subseteq V$ form a basis for $\mathbb{R}^{\mathcal{P}(V)}$. This can be seen considering each χ_B as a column vector and ordering them by the size of B, producing an upper triangular matrix with ones in the diagonal. Furthermore, this basis is multiplicative with respect the union operation, namely for any $A, A', B \subseteq V$,

$$\chi_B(A \cup A') = \chi_B(A)\chi_B(A'). \tag{3.8}$$

We also consider the dual basis χ_B^* for $B \subseteq V$ (called Möbius function), defined via the relations

$$\left\langle \chi_A, \chi_B^* \right\rangle = \begin{cases} 1 & \text{if } A = B, \\ 0 & \text{otherwise.} \end{cases} \tag{3.9}$$

The function χ_B^* can be written explictly:

$$\chi_B^*(A) = \begin{cases} (-1)^{|A\setminus B|} & \text{if } A \supseteq B, \\ 0 & \text{otherwise.} \end{cases}$$

Using (3.9) we may easily express a function $f \in \mathbb{R}^{\mathcal{P}(V)}$ in terms of these bases:

$$f(A) = \sum_{B\subseteq V} \left\langle f, \chi_B^* \right\rangle \chi_B(A). \tag{3.10}$$

We say that a function $f : \mathcal{P}(V) \longrightarrow \mathbb{R}$ is of *positive type* if the matrix $M(f) \in \mathcal{S}^{\mathcal{P}(V)}$ defined by

$$M(f)(A, B) := f(A \cup B)$$

is positive semidefinite. The matrix $M(f)$ is called a *moment matrix*, since each entry (A, B) depends only on the union $A \cup B$. The following theorem (see Theorem 5.2.3 in [LV12]) is fundamental to compute $\alpha(G)$ with a semidefinite program, it shows that the condition $M(f) \succeq 0$ implies that f is a nonnegative combination of the functions χ_B:

Theorem 3.2.2. *A function $f : \mathcal{P}(V) \longrightarrow \mathbb{R}$ is of positive type if and only if*

$$\left\langle f, \chi_B^* \right\rangle = \sum_{B \subseteq A \subseteq V} (-1)^{|A \setminus B|} f(A) \geq 0$$

for all $B \subseteq V$.

Proof. The sufficiency follows from (3.10) once we observe that each χ_B is of positive type. This in turn follows from (3.8). Indeed, if $g : \mathcal{P}(V) \longrightarrow \mathbb{R}$, then

$$\sum_{S,T \in \mathcal{P}(V)} \chi_B(S \cup T) g(S) g(T) = \left(\sum_{S \in \mathcal{P}(V)} \chi_B(S) g(S) \right)^2 \geq 0.$$

The necessity part also follows from (3.10). Suppose that $\left\langle f, \chi_B^* \right\rangle < 0$ for some $B \subseteq V$ and consider the double sum with χ_B^*:

$$\begin{aligned}
\sum_{S,T \in \mathcal{P}(V)} f(S \cup T) \chi_B^*(S) \chi_B^*(T) &= \sum_{S,T \in \mathcal{P}(V)} \sum_{A \subseteq V} \left\langle f, \chi_A^* \right\rangle \chi_A(S \cup T) \chi_B^*(S) \chi_B^*(T) \\
&= \sum_{A \subseteq V} \left\langle f, \chi_A^* \right\rangle \sum_{S,T \in \mathcal{P}(V)} \chi_A(S) \chi_A(T) \chi_B^*(S) \chi_B^*(T) \\
&= \sum_{A \subseteq V} \left\langle f, \chi_A^* \right\rangle \left\langle \chi_A, \chi_B^* \right\rangle^2 \\
&= \left\langle f, \chi_B^* \right\rangle < 0,
\end{aligned}$$

hence f is not of positive type. ∎

Theorem 3.2.2 and Equation (3.10) show that $M(y) \succeq 0$ if and only if y is a nonnegative combination of the functions χ_B. Since $\chi_B(\emptyset) = 1$ for all $B \subseteq V$, adding the constraint $y(\emptyset) = 1$ we have that y must be a convex combination of the functions χ_B. This allows us to express $\alpha(G)$ as the optimal value of a semidefinite program:

$$\begin{aligned}
\max \ & \sum_{u \in V} y(\{u\}), \\
& y : \mathcal{P}(V) \longrightarrow \mathbb{R}, \\
& y(S) = 0 \text{ for all } S \subseteq V \text{ that is not independent}, \\
& y(\emptyset) = 1, \\
& M(y) \succeq 0.
\end{aligned} \tag{3.11}$$

Indeed, the optimal value of (3.11) is at least $\alpha(G)$ since for any $B \subseteq V$ independent, χ_B

is feasible for it and $\sum_{u\in V}\chi_B(\{u\}) = |B|$. Also, the optimal value of (3.11) is at most $\alpha(G)$ since as aforementioned, if y is feasible for (3.11), then from $M(y)\succeq 0$ and $y(\emptyset)=1$ we get that y is a convex combination of the functions χ_B and from "$y(S)=0$ for all $S\subseteq V$ that is not independent", we get that y is a convex combination of χ_B such that B is independent and hence $\sum_{u\in V} y(\{u\}) \leq \max_{B \text{ is independent}} \sum_{u\in V}\chi_B(\{u\})$.

Program (3.11) is not an efficient method to compute $\alpha(G)$ since $M(y)$ has one row for each subset of V and simply writing it down is harder than enumerating all subsets of V. Instead, the usefulness of it is to generate relaxations that are more treatable. This can be done by replacing $M(y)\succeq 0$ with some principal submatrix of moderate size.

Let $\mathcal{P}_t(V)$ be the family of all subsets of V of size at most t. For $y\in\mathcal{P}(V)\longrightarrow\mathbb{R}$, we let the *truncated moment matrix* $M_t(y)\in\mathcal{S}^{\mathcal{P}_t(V)}$ be the principal submatrix of $M(y)$ indexed by $\mathcal{P}_t(V)$. When t is fixed, the size of $M_t(y)$ is bounded by a polynomial in $|V|$ and when $t\longrightarrow|V|$ we recover $M(y)$. Note that under the constraints $y(S)=0$ for all $S\subseteq V$ that is not independent, $M_{\alpha(G)}(y)\succeq 0$ is already equivalent to $M(y)\succeq 0$. Replacing $M(y)$ by $M_t(y)$ in (3.11) we get the t-th step of Lasserre hierarchy, whose optimal value we denote by $\mathrm{las}_t(G)$:

$$\begin{aligned} \max \sum_{u\in V} & y(\{u\}), \\ & y:\ \mathcal{P}_{2t}(V)\longrightarrow\mathbb{R}, \\ & y(S)=0 \text{ for all } S\subseteq V \text{ that is not independent}, \\ & y(\emptyset)=1, \\ & M_t(y)\succeq 0. \end{aligned} \tag{3.12}$$

It can be shown that $\mathrm{las}_1(G)=\theta(G)$, therefore by the above discussion we have the following chain of inequalities

$$\alpha(G)=\mathrm{las}_{|V|}(G)=\mathrm{las}_{\alpha(G)}(G)\leq\cdots\leq\mathrm{las}_1(G)=\theta(G).$$

3.2.3 Three point bounds

In (3.12) we only use subsets of size at most $2t$ in the construction of $M_t(y)$, so we could change the domain of y, from $\mathcal{P}(V)$ to $\mathcal{P}_{2t}(V)$. This observation leads to a rough way of measuring the size of the semidefinite program: We say that a relaxation of (3.11) is a *k-point bound* if only subsets of size at most k are used in the definition of the program. In this way, program (3.2) is a 2-point bound and more generally, program (3.12) is a $2t$-point bound.

In some applications the 4-point bound defined in (3.12) with $t=2$ is already too big to be computed. This motivates the consideration of other strategies to select principal submatrices of $M(y)$, as done by Gvozdenovic, Laurent and Vallentin [GLV09] and in Section 4.3 of Bachoc, Gijswijt, Schrijver, and Vallentin [Bac+12]. Here we aim especially to three point bounds lying in between $\theta(G)$ and $\mathrm{las}_2(G)$, as done initially by Schrijver [Sch05] to upper bound the size of error detecting binary codes.

For each $v\in V$ and $y:\ \mathcal{P}(V)\longrightarrow\mathbb{R}$, we let $M_v(y)\in\mathcal{S}^{\mathcal{P}_1(V)}$ be the matrix defined by

$$M_v(y)(A,B) := y(\{v\} \cup A \cup B),$$

for $A, B \in \mathcal{P}_1(V)$. This is a principal submatrix of $M_2(y)$ indexed by $\{\{v\} \cup A : A \in \mathcal{P}_1(V)\}$ whose entries depend on sets of at most three elements. It is convenient to let the indices be a multiset and have some rows repeated, note that $\mathcal{P}_1(V)$ includes $\emptyset$ and the rows associated to $A = \emptyset$ and to $A = \{v\}$ are the same.

The constraint $M_1(y) \succeq 0$ can also be made stronger in a three point bound. Let $C \subseteq V$ be a clique (i.e. any two elements from C are connected by an edge) and consider the principal submatrix $\tilde{M}_C(y)$ of $M_2(y)$ indexed (as a multiset) by

$$\mathcal{P}_1(V) \cup_{v \in C} \{\{v\} \cup A : A \in \mathcal{P}_1(V)\}.$$

We see $\tilde{M}_C(y)$ as a block-matrix with $(|C|+1) \times (|C|+1)$ blocks of size $\mathcal{P}_1(V) \times \mathcal{P}_1(V)$. Using the constraints $y(S) = 0$ for all $S \subseteq V$ that is not independent, we have that only the first row, column and the diagonal blocks are nonzero. For instance, if $C = \{u, v, t\}$, then:

$$\tilde{M}_C(y) = \begin{pmatrix} M_1(y) & M_u(y) & M_v(y) & M_t(y) \\ M_u(y) & M_u(y) & 0 & 0 \\ M_v(y) & 0 & M_v(y) & 0 \\ M_t(y) & 0 & 0 & M_t(y) \end{pmatrix}.$$

Since $\tilde{M}_C(y)$ is a principal submatrix of $M_2(y)$ (up to some repetition of rows and columns), the constraint $M_2(y) \succeq 0$ can be relaxed to $\tilde{M}_C(y) \succeq 0$. Denoting the identity matrix in $\mathcal{S}^{\mathcal{P}_1(V)}$ by I, this can be simplified once we multiply $\tilde{M}_C(y)$ by the block-matrix $(I|-I|-I|-I)$ on the left and $(I|-I|-I|-I)^{\mathsf{T}}$ on the right:

$$(I|-I|-I|-I)\tilde{M}_C(y)(I|-I|-I|-I)^{\mathsf{T}} = M_1(y) - M_u(y) - M_v(y) - M_t(y).$$

Completing the block-matrix $(I|-I|-I|-I)$ with blocks I in the diagonal, we get an invertible transformation, namely

$$\begin{pmatrix} I & -I & -I & -I \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{pmatrix},$$

which shows that the condition $\tilde{M}_C(y) \succeq 0$ is equivalent to the constraints $M_1(y) - M_u(y) - M_v(y) - M_t(y) \succeq 0$, $M_u(y) \succeq 0$, $M_v(y) \succeq 0$, and $M_t(y) \succeq 0$.

The same argument holds for cliques of any size, leading to the following semidefinite program:

$$\begin{aligned}
&\max \sum_{u\in V} y(\{u\}),\\
&\quad y : \mathcal{P}_3(V) \longrightarrow \mathbb{R},\\
&\quad y(S) = 0 \text{ for all } S \subseteq V \ \text{ that is not independent},\\
&\quad y(\emptyset) = 1,\\
&\quad M_v(y) \succeq 0 \ \text{ for all } v \in V,\\
&\quad M_1(y) - \sum_{v\in C} M_v(y) \succeq 0 \ \text{ for every clique } C \subseteq V.
\end{aligned}$$

Other variations of the above strategy are also possible. In Section 4.2.1 we see a variation designed to have matrices indexed by V instead of $\mathcal{P}_1(V)$.

3.3 The Cohn-Elkies bound for the density of translative packings of convex bodies

In this section we consider the problem of upper bounding the maximum density of a translational packing of a convex body $K \subset \mathbb{R}^n$. Namely,

$$\Delta_T(K) := \sup\{\delta(\mathcal{P}) : \mathcal{P} \text{ is a translational packing of } K\}.$$

We present the bound from Cohn and Elkies [CE03] and show how it can be derived from the Lovász theta number (3.7). A similar presentation can be found in the lecture notes of Oliveira [Oli16].

A packing $\mathcal{P}$ is *periodic* if there is a lattice Λ such that $\mathcal{P} + v = \mathcal{P}$ for any $v \in \Lambda$. A translative periodic packing can be written as

$$\mathcal{P} = \bigcup_{v\in\Lambda} \bigcup_{j=1}^{m} (K + x_j + v), \tag{3.13}$$

for some $x_1, \dots, x_m \in \mathbb{R}^n/\Lambda$ such that $\operatorname{int}(K + x_j + v) \cap \operatorname{int}(K + x_k + u) = \emptyset$ if $(v, j) \neq (u, k)$. The density of a periodic packing $\mathcal{P}$ is simply

$$\delta(\mathcal{P}) = \frac{m \operatorname{vol}(K)}{\operatorname{vol}(\mathbb{R}^n/\Lambda)}. \tag{3.14}$$

The main fact about periodic packings is that any packing can be approximated by a periodic packing large enough (see Appendix A of Cohn and Elkies [CE03]), so we may consider only them when bounding $\Delta_T(K)$:

$$\Delta_T(K) = \sup\{\delta(\mathcal{P}) : \mathcal{P} \text{ is a translational periodic packing of } K\}.$$

Now we fix a lattice Λ and consider the problem of bounding the density of periodic packings for this fixed lattice. The main advantage of this procedure is that it replaces the

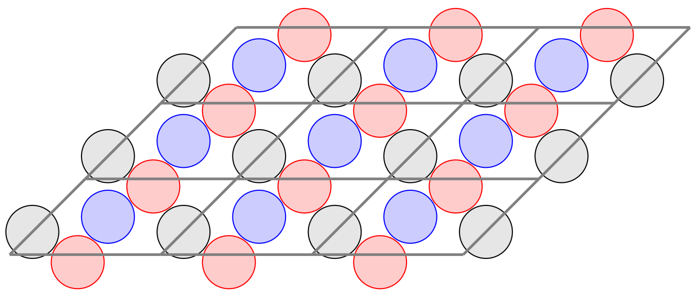

Figure 3.1: *A periodic packing of circles with three copies in each fundamental domain.*

unbounded domain $\mathbb{R}^n$ by the compact $\mathbb{R}^n/\Lambda$ and now the graph that models this packing problem is a compact topological packing graph, as mentioned in Section 3.1. In particular, the graph has a finite independence number and we may adapt the programs presented in the previous section to upper bound it. We replace the positive semidefinite matrices by the positive and continuous kernels seen in Section 2.2. Using 1 to denote the constant one kernel, Program (3.7) can be rewritten as

$$\begin{aligned} \min\ & \lambda, \\ & \lambda \in \mathbb{R},\ Z \in \mathcal{C}(\mathbb{R}^n/\Lambda \times \mathbb{R}^n/\Lambda), \\ & Z - 1 \succeq 0, \\ & Z(x,x) \le \lambda,\ \text{for all } x \in \mathbb{R}^n/\Lambda, \\ & Z(x,y) \le 0,\ \text{if } v + y - x \notin K - K \text{ for all } v \in \Lambda, \end{aligned} \tag{3.15}$$

If (Z, λ) is a feasible solution, then λ upper bounds the number of copies of K in a fundamental domain of the lattice. Here we replaced the packing condition "$\operatorname{int}(K-y) \cap \operatorname{int}(K-x+v) = \emptyset$" by "$v + y - x \notin K - K$" in the program above. We use the continuity of Z to ommit the interior and also use that $(K - y) \cap (K - x + v) = \emptyset$ if and only if $v + y - x \notin K - K$.

The next step is symmetrization. The program above is invariant with respect to the action of $\mathbb{R}^n/\Lambda$: if $Z \in \mathcal{C}(\mathbb{R}^n/\Lambda \times \mathbb{R}^n/\Lambda)$ is feasible for (3.15), so is $Z_w(x,y) := Z(x+w, y+w)$ for any $w \in \mathbb{R}^n/\Lambda$. Therefore

$$\overline{Z}(x,y) := \frac{1}{\operatorname{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n/\Lambda} Z(x+w, y+w)\, \mathrm{d}w$$

is also feasible with same objective value and it satisfies $\overline{Z}(x+w, y+w) = \overline{Z}(x,y)$ for any $x, y, w \in \mathbb{R}^n/\Lambda$. Hence we may search for invariant solutions in (3.15) and since $\overline{Z}(x,y)$ depends only on the difference $x - y$, we may reformulate (3.15) in terms of a function in $\mathcal{C}(\mathbb{R}^n/\Lambda)$:

$$\begin{aligned} \min\ & g(0), \\ & g \in \mathcal{C}(\mathbb{R}^n/\Lambda), \\ & g - 1 \text{ is of positive type}, \\ & g(x) \le 0,\ \text{if } v + x \notin K - K \text{ for all } v \in \Lambda. \end{aligned} \tag{3.16}$$

The constraint "$g - 1$ is of positive type" stands exactly for what it is replacing, namely, the kernel $Z(x, y) - 1 = g(x - y) - 1$ must be positive. Using the theory of positive and invariant kernels from Section 2.2 and specially Theorem 2.2.2, this constraint can be rewritten in terms of the Fourier coefficients of g, as saw in Theorem 2.4.4:

$$g(x) \sim \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{m \in \Lambda^*} \hat{g}_m e^{2\pi i \langle m,x \rangle},$$

where the symbol $\sim$ stands for an equality in the $L^2(\mathbb{R}^n/\Lambda)$-norm and for each $m \in \Lambda^*$,

$$\hat{g}_m = \int_{\mathbb{R}^n/\Lambda} g(x) e^{-2\pi i \langle m,x \rangle}\, \mathrm{d}x.$$

We have that "$g - 1$ is of positive type" if and only if $\hat{g}_0 \geq \mathrm{vol}(\mathbb{R}^n/\Lambda)$ and $\hat{g}_m \geq 0$ for all $m \in \Lambda^* \setminus \{0\}$.

The last step is removing the dependence on Λ. For that we make a program whose variable is a function $f \in C(\mathbb{R}^n)$ such that, given a lattice Λ, we may define

$$g(x) := \mathrm{vol}(\mathbb{R}^n/\Lambda) \sum_{v \in \Lambda} f(x + v) \tag{3.17}$$

that is feasible for (3.16).

The function f must satisfy the assumptions from Theorem 2.4.16, namely that exists $c, \delta > 0$ so that $|f(x)| < C(1 + |x|)^{-n-\delta}$ and $|\hat{f}(x)| < C(1 + |x|)^{-n-\delta}$ for all $x \in \mathbb{R}^n$, so we can use the Poisson summation formula and get

$$g(x) = \sum_{u \in \Lambda^*} \hat{f}(u) e^{2\pi i \langle x,u \rangle}.$$

This shows that $\hat{g}_m = \mathrm{vol}(\mathbb{R}^n/\Lambda)\hat{f}(m)$ for all $m \in \Lambda^*$. Therefore in order to satisfy the constraint "$g - 1$ is of positive type", we must have $\hat{f}(0) \geq 1$ and $\hat{f}(m) \geq 0$ for all $m \in \Lambda^*$. Since we want to remove the dependence on Λ, we need $\hat{f}(\xi) \geq 0$ for all $\xi \in \mathbb{R}^n$.

To satisfy the constraints "$g(x) \leq 0$, if $v + x \notin K - K$ for all $v \in \Lambda$", we use the constraint $f(x) \leq 0$ for $x \notin K - K$. If $v + x \notin K - K$ for all $v \in \Lambda$, then all terms in the right-hand side of (3.17) are nonpositive and hence $g(x) \leq 0$. Using this constraint we get

$$g(0) = \mathrm{vol}(\mathbb{R}^n/\Lambda) \sum_{v \in \Lambda} f(v) \leq \mathrm{vol}(\mathbb{R}^n/\Lambda) f(0),$$

provided that $v \notin K - K$ for all $v \in \Lambda \setminus \{0\}$, a property that holds for any periodic packing of K with the lattice Λ.

Using (3.14), the density of any periodic packing is upper bounded by

$$\delta(\mathcal{P}) = \frac{m\,\mathrm{vol}(K)}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \leq \mathrm{vol}(K) f(0).$$

This leads to the bound of Cohn and Elkies [CE03] for the maximum density of translative packings of a convex body.

Theorem 3.3.1 (Cohn-Elkies). *Let $K \subset \mathbb{R}^n$ be a convex body and $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ be a function for which there exists $c, \delta > 0$ so that $|f(x)| < C(1 + |x|)^{-n-\delta}$ and $|\hat{f}(x)| < C(1 + |x|)^{-n-\delta}$ for all $x \in \mathbb{R}^n$ and satisfies the conditions*

(a) $\hat{f}(0) \geq 1$,

(b) $\hat{f}(\xi) \geq 0$ *for all* $\xi \in \mathbb{R}^n$,

(c) $f(x) \leq 0$ *for all* $x \notin K - K$.

Then $\Delta_T(K) \leq f(0)\mathrm{vol}(K)$.

Next we give a direct proof of this theorem, which summarizes the discussion above.

Proof. Since the density of any traslative packing can be approximated by a periodic translative packing, we fix a lattice Λ and a periodic packing

$$\mathcal{P} = \bigcup_{v \in \Lambda} \bigcup_{j=1}^{m} (K + x_j + v).$$

Consider the sum

$$\sum_{v \in \Lambda} \sum_{j,k=1}^{m} f(v + x_j - x_k).$$

By one hand,

$$\sum_{v \in \Lambda} \sum_{j,k=1}^{m} f(v + x_j - x_k) \leq m f(0),$$

since if $v \neq 0$ or $j \neq k$, $\mathrm{int}(x_k + K) \cap \mathrm{int}(v + x_j + K) = \emptyset \iff v + x_j - x_k \notin \mathrm{int}(K - K)$ and condition (c) applies. By the other hand, using Poisson summation (Theorem 2.4.16) we have

$$\begin{aligned}
\sum_{v \in \Lambda} \sum_{j,k=1}^{m} f(v + x_j - x_k) &= \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{u \in \Lambda^*} \sum_{j,k=1}^{m} \hat{f}(u) e^{2\pi i \langle u, x_j - x_k \rangle} \\
&= \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{u \in \Lambda^*} \hat{f}(u) \Big| \sum_{j=1}^{m} e^{2\pi i \langle u, x_j \rangle} \Big|^2 \\
&\geq \frac{\hat{f}(0)}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} m^2 \geq m \frac{\delta(\mathcal{P})}{\mathrm{vol}(K)},
\end{aligned}$$

where we have used conditions (a) and (b). Therefore $\delta(\mathcal{P}) \leq f(0)\mathrm{vol}(K)$. Since the same bound holds for any translative periodic packing of K, we get $\Delta_T(K) \leq f(0)\mathrm{vol}(K)$. □

3.3.1 Formulation as a polynomial optimization problem

Theorem 3.3.1 is an elegant method to upper bound $\Delta_T(K)$, however it gives no clues on how to find functions that satisfy its hypothesis. The case when K is not a ball is considerable harder, see Dostert [Dos17] and Dostert, Guzman, Oliveira, and Vallentin [Dos+17] for details. Let $B_r^n \subset \mathbb{R}^n$ be the ball of radius r in $\mathbb{R}^n$, henceforth we assume $K = B_1^n$ and show an approach using semidefinite programming to find these functions, as described in Section 7 of Oliveira and Vallentin [OV15].

When $K = B_1^n$, condition (c) from Theorem 3.3.1 is $f(x) \le 0$ for all $\|x\| \ge 2$. If f is a function that satisfies the conditions from Theorem 3.3.1, then since the action of the orthogonal group commutes with the Fourier transform, for any $A \in \mathrm{O}(n)$, $(A \cdot f)(x) := f(A^\mathsf{T} x)$ is also feasible and so is $\overline{f}(x) := \int_{\mathrm{O}(n)} f(A^\mathsf{T} x)\, \mathrm{d}\mu(A)$, where the integration is with respect the Haar measure of $\mathrm{O}(n)$ normalized so that $\mu(\mathrm{O}(n)) = 1$. Therefore we may assume that f is radial when looking for feasible functions in Theorem 3.3.1.

We specify f via its Fourier transform $\hat{f}$, fixing an integer d and defining it as

$$\hat{f}(\xi) := p(\|\xi\|) e^{-\pi\|\xi\|^2}, \tag{3.18}$$

where p is an even polynomial of degree at most $2d$. We use $e^{-\pi\|\xi\|^2}$ because in this form both f and $\hat{f}$ are Schwartz functions satisfying the decaying conditions from Theorem 3.3.1. To satisfy $\hat{f}(\xi) \ge 0$ for all $\xi \in \mathbb{R}^n$ we must have p nonnegative, which can be achieved writing it as a sum of squares. See e.g., the survey of Laurent [Lau09] about polynomial optimization and sum of squares, next we show how this condition can be written with a semidefinite program.

For $l \ge 0$, let $\mathcal{B}_l$ be a basis of the space of univariate polynomials of degree at most l (e.g., the monomial basis) and write $z_l(t)$ for the column vector containing the polynomials of $\mathcal{B}_l$ evaluated at $t \in \mathbb{R}$. A polynomial p of degree $2d$ is a sum of squares if and only if there exists a positive semidefinite matrix $Q \in \mathcal{S}^{d+1}$ such that

$$p(t) = z_d(t)^\mathsf{T} Q z_d(t) = \left\langle (z_d z_d^\mathsf{T})(t), Q \right\rangle . \tag{3.19}$$

To specify that p is an even polynomial we use the constraint

$$p(t) = \left\langle (z_d z_d^\mathsf{T})(t), Q \right\rangle = \sum_{k=0}^{d} a_k t^{2k}.$$

This is an equality between polynomials of degree $2d$, to express it in a semidefinite program we must split it into $2d + 1$ equalities between the coefficients along a basis $\mathcal{B}_{2d}$. We use the constraint above for simplicity, but it is not the best way to ensure that p is even. Formula (3.19) can be rewritten with smaller matrices in such a way that it automatically generates an even polynomial. See Gatermann and Parrilo [GP04] for the theory of sum of squares for invariant polynomials and also Section 13 of Oliveira [OV15] for this specific application. The constraint "$\hat{f}(0) \ge 1$" becomes simply $a_0 \ge 1$.

Next we apply the Fourier inversion on (3.18) to retrieve f. We use the formula (see Lemma 5.2 in de Laat, Oliveira, and Vallentin [LOV14]):

$$\int_{\mathbb{R}^n} \|\xi\|^{2k} e^{-\pi\|\xi\|^2} e^{2\pi i\langle \xi, x\rangle}\, \mathrm{d}\xi = k!\pi^{-k} e^{-\pi\|x\|^2} L_k^{n/2-1}(\pi\|x\|^2), \tag{3.20}$$

where $L_k^{n/2-1}$ is the Laguerre polynomial of degree k with parameter $n/2 - 1$. Integrating each monomial from p, we get

$$f(x) = \sum_{k=0}^{d} a_k k! \pi^{-k} L_k^{n/2-1}(\pi \|x\|^2) e^{-\pi\|x\|^2}.$$

To ensure the constraint "$f(x) \leq 0$ for all $\|x\| \geq 2$" we use sum of squares again and write it as

$$\sum_{k=0}^{d} a_k k! \pi^{-k} L_k^{n/2-1}(\pi t^2) = -r(t) - (t^2 - 4)s(t),$$

where r and s are sum of squares polynomials respectively of degree at most $2d$ and $2d-2$, which can be represented by expressions similar to (3.19).

Putting all these constraints together, we produce a semidefinite program for which any feasible solution produces an upper bound for $\Delta_T(B_1^n)$:

$$\begin{aligned}
\min \ & \sum_{k=0}^{d} a_k k! \pi^{-k} L_k^{n/2-1}(0) \mathrm{vol}(B_1^n), \\
& Q, R \in \mathcal{S}_{\geq 0}^{d+1},\ S \in \mathcal{S}_{\geq 0}^{d-1},\ a_0, \ldots, a_d \in \mathbb{R},\ a_0 \geq 1, \\
& \left\langle (z_d z_d^{\mathsf{T}})(t), Q \right\rangle = \sum_{k=0}^{d} a_k t^{2k}, \\
& \sum_{k=0}^{d} a_k k! \pi^{-k} L_k^{n/2-1}(\pi t^2) + \left\langle (z_d z_d^{\mathsf{T}})(t), R \right\rangle + (t^2 - 4) \left\langle (z_{d-1} z_{d-1}^{\mathsf{T}})(t), S \right\rangle = 0.
\end{aligned} \tag{3.21}$$

As noted in Section 5.3 of de Laat, Oliveira, and Vallentin [LOV14], the choice of the basis of polynomials $\mathcal{B}_d$ used to express the sum of squares polynomials, as well to setup the equality constraints between polynomials in (3.21), greatly affects the numerical stability of the semidefinite program. In practice the monomial basis performs poorly.

3.3.2 Sharp bounds

Numerical computations can be used to produce explicit bounds for $\Delta_T(B_1^n)$ in several dimensions with Theorem 3.3.1. Cohn and Elkies [CE03] computed bounds for dimensions 4 to 36 using a technique different from the one presented above but that gives similar results since it also relies in approximating a general Schwartz function by a function of the form $f(x) = p(\|x\|)e^{-\pi\|x\|^2}$, where p is a polynomial with some bounded degree.

There is no reason to expect that these computations will produce bounds that match the best known packing densities in each dimension or even the true value of $\Delta_T(B_1^n)$. Indeed, the analogous bound for the independence number of a finite graph, the Lovász theta number seem in Section 3.2.1, is not sharp in general. However, Cohn and Elkies [CE03] observed that for dimensions 8 and 24, the bounds they obtained could numerically approximate the packing densities of the E_8 and Leech lattices respectively and hence they conjectured that Theorem 3.3.1 could be used to prove the optimality of these packings.

A function that produces a sharp bound must satisfy conditions much stronger than the assumptions from Theorem 3.3.1. While functions of the form $f(x) = p(\|x\|)e^{-\pi\|x\|^2}$ with a polynomial p can approximate other Schwartz functions, they cannot match the optimal bound. To understand why, we revisit the proof of Theorem 3.3.1 replacing the inequalities by equalities and letting $m = 1$, since the cases of interest are lattice packings.

$$f(0) \leq \sum_{v\in\Lambda} f(v) = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{u\in\Lambda^*} \hat{f}(u) \leq \frac{\hat{f}(0)}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \leq \frac{\delta(\mathcal{P})}{\mathrm{vol}(B_1^n)}.$$

To have an equality above we need $f(v) = 0$ for all $v \in \Lambda \setminus \{0\}$, $\hat{f}(u) = 0$ for all $u \in \Lambda^* \setminus \{0\}$, $\hat{f}(0) = 1$ and $f(0) = \Delta_T(B_1^n)/\mathrm{vol}(B_1^n)$.

In the case $n = 8$, the E_8 lattice can be normalized so that $E_8^* = E_8$. In this normalization $\mathrm{vol}(\mathbb{R}^n/E_8) = 1$ and E_8 has vectors of length $\sqrt{2k}$ for $k = 1, 2, \ldots$. Hence we have a packing $\mathcal{P}$ of spheres of radius $r = \sqrt{2}/2$ centered at the vectors of E_8 and the density of this packing is $\delta(\mathcal{P}) = \mathrm{vol}(B_r^8) = \pi^4/384 = 0.2536\ldots$.

We search for a function that satisfy the conditions above with $f(0) = \delta(\mathcal{P})/\mathrm{vol}(B_r^8) = 1$. For $\eta \in S^{n-1}$, since $f(r\eta) \leq 0$ for all $r \geq \sqrt{2}$, we must also have $\frac{d}{dr}f(r\eta) = 0$ for $r = \sqrt{2k}$, $k = 2, 3, \ldots$ and since $\hat{f}(r\eta) \geq 0$ for all $r \geq 0$, we must have $\frac{d}{dr}\hat{f}(r\eta) = 0$ for $r = \sqrt{2k}$, $k = 1, 2, \ldots$.

The function with these characteristics was found by Viazovska [Via17] using integral transforms of certain quotients of modular forms. Soon after, this construction was extended to the Leech lattice in dimension 24 by Cohn, Kumar, Miller, Radchenko, and Viazovska [Coh+17].

Chapter 4

k-point semidefinite programming bounds for equiangular lines

This chapter is based on the publication "D. de Laat, F.C. Machado, F.M. de Oliveira Filho, F. Vallentin, *k-point semidefinite programming bounds for equiangular lines*, arXiv:1812.06045, *Mathematical Programming*, 2021, 35 pages".

Abstract. We propose a hierarchy of k-point bounds extending the Delsarte-Goethals-Seidel linear programming 2-point bound and the Bachoc-Vallentin semidefinite programming 3-point bound for spherical codes. An optimized implementation of this hierarchy allows us to compute 4, 5, and 6-point bounds for the maximum number of equiangular lines in Euclidean space with a fixed common angle.

4.1 Introduction

Given $D \subseteq [-1, 1)$, a subset C of the unit sphere $S^{n-1} = \{ x \in \mathbb{R}^n : \|x\| = 1 \}$ is a *spherical D-code* if $x \cdot y \in D$ for all distinct $x, y \in C$, where $x \cdot y$ is the Euclidean inner product between x and y. The maximum cardinality of a spherical D-code in S^{n-1} is denoted by $A(n, D)$.

Different sets D describe different problems that can be treated with similar techniques. The most important cases are D being an interval and D being a finite set. If $D = [-1, \cos(\pi/3)]$, then $A(n, D)$ is the *kissing number*, the maximum number of pairwise nonoverlapping unit spheres that can touch a central unit sphere.

A fundamental tool for computing upper bounds for $A(n, D)$ is the *linear programming bound* of Delsarte, Goethals, and Seidel [DGS77], which is an adaptation of the Delsarte bound [Del73] to the sphere. The linear programming bound was one of the first nontrivial upper bounds for the kissing number and is the optimal value of a convex optimization problem. It is a 2*-point bound*, because it takes into account interactions between pairs of points on the sphere: pairs $\{x, y\}$ with $x \cdot y \notin D$ correspond to constraints in the optimization problem. Bachoc and Vallentin [BV08] extended the linear programming bound to a 3-*point bound* by taking into account interactions between triples of points, extending the three-point bound by Schrijver [Sch05] for binary codes. The resulting *semidefinite programming bound* gives the best known upper bounds for the kissing number for all dimensions $3 \leq n \leq 24$, although in dimensions $n = 3, 4, 8$, and 24 the optimal values were already known by other methods.

In the same paper in which the linear programming bound was proposed, Delsarte, Goethals, and Seidel [DGS77] considered its application to bound $A(n, D)$ when D is finite and also to the related problem of bounding $A(n, D)$ for all D with a given size $|D| = s$. The semidefinite programming bound from Bachoc and Vallentin was first computed for these problems by Barg and Yu [BY13].

In this paper, we give a hierarchy of k-*point bounds* that extend both the linear and semidefinite programming bounds. We model the parameter $A(n, D)$ as the independence number of a graph, namely the infinite graph with vertex set S^{n-1} in which two vertices x and y are adjacent if $x \cdot y \notin D$. The linear programming bound corresponds to an extension of the Lovász theta number to this infinite graph [Bac+09]. In Section 4.2, we derive our hierarchy from a generalization [LV15] of Lasserre's hierarchy to a class of infinite graphs that comprises the graph being considered. The first level of our hierarchy is the Lovász theta number, and is therefore equivalent to the linear programming bound; the second level is the semidefinite programming bound by Bachoc and Vallentin, as shown in Section 4.5.2. This puts the 2 and 3-point bounds in a common framework and shows how these relate to the Lasserre hierarchy.

For the case where D is infinite, we give a precise reason why it is difficult to compute the problems in this hierarchy when $k \geq 4$. This might explain why so far nobody has been able to compute a 4-point bound generalization of the 2 and 3-point bounds for the kissing number problem. For the case where D is finite there is no such obstruction, and though our hierarchy is not as strong, in theory, as the Lasserre hierarchy, it is computationally less expensive. This allows us to use it to compute 4, 5, and 6-point bounds for the maximum number of equiangular lines with a certain angle, a problem that corresponds to the case $|D| = 2$. Aside from a previous result of de Laat [Laa19], which uses Lasserre's hierarchy directly, this is the first successful use of k-point bounds for $k > 3$ for geometrical problems; it yields improved bounds for the number of equiangular lines with given angles in several dimensions.

To perform computations, we transform the resulting problems into semidefinite programming problems. To this end, for a given $k \geq 2$ we use a characterization of kernels $K : S^{n-1} \times S^{n-1} \longrightarrow \mathbb{R}$ on the sphere that are invariant under the action of the subgroup of the orthogonal group that stabilizes $k - 2$ given points. For $k = 2$, this characterization was given by Schoenberg [Sch42] and for $k = 3$, by Bachoc and Vallentin [BV08]; Musin [Mus08] extended these two results for $k > 3$; a similar result is given by Kuryatnikova and Vera [Olg19].

Still, a naive implementation of our approach would be too slow even to generate the problems for $k = 5$. The implementation available with the arXiv version of [Laa+21] was carefully written to deal with the orbits of k points in the sphere in an efficient way; this allows us to generate problems even for $k = 6$. This implementation could be of interest to others working on similar problems.

4.1.1 Equiangular lines

A set of *equiangular lines* is a set of lines through the origin such that every pair of lines defines the same angle. If this angle is α, then such a set of equiangular lines corresponds to a spherical D-code where $D = \{a, -a\}$ and $a = \cos(\alpha)$. So we are interested in finding $A(n, \{a, -a\})$ for a given $a \in [-1, 1)$ and also in finding the maximum number of equiangular lines with any given angle, namely

$$M(n) = \max\{\, A(n, \{a, -a\}) \,:\, a \in [-1, 1) \,\}.$$

The study of $M(n)$ started with Haantjes [Haa48] in 1948. He showed that $M(2) = 3$ and that the optimal configuration is a set of lines on the plane having a common angle of 60 degrees. He also showed that $M(3) = 6$; the optimal configuration is given by the lines going through opposite vertices of a regular icosahedron, which have a common angle of 63.43 … degrees. These two constructions provide lower bounds; in both cases, Gerzon's bound, which states that $M(n) \leq n(n+1)/2$ (see Theorem 4.6.1 below which is proven for example in Matoušek's book [Mat10, Miniature 9]), provides matching upper bounds.

In the setting of equiangular lines, the LP bound coincides with van Lint and Seidel's relative bound ([LS66], see also, Theorem 4.6.5). The 3-point SDP bound was first specialized to this setting by Barg and Yu [BY13]. No k-point bound has been computed or formulated for $k \geq 4$ for equiangular lines or for any other spherical code problem. Gijswijt, Mittelmann, and Schrijver [GMS12] computed 4-point SDP bounds for binary codes and Litjens, Polak, and Schrijver [LPS17] extended these 4-point bounds to q-ary codes.

Next to being fundamental objects in discrete geometry, equiangular lines have applications, for example in the field of compressed sensing: Only measurement matrices whose columns are unit vectors determining a set of equiangular lines can minimize the coherence parameter [FR13, Chapter 5].

In general, it is a difficult problem to determine $M(n)$ for a given dimension n. Currently, the first open case is dimension $n = 17$ where it is known that $M(17)$ is either 48 or 49; see Table 4.1. Sequence A002853 in The On-Line Encyclopedia of Integer Sequences [Slo18] is $M(n)$.

4.2 Derivation of the hierarchy

In this section we derive a hierarchy of bounds for the independence number of a graph. We first derive this for finite graphs and then we show how this can be extended to a larger class, which includes the infinite graphs that we use to model the geometric problems described in the introduction. We provide detailed arguments to justify each step of the derivation, but Proposition 4.2.1 at the end of the section has a direct and simple proof for the validity of the bound we use in the rest of the paper.

Let $G = (V, E)$ be a graph. A subset of V is *independent* if it does not contain a pair of adjacent vertices. The *independence number* of G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set. For an integer $k \geq 0$, let I_k be the set of independent sets in G of size at most k and $I_{=k}$ be the set of independent sets in G of size exactly k.

4.2.1 Definition of the hierarchy for finite graphs

Assume for now that G is finite. We can obtain upper bounds for the independence number via the Lasserre hierarchy [Las02] for the independent set problem, whose t-th step, as shown by Laurent [Lau03], can be formulated as

$$\max\left\{ \sum_{S\in I_{=1}} \nu_S \;:\; \nu \in \mathbb{R}^{I_{2t}}_{\geq 0},\; \nu_\emptyset = 1,\; \text{and } M(\nu) \succeq 0 \right\}, \tag{4.1}$$

where $M(\nu)$ is the matrix indexed by $I_t \times I_t$ such that

$$M(\nu)_{J,J'} = \begin{cases} \nu_{J\cup J'} & \text{if } J \cup J' \text{ is independent;} \\ 0 & \text{otherwise} \end{cases} \tag{4.2}$$

and $M(\nu) \succeq 0$ means that $M(\nu)$ is positive semidefinite. It is easily seen that this hierarchy bounds the independence number from above since for an independent set $C \subseteq V$, the vector $\nu \in \mathbb{R}^{I_{2t}}$ defined by $\nu_S = 1$ if $S \subseteq C$ and $\nu_S = 0$ otherwise is such that $M(\nu)$ is a principal submatrix of $\nu\nu^{\mathsf{T}}$ and hence is a feasible solution to (4.1) with value $\sum_{S\in I_{=1}} \nu_S = |C|$. It is also shown [Lau03] that this hierarchy converges to the independence number in at most $\alpha(G)$ steps.

To produce an optimization program where the variables are easier to parameterize, we construct in two stages a weaker hierarchy with matrices indexed only by the vertex set of the graph. First, we modify the problem to remove $\emptyset$ from the domain of ν; this gives the possibly weaker problem

$$\max\left\{ 1 + 2\sum_{S\in I_{=2}} \nu_S \;:\; \nu \in \mathbb{R}^{I_{2t}\setminus\{\emptyset\}}_{\geq 0},\; \sum_{S\in I_{=1}} \nu_S = 1,\; \text{and } M(\nu) \succeq 0 \right\}, \tag{4.3}$$

where $M(\nu)$ is now considered as a matrix indexed by $(I_t \setminus \{\emptyset\}) \times (I_t \setminus \{\emptyset\})$. To see how problem (4.3) is a weaker version of problem (4.1) and thus still an upper bound for the independence number, let $\nu \in \mathbb{R}^{I_{2t}}$ be a feasible solution for (4.1) and define $\overline{\nu} \in \mathbb{R}^{I_{2t}\setminus\{\emptyset\}}$ as $\overline{\nu}_S = \nu_S / (\sum_{Q\in I_{=1}} \nu_Q)$. One can check that $\overline{\nu}$ is feasible for (4.3) and $\sum_{S\in I_{=1}} \nu_S \leq 1 + 2\sum_{S\in I_{=2}} \overline{\nu}_S$. To justify this last inequality, apply the Schur complement to the submatrix of $M(\nu)$ indexed by I_1 to conclude that the matrix

$$\left(\nu_{\{u,v\}} - \nu_{\{u\}}\nu_{\{v\}}\right)_{u,v\in V}$$

indexed by $I_{=1} \simeq V$ (set $\nu_{\{u,v\}} = 0$ if $\{u, v\}$ is not independent) is positive semidefinite and hence

$$\left(\sum_{u\in V} \nu_{\{u\}}\right)^2 \leq \sum_{u,v\in V} \nu_{\{u,v\}},$$

which implies the desired inequality.

Second, we construct a weaker hierarchy by only requiring certain principal submatrices of $M(\nu)$ to be positive semidefinite, an approach similar to the one employed by Gvozdenović, Laurent, and Vallentin [GLV09]. For this we fix $k \geq 2$ and, for each $Q \in I_{k-2}$, define the matrix $M_Q(\nu): V \times V \longrightarrow \mathbb{R}$ by

$$M_Q(\nu)(x,y) = \begin{cases} \nu_{Q \cup \{x,y\}} & \text{if } Q \cup \{x,y\} \in I_k; \\ 0 & \text{otherwise} \end{cases}$$

and replace the condition '$M(\nu) \succeq 0$' by '$M_Q(\nu) \succeq 0$ for all $Q \in I_{k-2}$'. With these conditions we can restrict the support of ν to the set $I_k \setminus \{\emptyset\}$, obtaining the relaxation

$$\max\left\{ 1 + 2\sum_{S \in I_{=2}} \nu_S : \nu \in \mathbb{R}_{\geq 0}^{I_k \setminus \{\emptyset\}},\ \sum_{S \in I_{=1}} \nu_S = 1,\ \text{and } M_Q(\nu) \succeq 0 \text{ for } Q \in I_{k-2} \right\}. \tag{4.4}$$

We now proceed to the computation of the dual of program (4.4). For that we use $\mathbb{R}^{V^2 \times I_{k-2}}$ to denote a collection of matrices $V \times V \longrightarrow \mathbb{R}$ indexed by $I_{I_{k-2}}$ and $\mathbb{R}_{\succeq 0}^{V^2 \times I_{k-2}}$ to denote that each of these matrices is positive semidefinite. We define a linear operator $M_k : \mathbb{R}^{I_k \setminus \{\emptyset\}} \longrightarrow \mathbb{R}^{V^2 \times I_{k-2}}$ by

$$M_k(\nu) = \big(M_Q(\nu)\big)_{Q \in I_{k-2}}$$

and write the constraints '$M_Q(\nu) \succeq 0$ for all $Q \in I_{k-2}$' as $M_k(\nu) \in \mathbb{R}_{\succeq 0}^{V^2 \times I_{k-2}}$. The adjoint operator is defined in such a way that the inner product between $M_k(\nu)$ and $T \in \mathbb{R}^{V^2 \times I_{k-2}}$ is equal to the inner product between ν and $M_k^*(T)$:

$$\begin{aligned} \sum_{Q \in I_{k-2}} \sum_{x,y \in V} M_Q(\nu)(x,y) T(x,y,Q) &= \sum_{Q \in I_{k-2}} \sum_{\substack{x,y \in V \\ Q \cup \{x,y\} \in I_k}} \nu_{Q \cup \{x,y\}} T(x,y,Q) \\ &= \sum_{S \in I_k \setminus \{\emptyset\}} \nu_S \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S \\ Q \cup \{x,y\} = S}} T(x,y,Q), \end{aligned}$$

so we conclude that the expression for $M_k^* : \mathbb{R}^{V^2 \times I_{k-2}} \longrightarrow \mathbb{R}^{I_k \setminus \{\emptyset\}}$ is

$$M_k^*(T)(S) = \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S \\ Q \cup \{x,y\} = S}} T(x,y,Q). \tag{4.5}$$

Using the duality theory of conic optimization as described e.g. by Barvinok [Bar02, Chapter IV], we can derive the following dual problem for (4.4):

$$\min\left\{ 1 + \lambda : \lambda \in \mathbb{R},\ T \in \mathbb{R}_{\succeq 0}^{V^2 \times I_{k-2}},\ \text{and } M_k^*(T) \leq \lambda \mathbb{1}_{I_{=1}} - 2\mathbb{1}_{I_{=2}} \right\}, \tag{4.6}$$

where $\mathbb{1}_{I_{=1}}$ and $\mathbb{1}_{I_{=2}}$ are the indicator functions of $I_{=1}$ and $I_{=2}$. It is a consequence of weak duality that program (4.6) gives an upper bound for the independence number. At the end of the next section we give a direct proof of this fact in a more general context.

4.2.2 Definition of the hierarchy for infinite graphs

We extend this hierarchy to infinite graphs in the same way that the Lasserre hierarchy is extended by de Laat and Vallentin [LV15]. This extension can be carried out for *compact topological packing graphs*; these are graphs whose vertex sets are compact Hausdorff spaces and in which every finite clique is contained in an open clique. The main consequences of this definition are that the independence number is finite and I_k, considered with the topology inherited from V, is the disjoint union of the compact and open sets $I_{=s}$ for $s = 0, \dots, k$ [LV15, Section 2]. We assume from now on that G is a compact topological packing graph.

The extension relies on the theory of conic optimization over infinite-dimensional spaces presented e.g. by Barvinok [Bar02]. The first step is to introduce the spaces for the variables of our problem; we will use both the space $\mathcal{C}(X)$ of continuous real-valued functions on a compact space X and its topological dual (with respect to the supremum norm) $\mathcal{M}(X)$, the space of signed Radon measures.

In the infinite setting, the nonnegative variable ν from (4.4) becomes a measure in the dual of the cone $\mathcal{C}(I_k \setminus \{\emptyset\})_{\geq 0}$ of continuous and nonnegative functions, namely

$$\mathcal{M}(I_k \setminus \{\emptyset\})_{\geq 0} = \{\, \nu \in \mathcal{M}(I_k \setminus \{\emptyset\}) \,:\, \nu(f) \geq 0 \text{ for all } f \in \mathcal{C}(I_k \setminus \{\emptyset\})_{\geq 0} \,\};$$

we observe that when V is finite, $\mathcal{M}(I_k \setminus \{\emptyset\})_{\geq 0}$ can be identified with $\mathbb{R}_{\geq 0}^{I_k \setminus \{\emptyset\}}$.

Let $\mathcal{C}(V^2 \times I_{k-2})_{\text{sym}}$ be the set of continuous real-valued functions on $V^2 \times I_{k-2}$ that are symmetric in the first two coordinates and let $\mathcal{M}(V^2 \times I_{k-2})_{\text{sym}}$ be the space of symmetric and signed Radon measures[1]. A kernel $K \in \mathcal{C}(V^2)$ is *positive* if for every finite $U \subseteq V$ the matrix $\big(K(x, y)\big)_{x,y \in U}$ is positive semidefinite. A function $T \in \mathcal{C}(V^2 \times I_{k-2})$ is *positive* if for every $Q \in I_{k-2}$ the kernel $(x, y) \mapsto T(x, y, Q)$ is positive. The set of all positive functions in $\mathcal{C}(V^2 \times I_{k-2})$ is a convex cone denoted by $\mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$; its dual cone is denoted by $\mathcal{M}(V^2 \times I_{k-2})_{\succeq 0}$.

Instead of extending the operator M_k from the finite case, a key step in this extension is to use its adjoint. Based on formula (4.5), we define the operator $B_k : \mathcal{C}(V^2 \times I_{k-2})_{\text{sym}} \longrightarrow \mathcal{C}(I_k \setminus \{\emptyset\})$ by

$$B_k T(S) = \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S \\ Q \cup \{x,y\} = S}} T(x, y, Q). \tag{4.7}$$

Note that, though the number of summands in (4.7) varies with the size of S, the function $B_k T$ is still continuous since, by the assumption that G is a topological packing graph, $I_k \setminus \{\emptyset\}$ can be written as the disjoint union of the compact and open subsets $I_{=s}$ for $s = 1, \dots, k$ and $B_k T$ is continuous in each of these parts. Furthermore, since the number of summands in (4.7) is bounded by a constant depending only on k, the operator B_k is itself continuous. Thus it has an adjoint $B_k^* : \mathcal{M}(I_k \setminus \{\emptyset\}) \longrightarrow \mathcal{M}(V^2 \times I_{k-2})_{\text{sym}}$. Using the adjoint, we define the *generalized k-point bound* for $k \geq 2$:

$$\Delta_k(G) = \sup\{\, 1 + 2\nu(I_{=2}) \,:\, \nu \in \mathcal{M}(I_k \setminus \{\emptyset\})_{\geq 0},\ \nu(I_{=1}) = 1, \text{ and } B_k^* \nu \in \mathcal{M}(V^2 \times I_{k-2})_{\succeq 0} \,\}. \tag{4.8}$$

[1] A measure $\mu \in \mathcal{M}(V^2 \times I_{k-2})$ is *symmetric* if $\mu(E \times E' \times C) = \mu(E' \times E \times C)$ for all Borel sets $E, E' \subseteq V$ and $C \subseteq I_{k-2}$.

Note that for a finite graph with the discrete topology this reduces to (4.4).

Again, using the duality theory of conic optimization [Bar02, Chapter IV], we can derive the following dual problem for (4.8):

$$\Delta_k(G)^* = \inf\{\, 1 + \lambda : \lambda \in \mathbb{R},\ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0},\ \text{and } B_k T \le \lambda \mathbb{1}_{I_{=1}} - 2\mathbb{1}_{I_{=2}} \,\}, \tag{4.9}$$

where $\mathbb{1}_{I_{=1}}$ and $\mathbb{1}_{I_{=2}}$ are the indicator functions of $I_{=1}$ and $I_{=2}$, which are continuous since G is a topological packing graph. From now on, we will denote both the optimal value of (4.9) and the optimization problem itself by $\Delta_k(G)^*$.

It is a direct consequence of weak duality that $\Delta_k(G)^*$ is an upper bound for the independence number of G, but it is instructive to see a direct proof.

Proposition 4.2.1. *If $G = (V, E)$ is a compact topological packing graph, then $\alpha(G) \le \Delta_k(G)^*$.*

Proof. Let $C \subseteq V$ be a nonempty independent set and let (λ, T) be a feasible solution of $\Delta_k(G)^*$. On the one hand, since $B_k T \le \lambda \mathbb{1}_{I_{=1}} - 2\mathbb{1}_{I_{=2}}$, we have

$$\sum_{\substack{S \subseteq C \\ |S| \le k,\ S \neq \emptyset}} B_k T(S) \le \binom{|C|}{1}\lambda + \binom{|C|}{2}(-2) = |C|(1 + \lambda - |C|).$$

On the other hand, since $T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$, we have

$$\begin{aligned} \sum_{\substack{S \subseteq C \\ |S| \le k,\ S \neq \emptyset}} B_k T(S) &= \sum_{\substack{S \subseteq C \\ |S| \le k,\ S \neq \emptyset}} \ \sum_{\substack{Q \subseteq S \\ |Q| \le k-2}} \ \sum_{\substack{x,y \in S \\ Q \cup \{x,y\} = S}} T(x, y, Q) \\ &= \sum_{\substack{Q \subseteq C \\ |Q| \le k-2}} \ \sum_{x,y \in C} T(x, y, Q) \ge 0 \end{aligned}$$

since, by the definition of $\mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$, the matrices $\big(T(x, y, Q)\big)_{x,y \in C}$ are positive semidefinite for all $Q \in I_{k-2}$. Putting it all together we get $|C| \le 1 + \lambda$. ☐

4.3 Symmetry reduction

Symmetry reduction plays a key role in the computation of $\Delta_k(G)^*$ in our application. We now see how to exploit symmetry to decompose the variable T of (4.9) in terms of simpler kernels from $\mathcal{C}(V^2)$. In this section we keep assuming that G is a compact topological packing graph and delay the specialization to the case where V is a sphere to the next section.

Let Γ be a compact group that acts continuously on V and that is a subgroup of the automorphism group[2] of the graph G. The group Γ acts coordinatewise on V^2, and this

[2] The *automorphism group* $\mathrm{Aut}(G)$ of a graph $G = (V, E)$ is the group of permutations $\sigma : V \longrightarrow V$ that respect the adjacency relation; that is, $\sigma(x)$ and $\sigma(y)$ are adjacent if and only if x and $y \in V$ are adjacent.

action extends to an action on $C(V^2)$ by

$$(\gamma K)(x, y) = K(\gamma^{-1}x, \gamma^{-1}y).$$

The group Γ acts continuously on I_t by

$$\gamma\emptyset = \emptyset \quad \text{and} \quad \gamma\{x_1, \dots, x_t\} = \{\gamma x_1, \dots, \gamma x_t\},$$

and hence it also acts on $C(V^2 \times I_{k-2})_{\mathrm{sym}}$ by

$$(\gamma T)(x, y, S) = T(\gamma^{-1}x, \gamma^{-1}y, \gamma^{-1}S).$$

If Γ acts on a set X, we denote by X^Γ the set of elements of X that are invariant under this action. In this way we write $C(V^2)^\Gamma$, $C(V^2 \times I_{k-2})^\Gamma_{\succeq 0}$, etc.

Given a feasible solution (λ, T) of $\Delta_k(G)^*$, the pair $(\lambda, \overline{T})$ with

$$\overline{T}(x, y, S) = \int_\Gamma T(\gamma^{-1}x, \gamma^{-1}y, \gamma^{-1}S)\, \mathrm{d}\gamma,$$

where we integrate against the Haar measure on Γ normalized so that the total measure is 1, is also feasible with the same objective value. So we may assume that T is invariant under the action of Γ.

Let $\mathcal{R}_{k-2}$ be a complete set of representatives of the orbits of I_{k-2}/Γ. For $R \in \mathcal{R}_{k-2}$, let $\mathrm{Stab}_\Gamma(R) = \{\, \gamma \in \Gamma : \gamma R = R \,\}$ be the stabilizer of R with respect to Γ and, for $Q \in \Gamma R$, let $\gamma_Q \in \Gamma$ be a group element such that $\gamma_Q Q = R$. When I_{k-2}/Γ is finite, we can decompose the space $C(V^2 \times I_{k-2})^\Gamma$ as a direct sum of simpler spaces.

The next proposition may seem rather technical but the main idea is to use the symmetry of $T \in C(V^2 \times I_{k-2})^\Gamma$ and the assumption that there is just a finite collection of representatives for the last coordinate to write $T(x, y, Q) = T(\gamma_Q x, \gamma_Q y, \gamma_Q Q)$ and express T by finitely many kernels, each of them representing T when its last coordinate is fixed; this is also the place where the stabilizer subgroups come into play.

Proposition 4.3.1. *If I_{k-2}/Γ is finite, then*

$$\Psi : \bigoplus_{R \in \mathcal{R}_{k-2}} C(V^2)^{\mathrm{Stab}_\Gamma(R)} \longrightarrow C(V^2 \times I_{k-2})^\Gamma$$

given by

$$\Psi((K_R)_{R \in \mathcal{R}_{k-2}})(x, y, Q) = K_{\gamma_Q Q}(\gamma_Q x, \gamma_Q y)$$

is an isomorphism that preserves positivity, that is, if $(K_R)_{R \in \mathcal{R}_{k-2}}$ is such that K_R is a positive kernel for each R, then $\Psi((K_R)_{R \in \mathcal{R}_{k-2}})$ is positive.

Proof. We first show that $(V^2 \times I_{k-2})/\Gamma$ is homeomorphic to the disjoint union

$$\bigcup_{R \in \mathcal{R}_{k-2}} V^2/\mathrm{Stab}_\Gamma(R) \times \{R\}.$$

More precisely, we show that

$$\psi : \bigcup_{R \in \mathcal{R}_{k-2}} V^2/\mathrm{Stab}_\Gamma(R) \times \{R\} \longrightarrow (V^2 \times I_{k-2})/\Gamma$$

given by $\psi(\mathrm{Stab}_\Gamma(R)(x, y), R) = \Gamma(x, y, R)$ is such a homeomorphism with inverse

$$\psi^{-1}(\Gamma(x, y, Q)) = (\mathrm{Stab}_\Gamma(\gamma_Q Q)(\gamma_Q x, \gamma_Q y), \gamma_Q Q). \tag{4.10}$$

Indeed, the map ψ is well defined because $\Gamma(x, y, R) = \Gamma(\gamma x, \gamma y, R)$ for all γ in $\mathrm{Stab}_\Gamma(R)$. For each $R \in \mathcal{R}_{k-2}$, the map $\psi_R : V^2/\mathrm{Stab}_\Gamma(R) \longrightarrow (V^2 \times I_{k-2})/\Gamma$ given by

$$\psi_R\big(\mathrm{Stab}_\Gamma(R)(x, y)\big) = \Gamma(x, y, R)$$

is continuous, as follows from the definition of quotient topology. By the definition of disjoint union topology, this implies ψ is continuous.

The map (4.10) is well defined, for if we replace γ_Q by $\xi\gamma_Q$, where $\xi \in \mathrm{Stab}_\Gamma(\gamma_Q Q)$, then the right-hand side of (4.10) does not change. Direct verification shows $\psi^{-1} \circ \psi$ and $\psi \circ \psi^{-1}$ are the identity maps.

Since $\mathcal{R}_{k-2}$ is finite, the domain of ψ is compact. So ψ is a continuous bijection between compact Hausdorff spaces, and hence a homeomorphism.

Now the proposition follows easily. Under the isomorphisms

$$\mathcal{C}\Bigg(\bigcup_{R \in \mathcal{R}_{k-2}} V^2/\mathrm{Stab}_\Gamma(R) \times \{R\}\Bigg) \simeq \bigoplus_{R \in \mathcal{R}_{k-2}} \mathcal{C}(V^2)^{\mathrm{Stab}_\Gamma(R)}$$

and

$$\mathcal{C}((V^2 \times I_{k-2})/\Gamma) \simeq \mathcal{C}(V^2 \times I_{k-2})^\Gamma,$$

the operator Ψ is equal to

$$\mathcal{C}\Bigg(\bigcup_{R \in \mathcal{R}_{k-2}} V^2/\mathrm{Stab}_\Gamma(R) \times \{R\}\Bigg) \longrightarrow \mathcal{C}((V^2 \times I_{k-2})/\Gamma), \qquad f \longmapsto f \circ \psi^{-1},$$

which is a well-defined isomorphism since ψ is a homeomorphism. Finally, it follows directly from the definitions of positive kernels and $\mathcal{C}(V^2 \times I_{k-2})^\Gamma_{\geq 0}$ that Ψ preserves positivity. $\square$

The above proposition shows that to characterize $\mathcal{C}(V^2 \times I_{k-2})^\Gamma$ we need to characterize the sets $\mathcal{C}(V^2)^{\mathrm{Stab}_\Gamma(R)}$ for $R \in \mathcal{R}_{k-2}$. In the next section we give this characterization for the case of spherical symmetry.

4.4 Parameterizing invariant kernels on the sphere by positive semidefinite matrices

From now on we assume $G = (V, E)$ is the graph where $V = S^{n-1}$ and where two distinct vertices $x, y \in S^{n-1}$ are adjacent if $x \cdot y \notin D$ for some $D \subseteq [-1, 1)$. We assume D is closed in order to make G a compact topological packing graph. Taking $\Gamma = \mathrm{O}(n)$, we are in the situation described in the previous section.

We observe that $I_{=m}/\mathrm{O}(n)$ can be represented by the set of $m \times m$ positive semidefinite matrices of rank at most n with ones in the diagonal and elements of D elsewhere, up to simultaneous permutations of the rows and columns. So the condition that $I_{k-2}/\mathrm{O}(n)$ is finite is fulfilled for any set D when $k = 2$ or 3 and it only holds for finite D when $k \geq 4$.

Let us see how to parameterize the cones

$$C(S^{n-1} \times S^{n-1})_{\geq 0}^{\mathrm{Stab}_{\mathrm{O}(n)}(R)} \quad \text{for } R \in \mathcal{R}_{k-2}$$

by positive semidefinite matrices. For simplicity, we only consider the case where every $R \in \mathcal{R}_{k-2}$ consists of linearly independent vectors; later on we will see that all cases considered in the computations satisfy this assumption.

Let $\{e_1, \ldots, e_n\}$ be the standard basis of $\mathbb{R}^n$ and fix $R \in \mathcal{R}_{k-2}$. By rotating a set $R \in \mathcal{R}_{k-2}$ if necessary, we may assume that R is contained in $\mathrm{span}(\{e_1, \ldots, e_m\})$, where $m = \dim(\mathrm{span}(R))$. The stabilizer subgroup of $\mathrm{O}(n)$ with respect to R is isomorphic to the direct product of two groups, namely

$$\mathrm{Stab}_{\mathrm{O}(n)}(R) \simeq \mathcal{S}_R \times \mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R)),$$

where $\mathcal{S}_R$ is isomorphic to a finite subgroup of $\mathrm{O}(m)$ that acts on the first m coordinates and acts on R as a permutation of its elements and $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$ is a group isomorphic to $\mathrm{O}(n - m)$ that acts on the last $n - m$ coordinates. Indeed, any rotation that leaves $\mathrm{span}(R)$ and its orthogonal complement invariant and acts in R as a permutation fixes R as a set and hence is from $\mathrm{Stab}_{\mathrm{O}(n)}(R)$. Conversely, any rotation that fixes R as a set will at most permute its elements and hence by linearity, leaves $\mathrm{span}(R)$ invariant; while by orthogonality, such a rotation also leaves the orthogonal complement invariant and hence is of the prescribed form.

If $k = 2$, then $R = \emptyset$ and $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R)) = \mathrm{O}(n)$. By a classical result of Schoenberg [Sch42], each positive $\mathrm{O}(n)$-invariant kernel $K : S^{n-1} \times S^{n-1} \longrightarrow \mathbb{R}$ is of the form

$$K(x, y) = \sum_{l=0}^{\infty} a_l P_l^n(x \cdot y)$$

for some nonnegative numbers $a_0, a_1, \ldots$ with absolute and uniform convergence, where P_l^n is the Gegenbauer polynomial of degree l in dimension n normalized so that $P_l^n(1) = 1$ (equivalently, P_l^n is the Jacobi polynomial with both parameters equal to $(n-3)/2$).

Kernels invariant under the stabilizer of one point were considered by Bachoc and

Vallentin [BV08] and kernels invariant under the stabilizer of more points were considered by Musin [Mus14]. The analogue of Schoenberg's theorem for kernels invariant under the stabilizer of one or more points is stated in terms of certain polynomials $P_l^{n,m}$, which were called by Musin [Mus14] "multivariate Gegenbauer polynomials".

For $0 \le m \le n-2$, $t \in \mathbb{R}$, and $u, v \in \mathbb{R}^m$, the polynomial $P_l^{n,m}$ is the $(2m+1)$-variable polynomial

$$P_l^{n,m}(t,u,v) = \big((1-\|u\|^2)(1-\|v\|^2)\big)^{l/2} P_l^{n-m}\left(\frac{t-u\cdot v}{\sqrt{(1-\|u\|^2)(1-\|v\|^2)}}\right),$$

where $\|v\| = \sqrt{v \cdot v}$. If we use the convention $\mathbb{R}^0 = \{0\}$, then $P_l^n(t) = P_l^{n,0}(t,0,0)$. Since the Gegenbauer polynomials are odd or even according to the parity of l, the function $P_l^{n,m}(t,u,v)$ is indeed a polynomial in the variables u, v, and t. Musin [Mus14] denotes $P_l^{n,m}$ by $G_l^{(n,m)}$ and Bachoc and Vallentin [BV08] denote $P_l^{n,1}$ by Q_l^{n-1}.

Fix $d \ge 0$, let $\mathcal{B}_l$ be a basis of the space of m-variable polynomials of degree at most l (e.g. the monomial basis), and write $z_l(u)$ for the column vector containing the polynomials in $\mathcal{B}_l$ evaluated at $u \in \mathbb{R}^m$. Let $Y_l^{n,m}$ be the matrix of polynomials

$$Y_l^{n,m}(t,u,v) = P_l^{n,m}(t,u,v) z_{d-l}(u) z_{d-l}(v)^\mathsf{T}.$$

The choice of d makes $Y_l^{n,m}$ a $\binom{d-l+m}{m} \times \binom{d-l+m}{m}$ matrix with $(2m+1)$-variable polynomials of degree at most $2d$ as its entries.

Given a matrix X with linearly independent columns, set $L(X) = B^{-1}X^\mathsf{T}$, where B is the matrix such that BB^T is the Cholesky factorization of $X^\mathsf{T}X$, which is unique since $X^\mathsf{T}X$ is positive definite. For each $R \in \mathcal{R}_{k-2}$, fix a matrix A_R whose columns are the vectors of R in some order. The rows of $L(A_R)$ span the same space as the columns of A_R because B is invertible, and by construction the rows of $L(A_R)$ are orthonormal:

$$L(A_R)L(A_R)^\mathsf{T} = B^{-1}A_R^\mathsf{T}A_R B^{-\mathsf{T}} = B^{-1}BB^\mathsf{T}B^{-\mathsf{T}} = I.$$

Therefore, for $x \in \mathbb{R}^n$, $L(A_R)x$ is a vector with the coordinates of the projection of x onto $\operatorname{span}(R)$ with respect to an orthonormal basis of the linear span.

The following theorem is a restatement of a result of Musin [Mus14, Corollary 3.2] in terms of invariant kernels and with adapted notation. We will only use the sufficiency part of the statement, proved in Section 2.3.2 for completeness.

For square matrices A, B of the same dimensions, write $\langle A, B\rangle = \operatorname{tr}(A^\mathsf{T}B)$ for their Frobenius inner product.

Theorem 4.4.1. *Let $R \subseteq S^{n-1}$ with $m = \dim(\operatorname{span}(R)) = |R| \le n-2$ and let A_R be a matrix whose columns are the vectors of R in some order. Fix $d \ge 0$ and, for each $0 \le l \le d$, let F_l be a positive semidefinite matrix with $\binom{d-l+m}{m}$ rows and columns. Then $K : S^{n-1} \times S^{n-1} \longrightarrow \mathbb{R}$ given by*

$$K(x,y) = \sum_{l=0}^{d} \Big\langle F_l, Y_l^{n,m}(x\cdot y, L(A_R)x, L(A_R)y)\Big\rangle \tag{4.11}$$

is a positive, continuous, and $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$*-invariant kernel. Conversely, every* $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$*-invariant kernel* $K \in C(S^{n-1} \times S^{n-1})_{\geq 0}$ *can be uniformly approximated by kernels of the above form.*

Theorem 4.4.1 gives us a parameterization of $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$-invariant kernels. To get a parameterization of $\mathrm{Stab}_{\mathrm{O}(n)}(R)$-invariant kernels we still have to deal with the symmetries in $\mathcal{S}_R$. By construction, for an orthogonal matrix $\sigma \in \mathcal{S}_R$ there is a permutation matrix P_σ such that $\sigma A_R = A_R P_\sigma$. Since $\sigma \in \mathrm{O}(n)$ and $A_R^\mathsf{T} A_R = A_R^\mathsf{T} \sigma^\mathsf{T} \sigma A_R = P_\sigma^\mathsf{T} A_R^\mathsf{T} A_R P_\sigma$, the elements of $\mathcal{S}_R$ correspond precisely to the symmetries of the Gram matrix $A_R^\mathsf{T} A_R$ under simultaneous permutations of rows and columns. Indeed, if the Gram matrix $A_R^\mathsf{T} A_R$ is invariant under a certain simultaneous permutation of rows and columns, then since R is linearly independent, this permutation defines a linear transformation of $\mathrm{span}(R)$ that preserves all inner products between vectors of R, whence it is orthogonal and therefore corresponds to an element of $\mathcal{S}_R$. This observation leads to the following corollary.

Corollary 4.4.2. *Let* $R \subseteq S^{n-1}$ *with* $m = \dim(\mathrm{span}(R)) = |R| \leq n-2$ *and let* A_R *be a matrix whose columns are the vectors of* R *in some order. Fix* $d \geq 0$ *and, for each* $0 \leq l \leq d$*, let* F_l *be a positive semidefinite matrix with* $\binom{d-l+m}{m}$ *rows and columns. Then* $K : S^{n-1} \times S^{n-1} \longrightarrow \mathbb{R}$ *given by*

$$K(x, y) = \sum_{l=0}^{d} \left\langle F_l, \Phi_l(R)(x, y) \right\rangle, \tag{4.12}$$

where

$$\Phi_l(R)(x, y) := \frac{1}{|\mathcal{S}_R|} \sum_{\sigma \in \mathcal{S}_R} Y_l^{n,m}(x \cdot y, L(A_R P_\sigma)x, L(A_R P_\sigma)y),$$

is a positive, continuous, and $\mathrm{Stab}_{\mathrm{O}(n)}(R)$*-invariant kernel.*

Proof. If K is given by (4.12), then by writing

$$K(x, y) = \frac{1}{|\mathcal{S}_R|} \sum_{\sigma \in \mathcal{S}_R} \sum_{l=0}^{d} \left\langle F_l, Y_l^{n,m}(x \cdot y, L(A_R P_\sigma)x, L(A_R P_\sigma)y) \right\rangle$$

we see using Theorem 4.4.1 that K is a sum of $|\mathcal{S}_R|$ positive, continuous, and $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$-invariant kernels, and hence it is itself positive, continuous, and $\mathrm{Stab}_{\mathrm{O}(n)}(\mathrm{span}(R))$-invariant.

Since, for every $\sigma \in \mathcal{S}_R$,

$$L(A_R P_\sigma)x = B^{-1} P_\sigma^\mathsf{T} A_R^\mathsf{T} x = B^{-1} A_R^\mathsf{T} \sigma^\mathsf{T} x = L(A_R)\sigma^\mathsf{T} x$$

(recall BB^T is the Cholesky decomposition of $A_R^\mathsf{T} A_R = (A_R P_\sigma)^\mathsf{T}(A_R P_\sigma)$), and since $x \cdot y = (\sigma^\mathsf{T} x) \cdot (\sigma^\mathsf{T} y)$, we have that

$$K(x, y) = \frac{1}{|\mathcal{S}_R|} \sum_{\sigma \in \mathcal{S}_R} K'(\sigma^\mathsf{T} x, \sigma^\mathsf{T} y), \tag{4.13}$$

where

$$K'(x, y) = \sum_{l=0}^{d} \left\langle F_l, Y_l^{n,m}(x \cdot y, L(A_R)x, L(A_R)y) \right\rangle.$$

Now it follows directly from (4.13) that K is $\mathrm{Stab}_{\mathrm{O}(n)}(R)$-invariant. □

4.5 Semidefinite programming formulations

Before giving the semidefinite programming formulations, let us discuss how the matrix-valued function $\Phi_l(R)(x, y)$ can be computed. We have

$$L(A_R P_\sigma)x = B^{-1} P_\sigma^{\mathsf{T}} A_R^{\mathsf{T}} x = B^{-1} P_\sigma^{\mathsf{T}} (A_R^{\mathsf{T}} x),$$

where BB^{T} is the Cholesky decomposition of $A_R^{\mathsf{T}} A_R = (A_R P_\sigma)^{\mathsf{T}} (A_R P_\sigma)$. This shows that $L(A_R P_\sigma)x$ depends only on the inner products between the vectors in the set $R \cup \{x\}$ and on the ordering of the columns of A_R. Since the size of R is bounded by $k - 2$, this also shows that all computations for setting up the problem can be done in a relatively small dimension depending on k and not on n.

4.5.1 An SDP formulation for spherical finite-distance sets

To write the full semidefinite programming formulation corresponding to (4.9), we use Corollary 4.4.2 together with the isomorphism from Proposition 4.3.1. Let $\mathcal{S}_{\succeq 0}^N$ denote the cone of $N \times N$ positive semidefinite matrices. If for $R \in \mathcal{R}_{k-2}$ and $0 \leq l \leq d$ we have $F_{R,l} \in \mathcal{S}_{\succeq 0}^N$, where $N = \binom{d-l+|R|}{|R|}$, then $T : S^{n-1} \times S^{n-1} \times I_{k-2} \longrightarrow \mathbb{R}$ given by

$$T(x, y, Q) = \sum_{l=0}^{d} \left\langle F_{\gamma_Q Q, l}, \Phi_l(\gamma_Q Q)(\gamma_Q x, \gamma_Q y) \right\rangle$$

is a function in $C(S^{n-1} \times S^{n-1} \times I_{k-2})_{\succeq 0}^{\mathrm{O}(n)}$ and hence, for $S \in \mathcal{R}_k \setminus \{\emptyset\}$, the expression for $B_k T(S)$ becomes

$$\begin{aligned} B_k T(S) &= \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S \\ \{x,y\} \cup Q = S}} T(x, y, Q) \\ &= \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S \\ \{x,y\} \cup Q = S}} \sum_{l=0}^{d} \left\langle F_{\gamma_Q Q, l}, \Phi_l(\gamma_Q Q)(\gamma_Q x, \gamma_Q y) \right\rangle \\ &= \sum_{\substack{Q \subseteq S \\ |Q| \leq k-2}} \sum_{l=0}^{d} \left\langle F_{\gamma_Q Q, l}, \sum_{\substack{x,y \in S \\ \{x,y\} \cup Q = S}} \Phi_l(\gamma_Q Q)(\gamma_Q x, \gamma_Q y) \right\rangle. \end{aligned}$$

Since the action of $\mathrm{O}(n)$ on $S^{n-1} \simeq I_{=1}$ is transitive, the quotient $I_{=1}/\mathrm{O}(n)$ has only one element. We set $\mathcal{R}_1 \setminus \mathcal{R}_0 = \{e_1\}$, where e_1 is the first canonical basis vector of $\mathbb{R}^n$. We replace the objective $1 + \lambda$ in (4.9) by $1 + B_k T(\{e_1\})$, which we can further simplify by noticing that $Y_0^{n,1}(1, 1, 1)$ is the all-ones matrix J_{d+1} of size $(d + 1) \times (d + 1)$ and $Y_l^{n,1}(1, 1, 1)$ is the zero matrix for $l > 0$. This gives the semidefinite programming formulation

$$\min \left\{ 1 + \sum_{l=0}^{d} F_{\emptyset,l} + \langle F_{\{e_1\},0}, J_{d+1} \rangle \; : \; F_{R,l} \in \mathcal{S}_{\succeq 0}^{\binom{d-l+|R|}{|R|}} \text{ for } 0 \leq l \leq d \text{ and } R \in \mathcal{R}_{k-2}, \right.$$

$$\sum_{\substack{Q\subseteq S\\|Q|\leq k-2}} \sum_{l=0}^{d} \Big\langle F_{\gamma_Q Q,l}, \sum_{\substack{x,y\in S\\ \{x,y\}\cup Q=S}} \Phi_l(\gamma_Q Q)(\gamma_Q x, \gamma_Q y)\Big\rangle \leq -2\mathbb{1}_{I_{=2}}(S) \text{ for } S\in \mathcal{R}_k\setminus\mathcal{R}_1 \Bigg\}.$$

For each fixed d this gives an upper bound for $\Delta_k(G)^*$ that converges to $\Delta_k(G)^*$ as d tends to infinity.

We give an efficient Julia [Bez+17] implementation to generate the semidefinite programming input files for the solver, which was essential to make computations with $k = 6$. This includes an efficient function for generating the representatives of the independent sets, a function for checking whether two sets of vectors are in the same orbit, an implementation of the function $\mathcal{F}$ that works entirely in dimension k, and finally a function for setting up the semidefinite programming problems, which works for general n, finite D, and k.

4.5.2 A precise connection between the Bachoc-Vallentin bound and the Lasserre hierarchy

The bound $\Delta_2(G)^*$ immediately reduces to the generalization of the Lovász ϑ number as given by Bachoc, Nebe, Oliveira, and Vallentin [Bac+09], which coincides with the LP bound [DGS77] after symmetry reduction. Here we show that $\Delta_3(G)^*$ can be interpreted as a nonsymmetric version of the Bachoc-Vallentin 3-point bound [BV08].

Suppose T is feasible for $\Delta_3(G)^*$. If $S = \{a, b\}$ with $a \neq b$, then

$$\begin{aligned} B_3T(\{a,b\}) &= \sum_{\substack{Q\subseteq S\\|Q|\leq 1}} \sum_{\substack{x,y\in S\\ Q\cup\{x,y\}=S}} T(x,y,Q)\\ &= T(a,b,\emptyset) + T(b,a,\emptyset) + T(a,b,\{a\}) + T(b,a,\{a\})\\ &\quad + T(b,b,\{a\}) + T(a,b,\{b\}) + T(b,a,\{b\}) + T(a,a,\{b\}). \end{aligned}$$

By using $T(x,y,\emptyset) = \sum_{l=0}^d F_{\emptyset,l} P_l^n(x\cdot y)$ and

$$\begin{aligned} T(x,y,\{z\}) &= \sum_{l=0}^{d} \Big\langle F_{\{e_1\},l}, \Phi_l\big(\{e_1\}\big)(\gamma_{\{z\}}x, \gamma_{\{z\}}y)\Big\rangle\\ &= \sum_{l=0}^{d} \Big\langle F_{\{e_1\},l}, Y_l^{n,1}(x\cdot y, x\cdot z, y\cdot z)\Big\rangle, \end{aligned}$$

we see that

$$B_3T(\{a,b\}) = 2\sum_{l=0}^{d} F_{\emptyset,l}P_l^n(a\cdot b) + 6\sum_{l=0}^{d} \Big\langle F_{\{e_1\},l}, S_l^n(a\cdot b, a\cdot b, 1)\Big\rangle,$$

where we use the notation $S_l^n = \frac{1}{6}\sum_{\sigma\in S_3} \sigma Y_l^{n,1}$, in which σ runs through the group of all permutations of three variables and acts on $Y_l^{n,1}$ by permuting its arguments.

If $|S| = 3$, say $S = \{a, b, c\}$, then

$$\begin{aligned} B_3 T(\{a,b,c\}) &= \sum_{\substack{Q \subseteq S \\ |Q| \le 1}} \sum_{\substack{x,y \in S \\ Q \cup \{x,y\} = S}} T(x,y,Q) \\ &= T(a,b,\{c\}) + T(b,a,\{c\}) + T(a,c,\{b\}) \\ &\quad + T(c,a,\{b\}) + T(b,c,\{a\}) + T(c,b,\{a\}) \\ &= 6 \sum_{l=0}^{d} \big\langle F_{\{e_1\},l}, S_l^n(a \cdot b, a \cdot c, b \cdot c) \big\rangle. \end{aligned}$$

Using the above expressions we see that the constraints $B_3 T(S) \le -2$ for $S \in I_{=2}$ and $B_3 T(S) \le 0$ for $S \in I_{=3}$ in $\Delta_3(G)^*$ are exactly the ones that appear in Theorem 4.2 of Bachoc and Vallentin [BV08]. Except for the presence of an *ad hoc* 2×2 matrix variable b that comes from a separate argument, both bounds are identical.

Remark 4.5.1. Recall that for our method it is essential that $I_{k-2}/\mathrm{O}(n)$ be finite and that $I_{=m}/\mathrm{O}(n)$ can be represented by the set of $m \times m$ positive semidefinite matrices of rank at most n with ones in the diagonal and elements of D elsewhere, up to simultaneous permutations of the rows and columns. So $I_{k-2}/\mathrm{O}(n)$ is finite for $k = 2, 3$, but infinite whenever D is infinite and $k \ge 4$. This explains why it is not clear how to compute a 4-point bound generalization of the LP [DGS77] and SDP [BV08] bounds for the size of spherical codes with given minimal angular distance. For the spherical finite-distance problem, however, the set $I_{k-2}/\mathrm{O}(n)$ is always finite, so that we can perform computations beyond $k = 3$.

4.6 Two-distance sets and equiangular lines

If $D = \{a, -a\}$ for some $0 < a < 1$, then the vectors in a spherical D-code correspond to a set of equiangular lines with common angle $\arccos a$. We set

$$M_a(n) = A\big(n, \{a, -a\}\big)$$

and write

$$M(n) = \max_{0<a<1} M_a(n)$$

for the maximum number of equiangular lines in $\mathbb{R}^n$ with any common angle.

A semidefinite programming bound based on the method of Bachoc and Vallentin [BV08], and hence equivalent to $\Delta_3(G)^*$, was applied to this problem by Barg and Yu [BY14] (see also the table computed by King and Tang [KT19]) which, together with previous results, determines $M(n)$ for most $n \le 43$.

Barg and Yu present [BY13, Eqs. (14)–(17)] a semidefinite programming formulation that corresponds exactly to the formulation given in Section 4.5.1 when $k = 3$ (except for an *ad hoc* 2×2 matrix). In the other papers [BY14; KT19; OY16; Yu17] where this semidefinite program is considered, a primal version is given instead, which is less convenient from the perspective of rigorous verification of bounds.

n	$M(n)$	a	SDP bound	n	$M(n)$	a	SDP bound
2	3	1/2	3	17	48–49	1/5	51
3	6	$1/\sqrt{5}$	6	18	56–60	1/5	61
4	6	1/3, $1/\sqrt{5}$	6	19	72–74	1/5	76
5	10	1/3	10	20	90–94	1/5	96
6	16	1/3	16	21	126	1/5	126
7–13	28	1/3	28	22	176	1/5	176
14	28	1/3, 1/5	30	23–41	276	1/5	276
15	36	1/5	36	42	276–288	1/5, 1/7	288
16	40	1/5	42	43	344	1/7	344

Table 4.1: *Known values for $M(n)$ for small dimensions together with the cosine a of the common angle between the lines. The values known exactly were determined by several authors [BY14; GSY20; Haa48; LS73; LS66]. Most lower bounds are collected by Lemmens and Seidel [LS73], except for dimensions 18, 19, and 20 [Yu18], [Tay71, p.123]. The remaining upper bounds [Gre18; GSY20; GY19] do not rely on semidefinite programming.*

In this paper we compute new upper bounds for $M_a(n)$ for $a = 1/5$, $1/7$, $1/9$, and $1/11$ and many values of n using $\Delta_k(G)^*$ with $k = 4$, 5, and 6. The results do not improve the known bounds for $M(n)$ but greatly improve the known bounds for $M_a(n)$ for certain ranges of dimensions; these results are presented in Section 4.6.2.

4.6.1 Overview of the literature

The literature on equiangular lines is vast; here is a summary.

Bounds for $M(n)$

The interest in $M(n)$ started with Haantjes [Haa48], who showed $M(3) = M(4) = 6$ in 1948. Since then, much progress has been made using different techniques, and $M(n)$ has been determined for many values of $n \le 43$. Table 4.1 presents the known values for $M(n)$ for small dimensions.

The most general bound for $M(n)$, called the *absolute bound*, is due to Gerzon:

Theorem 4.6.1 (Gerzon, cf. Lemmens and Seidel [LS73]). *We have*

$$M(n) \le \frac{n(n+1)}{2}.$$

Moreover, if equality holds, then $n = 2$, $n = 3$, or $n = l^2 - 2$ for some odd integer l and the cosine of the common angle is $a = 1/l$.

The four cases where it is known that the bound is attained are $n = 2, 3, 7$, and 23. Delsarte, Goethals and Seidel [DGS77, Example 8.3] show that equality holds if and only if the union of the code with its antipodal code is a tight spherical 5-design, and in this case Cohn and Kumar [CK07] show this union is a universally optimal code (which means it minimizes every completely monotonic potential function in the squared chordal distance). Bannai, Munemasa, and Venkov [BMV04] and Nebe and Venkov [NV12] show that there are infinitely many odd integers l for which no tight spherical 5-design exists in S^{n-1} with $n = l^2 - 2$, so that Gerzon's bound cannot be attained in those dimensions. This list starts with $l = 7, 9, 13, 21, 25, 45, 57, 61, 69, 85, 93, \ldots$ (resp. $n = 47, 79, 167, 439, 623, 2023, 3247, 3719, 4759, 7223, 8647, \ldots$). For the remaining possible dimensions, attainability is an open problem.

For the dimensions that are not of the form $l^2 - 2$ for some odd integer l, the absolute bound can be improved:

Theorem 4.6.2 (Glazyrin and Yu [GY18] and King and Tang [KT19])**.** *Let l be the unique odd integer such that $l^2 - 2 \le n \le (l+2)^2 - 3$. Then,*

$$M(n) \le \begin{cases} \dfrac{n(l+1)(l+3)}{(l+2)^2 - n}, & n = 44, 45, 46, 76, 77, 78, 117, 118, 166, 222, 286, 358; \\[2ex] \dfrac{(l^2-2)(l^2-1)}{2}, & \textit{for all other } n \ge 44. \end{cases}$$

Furthermore, if the bound is attained, then the cosine of the angle between the lines is $a = 1/(l+2)$ for the first case and $a = 1/l$ for the second.

Glazyrin and Yu also proved another theorem [GY18, Theorem 4] about the codes that attain the bound from Theorem 4.6.2:

Theorem 4.6.3 (Glazyrin and Yu [GY18])**.** *Suppose l is a positive odd integer. If X is a $\{1/l, -1/l\}$-spherical code of size $(l^2-2)(l^2-1)/2$ contained in S^{n-1} with $n \le 3l^2 - 16$, then X must belong to a (l^2-2)-dimensional subspace.*

Since $(l+2)^2 - 3 \le 3l^2 - 16$ for $l \ge 5$, this last theorem implies that if the second bound from Theorem 4.6.2 is attained, then Gerzon's bound also has to be attained for $n = l^2 - 2$. For the first two cases where tight spherical 5-designs do not exist, this implies $M(n) \le 1127$ for $47 \le n \le 75$ and $M(n) \le 3159$ for $79 \le n \le 116$. The following theorem is adapted from Larman, Rogers, and Seidel [LRS77, Theorem 2]:

Theorem 4.6.4 (Larman, Rogers, and Seidel [LRS77])**.** *We have*

$$M(n) \le \max\{2n+3, M_{1/3}(n), M_{1/5}(n), \ldots, M_{1/l}(n)\},$$

where l is the largest odd integer such that $l \le \sqrt{2n}$.

Most of the results for $M(n)$ rely on Theorem 4.6.4, which shows that to bound $M(n)$ one just has to consider finitely many angles. This motivates the consideration of $M_a(n)$ when $1/a$ is an odd integer.

Bounds for $M_a(n)$

Bounds for fixed a are known as relative bounds, as opposed to Gerzon's absolute bound from Theorem 4.6.1. The first relative bound is due to van Lint and Seidel [LS66]:

Theorem 4.6.5 (van Lint and Seidel [LS66])**.** *If $n < 1/a^2$, then*

$$M_a(n) \leq \frac{n(1-a^2)}{1-na^2}.$$

As shown by Glazyrin and Yu [GY18, Theorem 5], Theorem 4.6.5 can be derived from the positivity of the Gegenbauer polynomials P_2^n, and indeed this is the bound given by the semidefinite programming techniques when $n \leq 1/a^2 - 2$. This bound is also the first case of Theorem 4.6.2.

After computing the semidefinite programming bound for many values of n and a, Barg and Yu [BY14] observed long ranges $1/a^2 - 2 \leq n \leq 3/a^2 - 16$ where the bound remained stable, matching Gerzon's bound (Theorem 4.6.1) at $n = 1/a^2 - 2$. Based on this observation, Yu [Yu17] proved the following theorem:

Theorem 4.6.6 (Yu [Yu17])**.** *If $n \leq 3/a^2 - 16$ and $a \leq 1/3$, then*

$$M_a(n) \leq \frac{(1/a^2-2)(1/a^2-1)}{2}.$$

An alternative proof for the previous theorem is given by Glazyrin and Yu [GY18, Theorem 6], where the use of the positivity of the Gegenbauer polynomials P_1^{n-1} and P_3^{n-1} is made more explicit. The bounds given by the semidefinite programming method were also used to prove the following theorem:

Theorem 4.6.7 (Okuda and Yu [OY16])**.** *If $3/a^2 - 16 \leq n \leq 3/a^2 + 6/a + 1$, then*

$$M_a(n) \leq 2 + \frac{(n-2)(1/a+1)^3}{(3/a^2 - 6/a + 2) - n}.$$

The bounds from Theorems 4.6.5, 4.6.6, and 4.6.7 coincide with the values given by the semidefinite programming formulation when $k = 3$ (see the points labeled "$\Delta_3(G)^*$ [BY14; KT19]" in Figures 4.1–4.4). Another source of relative bounds is a technique called pillar decomposition, introduced by Lemmens and Seidel [LS73] and used to determine $M_{1/3}(n)$:

Theorem 4.6.8 (Lemmens and Seidel [LS73])**.** *If $n \geq 15$, then*

$$M_{1/3}(n) = 2n - 2.$$

For $a = 1/5$, they obtained results that lead to the following conjecture:

Conjecture 4.6.9 (Lemmens and Seidel [LS73]). *We have*

$$M_{1/5}(n) = \begin{cases} 276 & \text{for } 23 \leq n \leq 185; \\ \lfloor \frac{3}{2}(n-1) \rfloor & \text{for } n \geq 185. \end{cases}$$

Note that 276 is the bound given by Theorem 4.6.6 when $a = 1/5$ and this shows (together with the fact that there exists a $\{-1/5, 1/5\}$-code of size 276 in dimension $n = 23$) that the conjecture is true for $n \leq 59$. In fact, the semidefinite programming bound computed by Barg and Yu [BY14] also shows $M_{1/5}(60) = 276$. Neumaier [Neu89] (see also [Gre+16, Corollary 6.6]) proved that there exists a large N such that $M_{1/5}(n) = \lfloor \frac{3}{2}(n-1) \rfloor$ for all $n > N$. Neumaier claimed, without a proof, that N should be at most 30251.

Recently, Lin and Yu [LY19] made progress in this conjecture by proving some claims from Lemmens and Seidel [LS73]. The only case still open is when the code has a set with 4 unit vectors with mutual inner products $-1/5$ and no such set with 5 unit vectors (up to replacement of some vectors by their antipodes).

Glazyrin and Yu [GY18] introduced a new method to derive upper bounds for spherical finite-distance sets. By using Gegenbauer polynomials together with the polynomial method, they proved a theorem that, specialized for two-distance sets, is:

Theorem 4.6.10 (Glazyrin and Yu [GY18]). *For all a, b, and n, we have*

$$A\big(n, \{a, b\}\big) \leq \frac{n+2}{1 - (n-1)/(n(1-a)(1-b))}$$

whenever the right-hand side is positive.

With this result, they proved the following relative bound, which provides the best bounds for moderately large values of n (see Figures 4.2–4.4):

Theorem 4.6.11 (Glazyrin and Yu [GY18]). *If $a \leq 1/3$, then*

$$\begin{aligned} M_a(n) &\leq n\left(\frac{(a^{-1}-1)(a^{-1}+2)^2}{3a^{-1}+5} + \frac{(a^{-1}+1)(a^{-1}-2)^2}{3a-5} + 2\right) + 2 \\ &\leq n\left(\frac{2}{3}a^{-2} + \frac{4}{7}\right) + 2. \end{aligned}$$

King and Tang [KT19] improved the pillar decomposition technique and got a better bound for $M_{1/5}(n)$ [KT19, Theorem 7]. Recently, Lin and Yu [LY19] further improved parts of their argument; by combining [LY19, Proposition 4.5] with the proof of [KT19, Theorem 7] we get:

Theorem 4.6.12 (Lin and Yu [LY19]). *If $n \geq 63$, then*

$$M_{1/5}(n) \leq 100 + 3A(n-4, \{1/13, -5/13\}).$$

The previous results give three competing methods to bound $M_{1/5}(n)$, each one being the best for a different range of dimensions. One can either use semidefinite programming to bound $M_{1/5}(n)$ directly, use Theorem 4.6.12 together with semidefinite programming to bound $A\big(n-4, \{1/13, -5/13\}\big)$, or use Theorem 4.6.10. King and Tang [KT19] made this comparison, computing the semidefinite programming bound $\Delta_3(G)^*$. See in Table 4.3 and in Figure 4.1 the comparison with the new semidefinite programming bound $\Delta_6(G)^*$.

Regarding asymptotic results, it is known that $M(n)$ is asymptotically quadratic in n: a quadratic lower bound in which the cosine of the angle between the lines, a, tends to zero as n increases can be found in [Gre+16, Corollary 2.8], while Theorem 4.6.1 gives a quadratic upper bound. For fixed a we have that $M_a(n)$ is linear in n. Bukh [Buk16] was the first to show a bound for $M_a(n)$ of the form $M_a(n) \le cn$, although with a large constant c. Theorem 4.6.11 has another linear bound good to give results for intermediate values of n, while the best asymptotic result is due to Jiang et al. [Jia+19]. They completely settled the value of $\lim_{n\to\infty} M_a(n)/n$ for every a in terms of a parameter called the *spectral radius order* $r(\lambda)$, which is defined for $\lambda > 0$ as the smallest integer r so there exists a graph with r vertices and adjacency matrix with largest eigenvalue exactly λ, and is defined $r(\lambda) = \infty$ in case no such graph exists.

Theorem 4.6.13 (Jiang et al. [Jia+19])**.** *Fix* $0 < a < 1$. *Let* $\lambda = (1-a)/(2a)$ *and* $r = r(\lambda)$ *be its spectral radius order. The maximum number* $M_a(n)$ *of equiangular lines in* $\mathbb{R}^n$ *with common angle* arccos a *satisfies*

(a) $M_a(n) = \lfloor r(n-1)/(r-1)\rfloor$ *for all sufficiently large* $n > n_0(a)$ *if* $r < \infty$.

(b) $M_a(n) = n + o(n)$ *as* $n \longrightarrow \infty$ *if* $r = \infty$.

Jiang et al. remarks that the $n_0(a)$ from their theorem may be really big, though. When $a = 1/(2r-1)$ for some positive integer r, then $\lambda = r-1$ and $r(\lambda) = r$ (since the complete graph on r vertices has spectral radius $r-1$). Theorem 4.6.13 confirms a conjecture made by Bukh [Buk16]:

Corollary 4.6.14 (Jiang et al. [Jia+19])**.** *If* $a = 1/(2r-1)$ *for some positive integer* $r \ge 2$, *then for all* n *sufficiently large,*

$$M_a(n) = \left\lfloor \frac{r(n-1)}{r-1} \right\rfloor.$$

There is a simple construction that achieves the value from Corollary 4.6.14. Let $a = 1/(2r-1)$ for some positive integer r and t, s be arbitrary positive integers. Then one can show that a matrix with t diagonal blocks, each of size r, and s diagonal blocks of size 1, with diagonal entries equal to 1, off-diagonal entries inside each block equal to $-a$, and all other entries equal to a is the Gram matrix of a $\{-a, a\}$-code in $S^{(r-1)t+s}$ of size $rt+s$. Letting $t = \lfloor (n-1)/(r-1)\rfloor$ and $s = n-1-(r-1)\lfloor (n-1)/(r-1)\rfloor$ we get the desired size.

4.6.2 New semidefinite programming bounds

As observed in Section 4.6, the semidefinite programming bounds computed by Barg and Yu [BY14] and King and Tang [KT19] correspond to $\Delta_3(G)^*$. In this paper we compute new upper bounds for $M_a(n)$ for $a = 1/5$, $1/7$, $1/9$, and $1/11$ and many values of n using

a	$(1/a^2-2)(1/a^2-1)/2$	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$
1/5	276	60	65	69	70
1/7	1128	131	145	158	169
1/9	3160	227	251	273	300
1/11	7140	347	381	413	448

Table 4.2: *By considering $\Delta_k(G)^*$ for $k \geq 4$ we find out that the maximum dimension n for which the bound $M_a(n) \leq (1/a^2-2)(1/a^2-1)/2$ is valid is larger than $3/a^2-16$ as given by Theorem 4.6.6 and $\Delta_3(G)^*$; the table shows the improved dimensions.*

$k = 4$, 5, and 6. Since every two-distance set with these angles and at most $k-2 \leq 4$ vectors is linearly independent, the assumption made in Section 4.4 is satisfied. We always use degree $d = 5$ for the polynomials since, as reported by Barg and Yu [BY13], no improvement is observed for larger values of d (but this may change if sets D with cardinality greater than 2 are considered). The semidefinite programs were produced using a script written in Julia [Bez+17] using Nemo [Fie+17], were solved with SDPA-GMP [Nak10], and the results were rigorously verified using the interval arithmetic library Arb [Joh17]. The rigorous verification procedure is much simpler than that for similar problems [Dos+17]. The scripts used to generate the programs and verify the results can be found with the arXiv version of this paper.

The results are presented in Figures 4.1–4.4 and Tables 4.3–4.6, where we compile the bounds for $M_a(n)$ for each n that is a multiple of 5; the best bounds are displayed in boldface. While it takes only a few seconds to generate and solve a single instance of the semidefinite programming problem for $k = 3$, the process takes about 5 days using a single core of an Intel i7-8650U processor for $k = 6$; that is why the tables have some missing values for $\Delta_6(G)^*$.

No improvements were obtained for $n \leq 3/a^2 - 16$; we observed in this case that $\Delta_6(G)^* = \Delta_3(G)^*$ which is equal to the values given by Theorems 4.6.5 and 4.6.6. Since this is the range of dimensions that influences $M(n)$, no improvements for $M(n)$ were obtained. We obtained great improvements for all dimensions $n > 3/a^2 - 16$, making the semidefinite programming bound competitive with the other methods (like Theorem 4.6.11) for more dimensions. Asymptotically, the semidefinite programming bounds behave badly, loosing even to Gerzon's bound.

In particular, we improved the range of dimensions for which the bound remains stable, showing that $n = 3/a^2 - 16$ from Theorem 4.6.6 is not optimal. Table 4.2 shows how much this range is increased for the values of a considered. This observation motivates the following two questions, where a is such that $1/a$ is an odd integer:

1. What is the smallest n such that $M_a(n) = (1/a^2-2)(1/a^2-1)/2$?
2. What is the smallest n such that $M_a(n) > (1/a^2-2)(1/a^2-1)/2$?

Question (1) is the more interesting of the two since if the smallest n is $1/a^2-2$, then

Gerzon's bound is attained. Theorem 4.6.3 makes progress in this direction, showing that Gerzon's bound is also attained if the smallest n is at most $3/a^2 - 16$; this is known not to be the case for many a (due to the nonexistence of some tight spherical 5-designs, as mentioned after Theorem 4.6.1), which implies $M_{1/7}(n) \leq 1127$ for $n \leq 131$ and $M_{1/9}(n) \leq 3159$ for $n \leq 227$. Table 4.2 also suggests that the constraint $n \leq 3/a^2 - 16$ in Theorem 4.6.3 may not be optimal.

Question (2) seems interesting because Table 4.2 shows that $n = 3/a^2 - 15$ is not a good candidate solution. In fact, the smallest n is likely much larger, as suggested by Conjecture 4.6.9 for $M_{1/5}(n)$ and the construction described after Corollary 4.6.14. Using this construction, we know that $(1/a^2-2)(1/a^2-1)/2$ is achieved when $n = (1/a^2-2)(1/a-1)^2/2+1$, which corresponds to the dimensions 185, 847, 2529, and 5951 for $a = 1/5$, 1/7, 1/9, and 1/11 respectively.

We also improve the bounds computed by King and Tang [KT19] for $M_{1/5}(n)$ by replacing their theorem [KT19, Theorem 7] by Theorem 4.6.12 and by using $\Delta_6(G)^*$ to compute better bounds for $A(n, \{1/13, -5/13\})$. Lin and Yu [LY19] observed that $A(n, \{1/13, -5/13\}) \geq 3n/2 - 3$ and therefore there is a limit to the power of this approach: it will never be able to prove Conjecture 4.6.9 no matter how much we increase k. In general, it is not clear how good the bound $\Delta_k(G)^*$ can be for $M_a(n)$ if one allows k to increase; in contrast, de Laat and Vallentin [LV15, Theorem 2] show that their version of the Lasserre hierarchy for compact topological packing graphs converges to the independence number if enough steps are computed. Whether such a convergence result holds for $\Delta_k(G)^*$ is an open question; in any case, it takes days to compute $\Delta_k(G)^*$ for $k = 6$, so one can expect that solving the resulting semidefinite programs for $k > 6$ will be hard in practice.

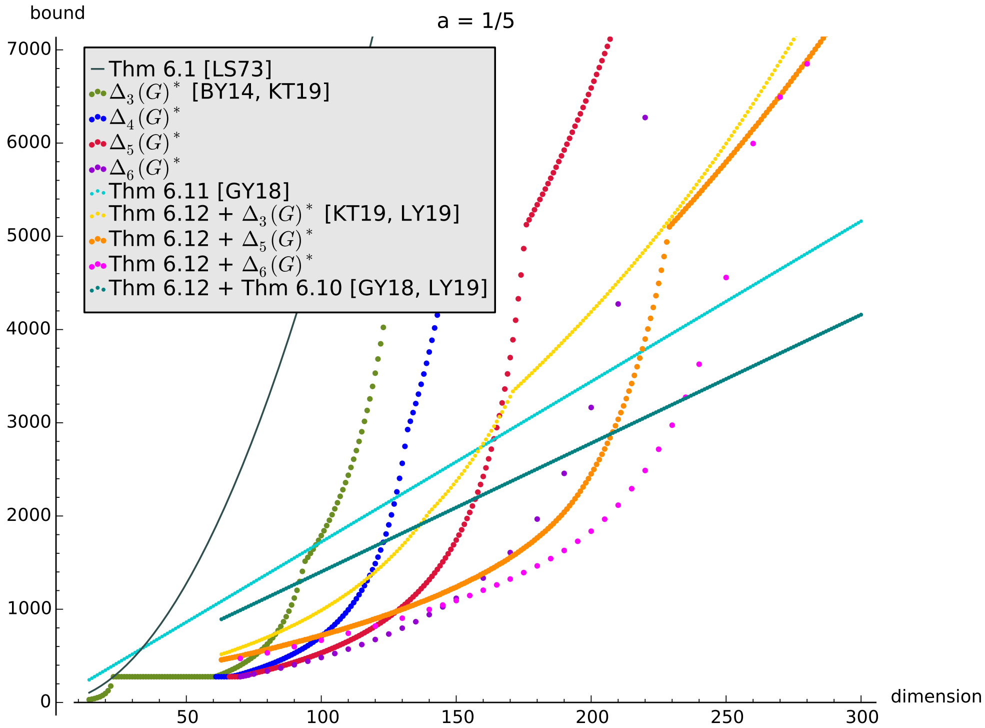

Figure 4.1: *Relative bounds for $M_{1/5}(n)$. In fact, King and Tang [KT19] computed a bound using $\Delta_3(G)^*$ together with a theorem [KT19, Theorem 7] weaker than Theorem 4.6.12; the result is similar though.*

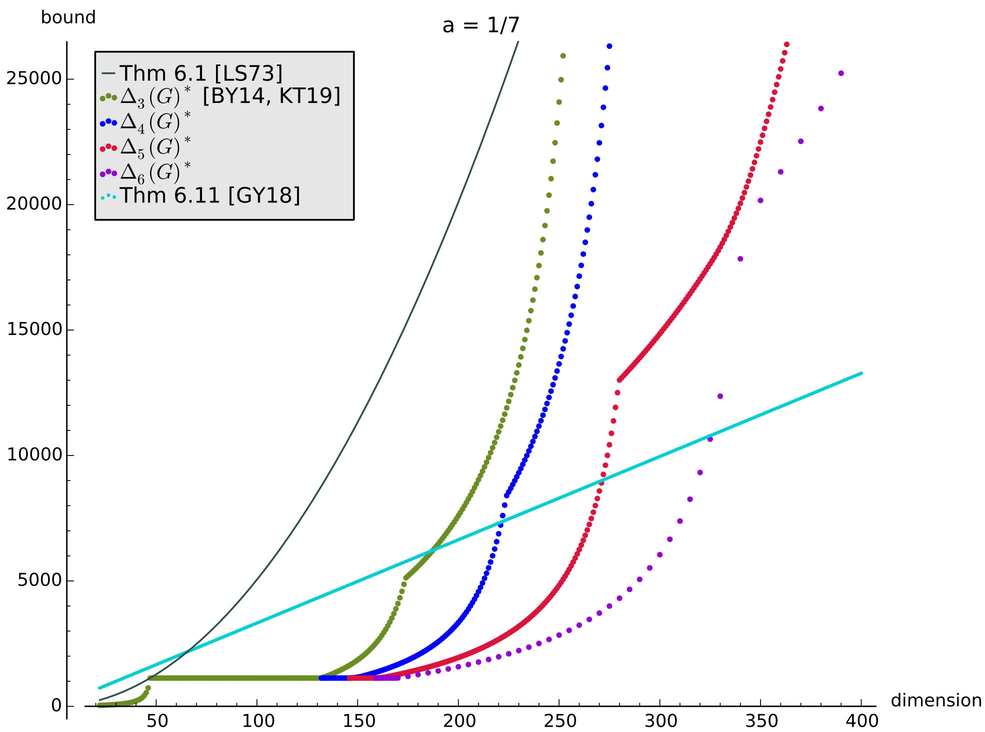

Figure 4.2: *Relative bounds for $M_{1/7}(n)$.*

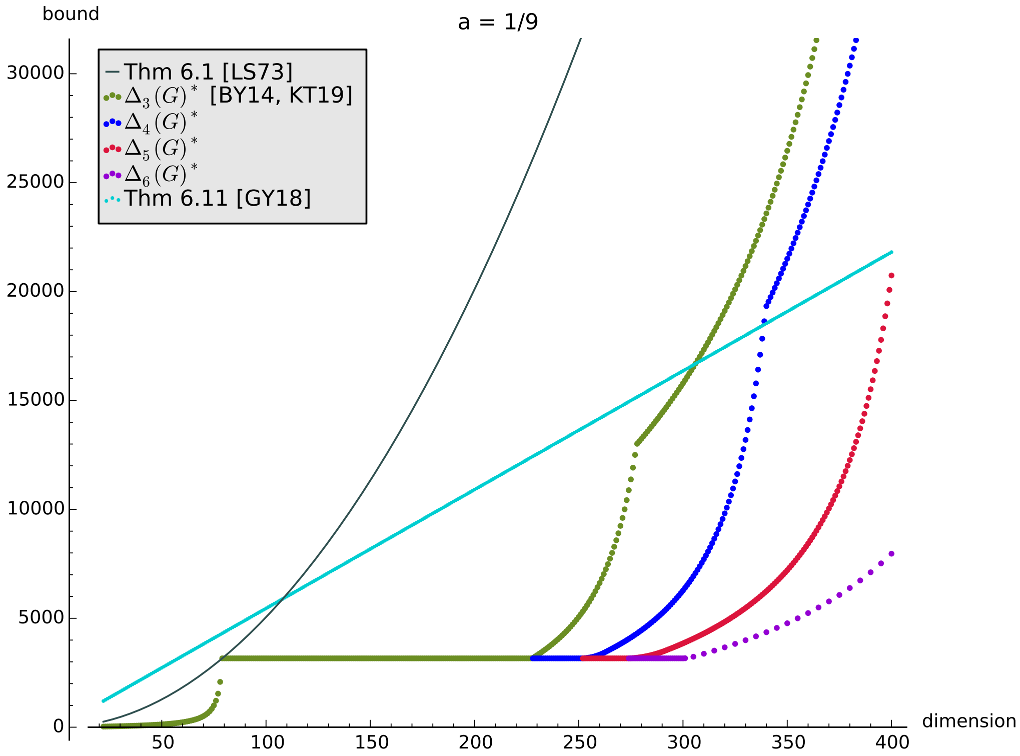

Figure 4.3: *Relative bounds for $M_{1/9}(n)$.*

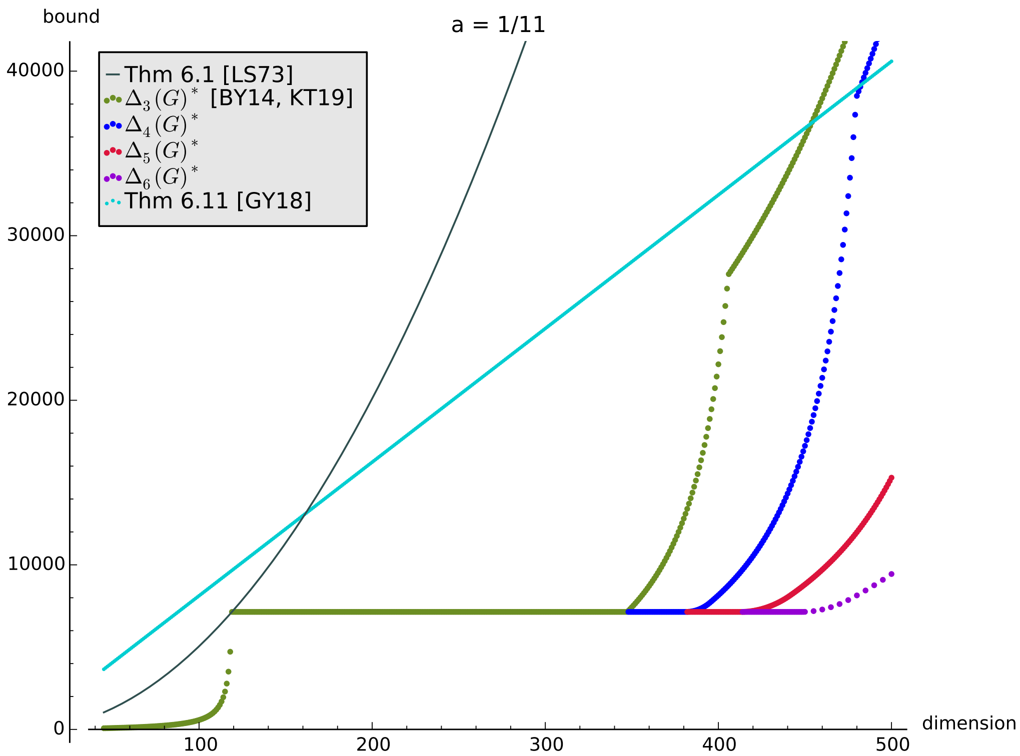

Figure 4.4: *Relative bounds for $M_{1/11}(n)$.*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.12 [LY19] + $\Delta_5(G)^*$**	**Thm 4.6.12 [LY19] + $\Delta_6(G)^*$**	**Thm 4.6.12 [LY19] + Thm 4.6.10 [GY18]**
60	**276**	**276**	**276**	**276**			
65	326	**276**	**276**	**276**	469		920
70	398	301	278	**276**	499	472	989
75	494	346	312	**305**	532		1057
80	626	397	348	**336**	568	532	1126
85	816	456	388	**369**	604		1195
90	1120	526	431	**404**	643	598	1264
95	1556	609	479	**442**	679		1333
100	1790	710	532	**482**	721	667	1402
105	2077	836	591	**525**	763		1471
110	2437	994	657	**572**	805	742	1540
115	2904	1203	732	**621**	850		1609
120	3532	1489	817	**675**	898	820	1677
125	4419	1905	915	**734**	946		1746
130	5770	2565	1028	**797**	1000	904	1815
135	8076	3206	1160	**866**	1054		1884
140	12896	3759	1317	**942**	1111	997	1953
145	29280	4450	1508	**1025**	1174	1045	2022
150		5307	1742	1117	1237	**1093**	2091
155		6131	2038		1309	**1147**	2160
160		6989	2424	1334	1384	**1204**	2229
165		8005	2948		1465	**1261**	2298
170		9166	3699	1608	1555	**1324**	2367
175		10401	4868		1654	**1393**	2436

Table 4.3: *Upper bounds for $M_{1/5}(n)$ by diverse methods, including new results with $\Delta_6(G)^*$. The best bound in each dimension is in boldface.*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.12 [LY19]** + $\Delta_5(G)^*$	**Thm 4.6.12 [LY19]** + $\Delta_6(G)^*$	**Thm 4.6.12 [LY19] + Thm 4.6.10 [GY18]**
180		11833	5339	1967	1765	**1465**	2504
185		13552	5623		1891	**1543**	2573
190		15647	5925	2457	2041	**1630**	2642
195		18244	6247		2224	**1729**	2711
200		21531	6591	3164	2452	**1837**	2780
205		25795	6960		2719	**1966**	2849
210		31508	7356	4274	3037	**2116**	2918
215		39487	7783		3421	**2293**	2987
220		51276	8243	6274	3898	**2488**	3056
225		70170	8741		4495	**2716**	3125
230		104611	9281	8667	5134	**2974**	3194
235			9870		5296	3274	**3263**
240			10514	9407	5458	3628	**3332**
245			11221		5626		**3401**
250			12001	10226	5797	4558	**3469**
255			12865		5971		**3538**
260			13828	11137	6148	5995	**3607**
265			14908		6328		**3676**
270			16128	12155	6511	6493	**3745**
275			17516		6700		**3814**
280			19122	13302	6889	6850	**3883**
285			21199		7084		**3952**
290			23982	14601	7285	7219	**4021**
295			27058		7489		**4090**
300			30840	16086	7696	7600	**4159**

Table 4.3: *continued*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**	n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**
125	**1128**	**1128**	**1128**	**1128**	4151	265	49145	19501	7254	**3465**	8797
130	**1128**	**1128**	**1128**	**1128**	4317	270	72667	22466	8584	**3717**	8963
135	1218	**1128**	**1128**	**1128**	4482	275	135319	26319	10427	**3998**	9129
140	1387	**1128**	**1128**	**1128**	4648	280		31427	13008	**4311**	9295
145	1593	**1128**	**1128**	**1128**	4814	285		36793	13442	**4663**	9461
150	1850	1163	**1128**	**1128**	4980	290		44064	13893	**5062**	9627
155	2178	1262	**1128**	**1128**	5146	295		54538	14363	**5519**	9793
160	2611	1381	1135	**1128**	5312	300		70925	14853	**6045**	9959
165	3211	1517	1188	**1128**	5478	305		100201	15364	**6660**	10125
170	4098	1670	1271	**1131**	5644	310			15897	**7386**	10291
175	5199	1846	1361	**1195**	5810	315			16453	**8257**	10457
180	5582	2051	1458	**1264**	5976	320			17035	**9322**	10623
185	6006	2290	1564	**1336**	6142	325			17644	**10653**	10789
190	6477	2575	1679	**1412**	6308	330			18309	12364	**10955**
195	7005	2919	1805	**1492**	6474	335			19106		**11121**
200	7597	3342	1944	**1578**	6640	340			20053	17840	**11287**
205	8269	3878	2097	**1668**	6806	345			21178		**11453**
210	9035	4575	2267	**1765**	6972	350			22494	20168	**11619**

Table 4.4: *Upper bounds for $M_{1/7}(n)$ by diverse methods, including new results with $\Delta_6(G)^*$. The best bound in each dimension is in boldface.*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**	n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**
215	9918	5522	2457	**1868**	7138	355			23893		**11785**
220	10946	6880	2670	**1978**	7304	360			25410	21307	**11951**
225	12158	8548	2911	**2096**	7470	365			27077		**12117**
230	13608	9314	3187	**2223**	7636	370			28923	22525	**12283**
235	15374	10181	3504	**2359**	7802	375			30981		**12449**
240	17571	11171	3872	**2507**	7968	380			33291	23833	**12615**
245	20378	12315	4307	**2667**	8134	385			35904		**12781**
250	24090	13652	4827	**2840**	8300	390			38885	25239	**12947**
255	29230	15238	5460	**3030**	8466	395			42316		**13112**
260	36818	17150	6247	**3237**	8632	400			46310	26756	**13278**

Table 4.4: *continued*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	Thm 4.6.11 [GY18]	n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	Thm 4.6.11 [GY18]
225	**3160**	**3160**	**3160**	**3160**	12269	315	18193	8654	4558	**3515**	17176
230	3306	**3160**	**3160**	**3160**	12542	320	19112	9815	4836	**3666**	17449
235	3642	**3160**	**3160**	**3160**	12814	325	20103	11281	5140	**3825**	17721
240	4035	**3160**	**3160**	**3160**	13087	330	21172	13192	5473	**3993**	17994
245	4502	**3160**	**3160**	**3160**	13360	335	22330	15784	5840	**4171**	18267
250	5063	**3160**	**3160**	**3160**	13632	340	23589	19333	6247	**4360**	18539
255	5752	3196	**3160**	**3160**	13905	345	24961	20385	6700	**4559**	18812
260	6617	3329	**3160**	**3160**	14177	350	26464	21506	7207	**4772**	19084
265	7737	3561	**3160**	**3160**	14450	355	28116	22707	7780	**4998**	19357
270	9243	3824	**3160**	**3160**	14723	360	29940	23999	8430	**5239**	19630
275	11377	4117	3167	**3160**	14995	365	31965	25395	9177	**5497**	19902
280	13235	4445	3219	**3160**	15268	370	34226	26911	10042	**5774**	20175
285	13816	4815	3317	**3160**	15540	375	36767	28563	11057	**6071**	20448
290	14434	5235	3461	**3160**	15813	380	39642	30373	12263	**6391**	20720
295	15091	5718	3647	**3160**	16086	385	42924	32365	13720	**6737**	20993
300	15791	6277	3849	**3160**	16358	390	46703	34571	15515	**7112**	21265
305	16538	6933	4067	**3235**	16631	395	51103	37026	17784	**7521**	21538
310	17336	7712	4302	**3372**	16904	400	56289	39779	20740	**7966**	21811

Table 4.5: *Upper bounds for $M_{1/9}(n)$ by diverse methods, including new results with $\Delta_6(G)^*$. The best bound in each dimension is in boldface.*

n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**	n	$\Delta_3(G)^*$ [BY14; KT19]	$\Delta_4(G)^*$	$\Delta_5(G)^*$	$\Delta_6(G)^*$	**Thm 4.6.11 [GY18]**
345	**7140**	**7140**	**7140**	**7140**	28011	425	30885	11309	7319	**7140**	34506
350	7426	**7140**	**7140**	**7140**	28417	430	31817	12186	7494	**7140**	34912
355	8028	**7140**	**7140**	**7140**	28823	435	32789	13185	7730	**7140**	35318
360	8715	**7140**	**7140**	**7140**	29229	440	33804	14332	8036	**7140**	35724
365	9506	**7140**	**7140**	**7140**	29635	445	34863	15665	8407	**7140**	36130
370	10426	**7140**	**7140**	**7140**	30041	450	35971	17232	8808	**7144**	36536
375	11511	**7140**	**7140**	**7140**	30447	455	37129	19100	9239	**7190**	36942
380	12809	**7140**	**7140**	**7140**	30853	460	38342	21365	9703	**7285**	37348
385	14389	7180	**7140**	**7140**	31259	465	39613	24170	10205	**7427**	37754
390	16354	7353	**7140**	**7140**	31665	470	40948	27732	10749	**7618**	38160
395	18866	7692	**7140**	**7140**	32071	475	42349	32408	11341	**7859**	38566
400	22187	8154	**7140**	**7140**	32477	480	43823	38495	11986	**8142**	38972
405	26786	8661	**7140**	**7140**	32883	485	45376	39896	12695	**8442**	39378
410	28304	9221	**7140**	**7140**	33289	490	47012	41346	13474	**8758**	39784
415	29130	9841	7146	**7140**	33695	495	48741	42853	14337	**9091**	40190
420	29990	10533	7204	**7140**	34100	500	50569	44424	15296	**9443**	40595

Table 4.6: *Upper bounds for $M_{1/11}(n)$ by diverse methods, including new results with $\Delta_6(G)^*$. The best bound in each dimension is in boldface.*

Chapter 5

The Fourier transform of a polytope

A *polyhedron* in $\mathbb{R}^d$ is any set defined by finitely many linear inequalities

$$\left\{(x_1,\dots,x_d)\in\mathbb{R}^d \;:\; a_{j1}x_1+\cdots+a_{jd}x_d\le b_j,\ j\in J\right\}, \tag{5.1}$$

with a_{ji}, $b_j\in\mathbb{R}$ and $|J|<\infty$. See Lecture 1 from Ziegler [Zie95] for the main facts and terminology about polyhedra. In particular, a bounded polyhedron is a *polytope*, which can also be described as the convex hull of a finite set of points [Zie95, Theorem 1.1]. The *dimension* $\dim(P)$ of a polytope P is the dimension of its affine hull. A *face* of a polytope P is any set of the form

$$F=P\cap\{(x_1,\dots,x_d)\in\mathbb{R}^d \;:\; a_1x_1+\cdots+a_dx_d=b\},$$

for a_i, $b\in\mathbb{R}$ such that $P\subset\{(x_1,\dots,x_d)\in\mathbb{R}^d \;:\; a_1x_1+\cdots+a_dx_d\le b\}$. A face of dimension 0 is a *vertex*, a face of dimension 1 is an *edge*, and a face of dimension $\dim(P)-1$ is a *facet* of P. We denote the set of all vertices of a polytope P by $V(P)$ and the set of all faces of a polytope by $\mathcal{F}(P)$. Note that $\emptyset, P\in\mathcal{F}(P)$.

A *rational polyhedron* is defined similarly to the polyhedra in (5.1), but with the additional requirement that the coefficients a_{ji}, $b_j\in\mathbb{Z}$. Similarly, we say that a subspace $V\subseteq\mathbb{R}^d$ is *rational* if it is defined by a set of equalities

$$V=\{x=(x_1,\dots,x_d)\in\mathbb{R}^d \;:\; a_{j1}x_1+\cdots+a_{jd}x_d=b_j,\ j\in J\},$$

with a_{ji}, $b_j\in\mathbb{Z}$ and $|J|\le d$. A polytope P is rational if and only if its vertices have rational coordinates, in this case there exists $m\in\mathbb{Z}$ such that $mP:=\{mx \;:\; x\in P\}$ is an *integer polytope*, a polytope that has vertices with integer coordinates.

In this chapter we study the Fourier transform of the indicator function of a d-dimensional polytope $P\subset\mathbb{R}^d$ (*Fourier transform of* P, for short), namely

$$\hat{\mathbb{1}}_P(\xi):=\int_P e^{-2\pi i\langle x,\xi\rangle}\,\mathrm{d}x.$$

As stated in Theorem 2.4.7, this function is uniformly continuous, $\hat{\mathbb{1}}_P(\xi) \longrightarrow 0$ as $\|\xi\| \longrightarrow \infty$ and $\sup_{\xi\in\mathbb{R}^d} |\hat{\mathbb{1}}_P(\xi)| = \mathrm{vol}(P) = \hat{\mathbb{1}}_P(0)$. Furthermore, since P is compact, by the dominated convergence theorem we may differentiate under the integral sign and conclude that $\hat{\mathbb{1}}_P$ is infinitely differentiable and analytic everywhere. In this chapter we discuss two common approaches to evaluate $\hat{\mathbb{1}}_P(\xi)$: the divergence and Brion's theorem. Both approaches are complementary in the sense that one uses information about the faces and the other uses the local information around the vertices of P.

As a motivating example, we mention the application of counting integer points in dilations of a convex body. For a d-dimensional compact convex body $C \subset \mathbb{R}^d$ and $t > 0$, let its *dilation* by t be $tC := \{tx : x \in C\}$ and

$$L_C(t) := |tC \cap \mathbb{Z}^d|$$

be its *integer point enumerator*. Since C is measurable, $L_C(t)$ grows as $\mathrm{vol}(C)t^d$ as $t \longrightarrow \infty$, however the difference

$$R_C(t) := L_C(t) - \mathrm{vol}(C)t^d \tag{5.2}$$

is much harder to estimate. Since $L_C(t) = \sum_{n\in\mathbb{Z}^d} \mathbb{1}_{tC}(n)$, in view of the Poisson summation formula (2.30), it is tempting to consider

$$\sum_{\xi\in\mathbb{Z}^d} \hat{\mathbb{1}}_{tC}(\xi) = \mathrm{vol}(C)t^d + \sum_{\xi\in\mathbb{Z}^d\setminus\{0\}} t^d \hat{\mathbb{1}}_C(t\xi),$$

and use the last series to estimate $R_C(t)$. Unfortunately this procedure is not correct, since $\mathbb{1}_{tC}$ does not satisfy the hypothesis from Theorem 2.4.16. It is necessary to approximate the function using some kind of summability method, whose details differ in each work. We take $\epsilon > 0$, consider the Gaussian $\phi_{d,\epsilon}(x) := \epsilon^{-d/2}e^{-\pi\|x\|^2/\epsilon}$ and let $\mathbb{1}_{tC} * \phi_{d,\epsilon}$ be an approximation for $\mathbb{1}_{tC}$ as $\epsilon \longrightarrow 0$. When C is a polytope, the first part of Lemma 2.5.2 shows that the approximation $\lim_{\epsilon\to 0} \mathbb{1}_{tC} * \phi_{d,\epsilon}(x)$ is equal to $\omega_{tC}(x)$, the solid angle of tC at x, which is equal to 1 if x is in the interior of tC, 0 if $x \notin tC$ and $0 < \omega_{tC}(x) < 1$ when x is in the boundary of tC.

For each fixed $\epsilon > 0$, Theorem 2.4.16 can be applied and with Lemma 2.5.2 we get

$$\sum_{n\in\mathbb{Z}^d} \omega_{tC}(n) - t^d\mathrm{vol}(C) = \lim_{\epsilon\longrightarrow 0} \sum_{\xi\in\mathbb{Z}^d\setminus\{0\}} t^d \hat{\mathbb{1}}_C(t\xi)\hat{\phi}_{d,\epsilon}(t\xi).$$

In order to estimate $R_C(t)$ with this approach, one has to compare the solid angle sum with $L_C(t)$ and study $\hat{\mathbb{1}}_C$ with more detail to estimate the series in the right-hand side.

When B is the unit disc in $\mathbb{R}^2$, the determination of $R_B(t)$ is the famous *Gauss circle problem*. In Section 8.3 of Travaglini [Tra14], the method outlined above is used to shown the result from Sierpinski:

$$|R_B(t)| := \left||\{n \in \mathbb{Z}^2 : \|n\| \le t\}| - \pi t^2\right| = O(t^{2/3}),$$

using the estimate $|\hat{\mathbb{1}}_B(\xi)| \le c(1 + |\xi|^{3/2})^{-1}$ for some $c > 0$. In Chapter 6, this method is used to study $R_P(t)$ when P is a rational polytope. In [Ran97], Randol uses this method to study $R_P(t)$ for a certain class of irrational polytopes.

Another application for the Fourier transform of a polytope is the production of interpolation formulas for bandlimited functions. See e.g., the work of Petersen and Middleton [PM62], or Chapter 14 from Higgins [Hig96].

5.1 Combinatorial Stokes Formula

The first method to evaluate $\hat{\mathbb{1}}_P(\xi)$ uses the divergence theorem (Theorem 2.3.4). The formula for $\hat{\mathbb{1}}_P(\xi)$ is obtained applying Theorem 2.3.4 to the polytope P and the vector field $x \mapsto ce^{-2\pi i\langle x,\xi\rangle}$, where $c \in \mathbb{R}^d$ is any vector such that $\langle c, \xi\rangle \neq 0$. For each facet F of P, we denote by n_F the outer unit normal vector along the facet F and use d_F to denote the relative Lebesgue measure on $\mathrm{aff}(F)$, so we get:

$$\hat{\mathbb{1}}_P(\xi) = \int_P e^{-2\pi i\langle x,\xi\rangle}\,\mathrm{d}x = \frac{-1}{2\pi i} \sum_{\substack{F\in\mathcal{F}(P)\\ \dim(F)=d-1}} \frac{\langle c, n_F\rangle}{\langle c,\xi\rangle} \int_F e^{-2\pi i\langle x,\xi\rangle}\,\mathrm{d}_F x, \tag{5.3}$$

Formula (5.3) appears in many places (see Section 5.1.1) and it is called "combinatorial Stokes formula" by Barvinok and Pommersheim [BP99].

Here we follow Diaz, Le, and Robins [DLR16], choose $c = \xi$ and apply the same procedure iteratively on each facet until we get a face orthogonal to ξ. Given any face F of P, define the *affine hull* $\mathrm{aff}(F)$ as the smallest affine space containing F and $\mathrm{lin}(F)$ as the linear subspace parallel to $\mathrm{aff}(F)$. If ξ is orthogonal to $\mathrm{lin}(F)$, then $e^{-2\pi i\langle x,\xi\rangle}$ is constant in $\mathrm{aff}(F)$ and $\int_F e^{-2\pi i\langle x,\xi\rangle}\,\mathrm{d}_F x = \mathrm{vol}(F)e^{-2\pi i\langle x_F,\xi\rangle}$, where x_F is any point in $\mathrm{aff}(F)$ and $\mathrm{vol}(F)$ is the volume of F with respect to the measure of $\mathrm{aff}(F)$.

Let Proj_F be the orthogonal projection onto $\mathrm{lin}(F)$ and for a facet G of F, denote by $N_F(G)$ the unit normal vector in $\mathrm{lin}(F)$ pointing outward to G. The *weight* on the pair (F, G) is defined as:

$$W_{(F,G)}(\xi) := \frac{-1}{2\pi i}\frac{\big\langle \mathrm{Proj}_F(\xi), N_F(G)\big\rangle}{\|\mathrm{Proj}_F(\xi)\|^2}.$$

The *face poset* of P consists of $\mathcal{F}(P)$ ordered by inclusion and a *chain* T of *length* $l(T) = k$ is a sequence of faces $T = (F_0 \longrightarrow F_1 \longrightarrow F_2 \longrightarrow \cdots \longrightarrow F_k)$ with $F_0 = P$ and F_j a facet of F_{j-1} for every j. Let $\mathfrak{C}_P$ be the collection of all chains in the face poset. The *admissible set* $S(T)$ of a chain $T = (F_0 \longrightarrow F_1 \longrightarrow F_2 \longrightarrow \cdots \longrightarrow F_k)$ is the set of all vectors orthogonal to $\mathrm{lin}(F_k)$ but not to $\mathrm{lin}(F_{k-1})$. For a point $\xi \in S(T)$, the *rational weight* $\mathcal{R}_T(\xi)$ is the product

$$\mathcal{R}_T(\xi) := \prod_{j=1}^{k} W_{(F_{j-1},F_j)}(\xi), \tag{5.4}$$

and the *exponential weight* $\mathcal{E}_T(\xi)$ is

$$\mathcal{E}_T(\xi) := \mathrm{vol}(F_k)e^{-2\pi i\langle \xi, x_{F_k}\rangle}, \tag{5.5}$$

where x_{F_k} is any point from $\mathrm{aff}(F_k)$, the last face from chain T, and $\mathrm{vol}(F_k)$ is its $(d-k)$-dimensional volume. Note that since $\xi \in S(T)$, the value of $\langle \xi, x_{F_k}\rangle$ does not depend on the choice of x_{F_k}.

With these definitions, via successive applications of (5.3), we get:

$$\hat{\mathbb{1}}_P(\xi) = \sum_{\substack{T\in\mathfrak{C}_P:\\ \xi\in S(T)}} \mathcal{R}_T(\xi)\mathcal{E}_T(\xi). \tag{5.6}$$

Note that $\mathcal{R}_T(\xi)$ is a homogeneous function of degree $-l(T)$. Formula (5.6) shows that if $\xi \in \mathbb{R}^d$ is a vector orthogonal to some face of dimension k and no face of dimension $k+1$, then $|\hat{\mathbb{1}}_P(t\xi)| = O(t^{-d+k})$. Vertices are faces of dimension 0 and every vector is orthogonal to the 0-dimensional space, hence for a generic vector, $|\hat{\mathbb{1}}_P(t\xi)| = O(t^{-d})$.

5.1.1 Similar applications

In this section we list some uses of the combinatorial Stokes formula (5.3), giving a more broad view of applications of the Fourier transform of P and in particular of (5.3). Often the development with the divergence theorem is a key step in the proofs of the main theorems in the cited works.

- Randol [Ran69] gives an estimate for the average order of growth of $\hat{\mathbb{1}}_P(\xi)$ when $P \subset \mathbb{R}^2$ is a polygon. The proof uses (5.3) and then bounds the integral over each edge. The result is then used to bound the average

$$\int_0^{2\pi} |R_{\theta P}(t)|\, \mathrm{d}\theta = O((\log t)^{3+\epsilon})$$

  for any $\epsilon > 0$, where θP represents a rotation of P by an angle θ and $R_{\theta P}(t)$ is defined as in (5.2). This kind of average under rotations allows for much stronger bounds, contrasting with $R_P(t)$ being of order $O(t)$ when P is a rational polygon.

- Skriganov [Skr98] and Skriganov and Starkov [SS00] improve the results from Randol [Ran69] and show that for an arbitrary polytope $P \subset \mathbb{R}^d$,

$$\int_{\mathrm{SO}(d)} |R_{UP}(t)|\, \mathrm{d}U = O((\log t)^{d-1+\epsilon})$$

  for any $\epsilon > 0$, where UP represents a rotation of P by $U \in \mathrm{SO}(d)$ and $R_{UP}(t)$ is defined as in (5.2) ([SS00, Theorem 2]). Section 11 from Skriganov [Skr98] outlines a method similar to the one described in the beginning of this chapter, while Equation (11.15) from [Skr98] is Equation (5.3) with $c = \xi$. Further, Lemma 11.3 from [Skr98] is very similar to Equation (5.6), however Skriganov only considers generic directions and hence only chains of length d in his development of $\hat{\mathbb{1}}_P(\xi)$.

- Lemma 1 from Barvinok [Bar92] and Lemma 2.5 from Barvinok [Bar93] are similar to Equation (5.3). Barvinok uses this formula to proof Brion's theorem, as we will see in detail in Section 5.2.1. Barvinok [Bar93] applies this theorem to give an algorithm to approximate the volume of a polytope and analises its complexity for integer polytopes in terms of the size of its vertices and the number of its edges.

- Let P be a rational polytope and $m \in \mathbb{Z}$ be such that mP has integer vertices. $L_P(t) := |tP \cap \mathbb{Z}^d|$ can be written as a *quasi-polynomial* function of t, that is, as an expression of the form

$$L_P(t) = \mathrm{vol}(P)t^d + e_{d-1}(t)t^{d-1} + \cdots + e_0(t),$$

for $t \in \mathbb{Z}$, $t > 0$. Each *quasi-coefficient* $e_k(t)$ is a periodic function with period dividing m and the function $L_P(t)$ is called the *Ehrhart quasi-polynomial* of P (see e.g., Beck and Robins [BR15]).

Barvinok [Bar06] gives a polynomial time algorithm to compute $e_{d-k}(t)$ for fixed k when P is a rational simplex. Lemma 3.1 from [Bar06] is formula (5.3) with $c = \xi$. Some of the techniques introduced in Section 4 from [Bar06] are used in Section 6.5.

- Let A and B be two sets formed by a finite union of polytopes in $\mathbb{R}^d$. We say that A and B are *equidecomposable* by translations along a lattice L if A and B can be written as finite unions $A = A_1 \cup \cdots \cup A_N$, $B = B_1 \cup \cdots \cup B_N$ with pairwise disjoint interiors such that $B_j = A_j + v_j$ for some $v_j \in L$, for all $1 \le j \le N$.

  Lev and Liu [LL19a] prove a characterization of sets that are equidecomposable as sets that have the same volume and same Hadwiger functionals $H_\Phi(A, L) = H_\Phi(B, L)$. Roughly, these functionals are a signed sum of volumes over chains of faces whose affine span are translates of each other along a vector from L (see Section 1.2 of [LL19a] for the precise definition). In the main step of the proof [LL19a, Lemma 4.2], the authors consider chains of faces of increasing length and use an inductive argument whose step is done with (5.3).

- Let A be a finite union of polytopes in $\mathbb{R}^d$. We say that A is *spectral* if there exists a countable set $\Lambda \subset \mathbb{R}^d$ such that the system of exponentials $\{e^{2\pi i\langle\lambda,x\rangle} : \lambda \in \Lambda\}$ is a complete orthonormal system for $L^2(A)$. The classical example is the Fourier series on the unit cube $[0,1]^d$, as stated in Theorem 2.4.4.

  Kolountzakis and Papadimitrakis [KP02] gave a necessary condition for a finite union of polytopes A be spectral, namely, the total area of the facets whose normal vector points to a direction has to be equal to the total area of the facets whose normal vector points to the opposite direction. In the proof, (5.3) is used to bound the growth of $\hat{\mathbb{1}}_A(\xi)$.

  Later, Lev and Liu [LL19b] extended this result and proved that if a set A is spectral, then its Hadwiger functionals $H_\Phi(A)$ (defined similarly to above, but without the lattice restriction) are all zero, meaning equivalently that A must be equidecomposable by translations to a cube. The divergence theorem is used [LL19b, Section 3] to approximate $\hat{\mathbb{1}}_A(\xi)$ in certain domains in terms of the contribution of only a few parallel chains of faces (see Theorem 4.1 and Lemma 5.1 of [LL19b] for the precise statement).

  Greenfeld and Lev [GL17] adapted the proof from Kolountzakis and Papadimitrakis [KP02] and proved that a spectral polytope in $\mathbb{R}^3$ tiles the space by translations, confirming a conjecture from Fuglede in the convex case. Formula (5.3) appears as Lemma 2.4 in [GL17]. Later, Lev and Matolcsi [LM19] extended the result for all dimensions.

5.2 The integral and exponential sum valuations

The maps that associates to each polytope its Fourier transform, its volume and the counting of its integer points are examples of valuations. Besides being very natural, the theory of valuations is useful not just to geberalize these maps but also to derive formulas that relates them. See McMullen and Schneider [MS83] and McMullen [McM93] for surveys. The definitions vary across the references, depending on the application in mind, here we follow Barvinok and Pommersheim [BP99] and the book of Barvinok [Bar08].

For a vector subspace $V \subseteq \mathbb{R}^d$, the *algebra of polyhedra* $\mathcal{P}(V)$ is the vector space spanned by the indicator functions $\mathbb{1}_P$ of all polyhedra $P \subset V$. A *valuation* in $\mathcal{P}(V)$ is any linear map from $\mathcal{P}(V)$ to some vector space. The ground field of $\mathcal{P}(V)$ changes across the references, varying between $\mathbb{Q}$, $\mathbb{R}$, and $\mathbb{C}$, here we consider $\mathcal{P}(V)$ as a complex vector space since we want to make a correspondence between the integral valuation that we will define below and the Fourier transform.

The indicator functions of polyhedra do not form a basis for $\mathcal{P}(V)$, since there are many linear relations among them. For instance, if $d = 2$, $A = [0,1]^2$, $B = [1,2] \times [0,1]$, and $C = \{1\} \times [0,1]$, then $\mathbb{1}_{A\cup B} = \mathbb{1}_A + \mathbb{1}_B - \mathbb{1}_C$. Therefore to define a valuation it is not enough to show how it behaves on indicator functions of polyhedra, but it is also necessary to show that it satisfies all these linear relations for it be well defined. So the following theorems (see e.g., Theorems 2.2, 2.3 and 2.5 from Barvinok and Pommersheim [BP99]) are not trivial.

Theorem 5.2.1. *There exists a unique valuation $\chi : \mathcal{P}(V) \longrightarrow \mathbb{C}$, called the* Euler characteristic*, such that $\chi(\mathbb{1}_P) = 1$ for each nonempty polyhedron $P \subset V$.*

Theorem 5.2.2. *Suppose that $A : V \longrightarrow W$ is an affine transformation. Then there is a unique valuation $\mathcal{A} : \mathcal{P}(V) \longrightarrow \mathcal{P}(W)$ such that $\mathcal{A}(\mathbb{1}_P) = \mathbb{1}_{AP}$ for each polyhedron $P \subset V$.*

If $P, Q \subset V$ are polyhedra in V, then the *Minkowski sum* $P + Q$ is defined as $P + Q := \{x + y : x \in P, y \in Q\}$.

Theorem 5.2.3. *There is a unique bilinear operation $* : \mathcal{P}(V) \times \mathcal{P}(V) \longrightarrow \mathcal{P}(V)$ such that $\mathbb{1}_P * \mathbb{1}_Q = \mathbb{1}_{P+Q}$ for any two polyhedra $P, Q \subset V$.*

The operation defined above is called *convolution* and it can be seen as a product, justifying the name "algebra of polyhedra". Specifically, it satisfies the commutative, associative and distributive properties. Further, $\mathbb{1}_{\{0\}}$ is the unit of the convolution and if $P \subset V$ is a k-dimensional polytope and relint(P) is its relative interior, then $(-1)^k \mathbb{1}_{-\mathrm{relint}(P)}$ is the inverse of $\mathbb{1}_P$. However, if P is an unbounded polyhedra, then there exists $f \in \mathcal{P}(V)$ nonzero such that $\mathbb{1}_P * f = 0$ (see Chapter 3 of Barvinok [Bar08] for the proofs of these statements). For $f, g \in \mathcal{P}(V)$ and $x \in V$, let $f(\cdot)g(x-\cdot)$ denote the function $y \mapsto f(y)g(x-y)$, then one may verify that

$$f * g(x) = \chi\big(f(\cdot)g(x-\cdot)\big),$$

so the convolution in $\mathcal{P}(V)$ is analogous to the convolution in $L^1(V)$ defined in Section 2.4.3, but with the integral replaced by the Euler characteristic (for a brief survey on applications of integration with the Euler characteristic, see Khovanskii and Pukhlikov [KP93]).

If F is a face of a polyhedron P, the *tangent cone* of P at F is the cone of directions that one can move from F and stay in P:

$$\operatorname{tcone}(P,F) := \{x + \lambda(y-x) : x \in F, y \in P, \lambda \geq 0\}.$$

The next theorem expresses the indicator function of a polytope in terms of the tangent cones of its vertices (see e.g., Barvinok [Bar08, Theorem 6.4]):

Theorem 5.2.4. *If $P \subset V$ be a polyhedron, then*

$$\mathbb{1}_P = \sum_{v \in V(P)} \mathbb{1}_{\operatorname{tcone}(P,v)} \quad \textit{modulo polyhedra with lines.}$$

That is, the difference $\mathbb{1}_P - \sum_{v\in V(P)} \mathbb{1}_{\operatorname{tcone}(P,v)}$ is a linear combination of indicator functions of polyhedra with lines.

Let $\mathcal{M}(\mathbb{C}V)$ be the space of meromorphic functions from $\mathbb{C}V := V \oplus iV$ to $\mathbb{C}$ (i.e., quotient between analytic functions in V with the denominator not constant 0). Next we define the exponential integral valuation, first proved by Lawrence [Law91] and independently, Khovanskii and Pukhlikov [PK92] (see Theorem 8.4 of Barvinok [Bar08]):

Theorem 5.2.5. *Let $V \subseteq \mathbb{R}^d$ be a subspace with a measure $\mathrm{d}x$. Then there exists a valuation $I : \mathcal{P}(V) \longrightarrow \mathcal{M}(\mathbb{C}V)$ such that for a polyhedron $P \subseteq V$,*

(a) If $\xi \in \mathbb{C}V$ is such that $|e^{\langle \xi, x\rangle}|$ is integrable over P, then

$$I(\mathbb{1}_P)(\xi) = \int_P e^{\langle \xi, x\rangle}\, \mathrm{d}x.$$

(b) If P contains a straight line, then $I(\mathbb{1}_P) = 0$.

(c) For every $c \in V$ and $\xi \in \mathbb{C}V$ regular for $I(\mathbb{1}_P)$,

$$I(\mathbb{1}_{P+c})(\xi) = e^{\langle \xi, c\rangle} I(\mathbb{1}_P)(\xi).$$

Note that I is a *solid valuation*, which means that when $P \subset V$ is not a full-dimensional polyhedron, then $I(\mathbb{1}_P) = 0$. Later we will consider different versions of this valuation, for different subspaces $V \subset \mathbb{R}^d$, with the understanding that each valuation has to be considered with an appropriate measure for each subspace V.

Condition (a) shows that $\hat{\mathbb{1}}_P(\xi) = I(\mathbb{1}_P)(-2\pi i \xi)$ when $V = \mathbb{R}^d$ and P is a d-dimensional polytope. However, when P is an unbounded polyhedron, $\mathbb{1}_P \notin L^1(\mathbb{R}^d)$ and the definition of the Fourier transform from Section 2.4.3 does not apply. The integral valuation is defined for arbitrary polyhedra and complex vectors $\xi \in \mathbb{C}^d$ which are regular for $I(\mathbb{1}_P)$. When $\hat{\mathbb{1}}_P$ is considered with complex vectors via the relation above, $\hat{\mathbb{1}}_P$ is called the *Fourier-Laplace transform of P*.

Theorems 5.2.4 and condition (b) from Theorem 5.2.5 imply that the integral valuation of a polyhedra can be expressed in terms of the integral valuations of the tangent cones of its vertices, which for some polytopes produces an effective method to compute it, as we will see in Section 5.2.1. This was first proved by Brion [Bri88] for rational polytopes and later proved for general polytopes by Barvinok [Bar92] and general polyhedra by Lawrence [Law91] and Khovanskii and Pukhlikov [PK92].

Theorem 5.2.6 (Brion). *If $P \subset V$ is a nonempty polyhedron, then*

$$I(\mathbb{1}_P) = \sum_{v \in V(P)} I(\mathbb{1}_{\mathrm{tcone}(P,v)}).$$

Next we consider that V is a rational subspace and we consider it together with a full dimensional and rational lattice $\Lambda \subset V \cap \mathbb{Q}^d$. The *algebra of rational polyhedra* $\mathcal{P}(\mathbb{Q}V)$ is the vector space spanned by the indicator functions of all rational polyhedra $P \subset V$ and all the cited theorems holds similarly within the rational polyhedra. In particular, if $P \subset V$ is a rational polyhedra, the tangent cones of each face also are rational and

$$\mathbb{1}_P = \sum_{v \in V(P)} \mathbb{1}_{\mathrm{tcone}(P,v)} \quad \text{modulo rational polyhedra with lines.} \tag{5.7}$$

Next we define the exponential sum valuation, a valuation very similar to the integral valuation (see Theorem 13.8b of Barvinok [Bar08]):

Theorem 5.2.7. *Let $V \subseteq \mathbb{R}^d$ be a rational subspace and $\Lambda \subset V$ be a rational spanning lattice. Then there exists a valuation $S : \mathcal{P}(\mathbb{Q}V) \longrightarrow \mathcal{M}(\mathbb{C}V)$ such that for a rational polyhedron $P \subseteq V$,*

(a) If $\xi \in \mathbb{C}V$ is such that $|e^{\langle \xi, x\rangle}|$ is absolutely summable over P, then

$$S(\mathbb{1}_P) = \sum_{P\cap\Lambda} e^{\langle \xi, x\rangle}.$$

(b) If P contains a straight line, then $S(\mathbb{1}_P) = 0$.

(c) For every $c \in \Lambda$ and $\xi \in \mathbb{C}V$ regular for $S(\mathbb{1}_P)$,

$$S(\mathbb{1}_{P+c})(\xi) = e^{\langle \xi, c\rangle} S(\mathbb{1}_P)(\xi).$$

Equation (5.7) and condition (b) from Theorem 5.2.7 also imply a discrete version of Brion's theorem:

Theorem 5.2.8 (Brion). *If $P \subset \mathbb{R}^d$ is a nonempty rational polyhedra, then*

$$S(\mathbb{1}_P) = \sum_{v \in V(P)} S(\mathbb{1}_{\mathrm{tcone}(P,v)}).$$

5.2.1 Brion's theorem

In this section we use Theorem 5.2.6 to derive an explicit formula for the Fourier transform of a polytope in terms of the tangent cones at its vertices. We begin introducing some notation and terminology about cones.

A *polyhedral cone* is a polyhedron $K \subset \mathbb{R}^d$ such that $0 \in K$ and for every $x \in K$ and

$\lambda \geq 0$, $\lambda x \in K$. This is equivalent to a polyhedron defined as in (5.1) with all $b_j = 0$. An *(affine) cone* is the translation of a cone by some vector $v \in \mathbb{R}^d$. We say that an affine cone is *pointed* if it does not contain any line, in this case v is the only vertex of the cone. Every pointed cone K has a set $w_1, \dots, w_m \in \mathbb{R}^d$ of *generators*, all lying in the same half-space, minimal and well defined up to scalar multiplication, such that it can be written as

$$K = \left\{ v + \lambda_1 w_1 + \cdots + \lambda_m w_m \, : \, \lambda_j \geq 0 \right\}.$$

If the cone has linearly independent generators, we say that the cone is *simplicial.*

Now we consider a full-dimensional simplicial cone $K \subset \mathbb{R}^d$ with generators $w_1, \dots, w_d \in \mathbb{R}^d$ and let $\det K$ denote the volume of the parallelepiped spanned by its generators. If $W \in \mathbb{R}^{d \times d}$ is the matrix with $w_1, \dots, w_d$ as columns, then $\det K = |\det W|$. For $\xi \in \mathbb{C}^d$, let $\operatorname{Re}(\xi)$ and $\operatorname{Im}(\xi)$ denote the real and imaginary parts of ξ, so that $\operatorname{Re}(\xi), \operatorname{Im}(\xi) \in \mathbb{R}^d$ and $\xi = \operatorname{Re}(\xi) + i\operatorname{Im}(\xi)$.

Lemma 5.2.9. *Let $K \subset \mathbb{R}^d$ be a d-dimensional simplicial affine cone with vertex $v \in \mathbb{R}^d$ and generators $w_1, \dots, w_d \in \mathbb{R}^d$, then for $\xi \in \mathbb{C}^d$ such that $\langle \operatorname{Re}(\xi), w_j \rangle < 0$ for all $1 \leq j \leq d$,*

$$\int_K e^{\langle \xi, x \rangle} \, \mathrm{d}x = (-1)^d \frac{\det K}{\langle \xi, w_1 \rangle \cdots \langle \xi, w_d \rangle} e^{\langle \xi, v \rangle}.$$

Proof. Let $W \in \mathbb{R}^{d \times d}$ be the matrix with $w_1, \dots, w_d$ as columns. Making the change of variables $x = v + Wu$ and denoting the nonnegative orthant by $\mathbb{R}^d_{\geq 0}$, we have

$$\begin{aligned} \int_K e^{\langle \xi, x \rangle} \, \mathrm{d}_K x &= \det K e^{\langle \xi, v \rangle} \int_{\mathbb{R}^d_{\geq 0}} e^{\langle W^\top \xi, u \rangle} \, \mathrm{d}u \\ &= \det K e^{\langle \xi, v \rangle} \prod_{j=1}^d \frac{e^{\langle \xi, w_j \rangle u_j}}{\langle \xi, w_j \rangle} \bigg|_{u_j = 0}^{\infty} \\ &= (-1)^d \frac{\det K}{\langle \xi, w_1 \rangle \cdots \langle \xi, w_d \rangle} e^{\langle \xi, v \rangle}, \end{aligned}$$

since $\operatorname{Re}(\langle \xi, w_j \rangle) < 0$ for every $1 \leq j \leq d$. □

Since meromorphic functions that coincide in an open set are equal, Lemma 5.2.9 gives a formula for $I(\mathbb{1}_K)(\xi)$ for a simplicial cone $K \subset \mathbb{R}^d$ and shows that the set of singular points of $I(\mathbb{1}_K)$ is the union of hyperplanes $\cup_{j=1}^d \{\xi \in \mathbb{C}^d \, : \, \langle \xi, w_j \rangle = 0\}$. Furthermore, since every pointed cone can be triangulated into simplicial cones with no new generators (see e.g., Beck and Robins [BR15, Section 3.2]), the integral valuation of a general cone can be written as a sum of expressions of the form above and using Brion's theorem 5.2.6, we have an expression for the integral valuation of any polyhedra.

Next we restate Theorem 5.2.6 for the Fourier transform of a polytope using a triangulation of the tangent cones of each vertex and Lemma 5.2.9.

Theorem 5.2.10 (Brion)**.** *If $P \subset \mathbb{R}^d$ is a d-dimensional polytope and for each $v \in V(P)$, $K_{v,1}, \dots, K_{v,M_v}$ are simplicial cones with disjoint interiors such that* $\operatorname{tcone}(P, v) = \bigcup_{j=1}^{M_v} K_{v,j}$

and for each $1 \le j \le M_v$, $w^v_{j,1}, \dots, w^v_{j,d}$ *are the generators of* $K_{v,j}$. *Then*

$$\hat{\mathbb{1}}_P(\xi) = \sum_{v \in V(P)} \sum_{j=1}^{M_v} \frac{e^{-2\pi i \langle v, \xi \rangle}}{(2\pi i)^d} \frac{\det K_{v,j}}{\langle w^v_{j,1}, \xi \rangle \dots \langle w^v_{j,d}, \xi \rangle}. \tag{5.8}$$

The formula above can be used to evaluate $\hat{\mathbb{1}}_P$ for complex ξ as well, whose meaning is given by the integral valuation: $\hat{\mathbb{1}}_P(\xi) = I(\mathbb{1}_P)(-2\pi i \xi)$. This extension of the Fourier transform to complex vectors is sometimes called "Fourier-Laplace transform". Since P is compact and $\hat{\mathbb{1}}_P(\xi)$ is continuous for all $\xi \in \mathbb{C}^d$, the formula above can also be used to evaluate $\hat{\mathbb{1}}_P(\xi)$ for $\xi \in \mathbb{C}^d$ that makes any of the denominators of (5.8) vanish, but an appropriate limiting procedure must be taken in these cases.

Example 5.2.11. *If* $P \subset \mathbb{R}^2$ *is the triangle* $P = \operatorname{conv}\{(0,0),(a,0),(0,b)\}$ *with* $a, b > 0$, *then* $w_1^{(0,0)} = (1,0)$, $w_2^{(0,0)} = (0,1)$, $w_1^{(a,0)} = (-1,0)$, $w_2^{(a,0)} = (-a,b)$, $w_1^{(0,b)} = (0,-1)$, $w_2^{(0,b)} = (a,-b)$, *and*

$$\hat{\mathbb{1}}_P(z) = \left(\frac{1}{2\pi i}\right)^2 \left(\frac{1}{z_1 z_2} + \frac{b e^{-2\pi i a z_1}}{(a z_1 - b z_2) z_1} + \frac{a e^{-2\pi i b z_2}}{(-a z_1 + b z_2) z_2}\right).$$

5.2.2 SI-interpolators

For a rational polytope $P \subset \mathbb{R}^d$, we have $I(P)(0) = \operatorname{vol}(P)$ and $S(P)(0) = |P \cap \mathbb{Z}^d|$, therefore a formula that relates $I(P)$ and $S(P)$ can be useful to determine the difference $R_P(t) := \left|\operatorname{vol}(tP) - |tP \cap \mathbb{Z}^d|\right|$. Berline and Vergne [BV07] developed such a formula expressing $S(P)$ in terms of the integral valuations of all faces $F \in \mathcal{F}(P)$ and the local information given by the tangent cones along each face. See also the works of Barvinok [Bar08] and Garoufalidis and Pommersheim [GP12].

For each rational subspace $V \subseteq \mathbb{R}^d$, let I_V be the integral valuation defined as in Theorem 5.2.5, but with the relative Lebesgue measure on V normalized so that $\det(V \cap \mathbb{Z}^d) = 1$. We also use I_V to denote the integral valuation on a rational translation of V.

For each rational subspace $V \subseteq \mathbb{R}^d$ and rational $v \in V$, let $\mathcal{A}_v(V) \subset \mathcal{P}(\mathbb{Q}V)$ be the subalgebra generated by the indicator functions of rational pointed affine cones contained in V and with vertex v. Using the Euclidean inner product $\langle , \rangle$ of $\mathbb{R}^d$, we identify the quotient $\mathbb{R}^d/V$ with the orthogonal complement $V^\perp$ of V, which is also a rational subspace of $\mathbb{R}^d$. When $K \subset V$ is a pointed affine cone and F is a proper face of K, the *transverse cone* of K along F is

$$\operatorname{trcone}(K, F) := \operatorname{tcone}(K, F)/\operatorname{lin}(F).$$

It is a pointed affine cone in $V/\operatorname{lin}(F)$.

Theorem 5.2.12 (Berline-Vergne [BV07])**.** *Let* $V \subseteq \mathbb{R}^d$ *be a rational subspace,* $\Lambda \subset V$ *be a rational spanning lattice and* S *be the associated exponential sum valuation. Then there exists a map* μ_V *that associates a meromorphic function from* $\mathcal{M}(\mathbb{C}V)$ *to each pointed affine cone in* V *such that:*

(a) $\mu_{\{0\}}(\{0\}) = 1$.

(b) *For any pointed affine cone $K \subset V$,*

$$S(\mathbb{1}_K)(\xi) = \sum_{F \in \mathcal{F}(K)} \mu_{V/\mathrm{lin}(F)}\big(\mathrm{trcone}(K,F)\big)(\xi/\mathrm{lin}(F)) I_{\mathrm{lin}(F)}(\mathbb{1}_F)(\xi), \tag{5.9}$$

where $\xi/\mathrm{lin}(F)$ is the orthogonal projection of ξ onto $\mathbb{C}V/\mathrm{lin}(F) = \mathbb{C}V^{\perp}$.

(c) *For any pointed affine cone $K \subset V$, the function $\mu_V(K)$ is analytic near* 0*.*

(d) *For any pointed affine cone $K \subset V$ and $x \in \Lambda$, $\mu_V(x + K) = \mu_V(K)$.*

(e) *For every rational vector $v \in V$, the function $M : \mathcal{A}_v(V) \longrightarrow \mathcal{M}(\mathbb{C}V)$ defined as $M(\mathbb{1}_K) := \mu_V(K)$ for each pointed affine cone $K \subset V$ with vertex v, is a valuation.*

The proof of this theorem is made by induction on the dimension of V. When $\dim(V) > 0$ and $K \subset V$ is a pointed affine cone with vertex v, formula (5.9) implies

$$\mu_V(K)(\xi) = e^{-\langle \xi, v\rangle}\Bigg(S(\mathbb{1}_K)(\xi) - \sum_{\substack{F \in \mathcal{F}(K)\\ \dim(F)>0}} \mu_{V/\mathrm{lin}(F)}\big(\mathrm{trcone}(K,F)\big)(\xi/\mathrm{lin}(F)) I_{\mathrm{lin}(F)}(\mathbb{1}_F)(\xi)\Bigg).$$

This formula defines $\mu_V(K)$ uniquely as a function in $\mathcal{M}(\mathbb{C}V)$, although as observed by Garoufalidis and Pommersheim [GP12], different inner products (or more generally, complement maps as defined in [GP12]) induce different orthogonal projections and different μ_V.

When $V_1 \subset V_2$ and K is a pointed affine cone in V_1, $\mu_{V_1}(K)$ is the composition of $\mu_{V_2}(K)$ with the orthogonal projection from V_2 to V_1 [BV07, Proposition 13]. Hence, making the composition with the orthogonal projection implicitly, the index V may be dropped from μ_V with no ambiguity.

The valuation and analytic properties of μ are proven in Propositions 15 and 18 of Berline and Vergne [BV07]. The valuation property of μ together with the Brion's theorem for S and I imply the following corollary ([BV07, Theorem 20]):

Corollary 5.2.13. *For any rational polyhedron $P \subset \mathbb{R}^d$,*

$$S(\mathbb{1}_P)(\xi) = \sum_{F \in \mathcal{F}(P)} \mu\big(\mathrm{trcone}(P,F)\big)(\xi) I_{\mathrm{lin}(F)}(\mathbb{1}_F)(\xi).$$

A function μ with this property is called a *SI-interpolator* by Garoufalidis and Pommersheim [GP12]. Its main application is to produce a local formula for the number of integer points in a rational polytope, that is, an expression in terms of the faces and the tangent cones along the faces of P.

More generally, let $P \subset \mathbb{R}^d$ be a rational polytope and h be a polynomial in d variables. We want to consider the sum

$$\sum_{x \in P \cap \mathbb{Z}^d} h(x).$$

Since $\mu\big(\mathrm{trcone}(P,F)\big)$ is an analytic function, we may use its Taylor expansion at 0 to define a differential operator for each face F of P:

$$D(P,F) := \mu\big(\mathrm{trcone}(P,F)\big)(\partial_x).$$

This operator satisfies:

$$D(P,F)e^{\langle \xi,x\rangle} = \mu\big(\mathrm{trcone}(P,F)\big)(\xi)e^{\langle \xi,x\rangle}.$$

Now, for the polynomial h we may define an associated differential operator

$$D_h := h(\partial_\xi),$$

which satisfies

$$D_h e^{\langle \xi,x\rangle} = h(x)e^{\langle \xi,x\rangle}.$$

Next, we take (5.9) and apply the definition of the operator $D(P,F)$ to get (d_F is the relative Lebesgue measure on $\mathrm{lin}(F)$ normalized so that $\det(\mathrm{lin}(F)\cap\mathbb{Z}^d) = 1$):

$$\begin{aligned}
S(\mathbb{1}_P)(\xi) &= \sum_{F\in\mathcal{F}(P)} \mu\big(\mathrm{trcone}(P,F)\big)(\xi) I_{\mathrm{lin}(F)}(\mathbb{1}_F)(\xi)\\
&= \sum_{F\in\mathcal{F}(P)} \int_F \mu\big(\mathrm{trcone}(P,F)\big)(\xi)e^{\langle \xi,x\rangle}\,\mathrm{d}_F(x)\\
&= \sum_{F\in\mathcal{F}(P)} \int_F D(P,F)e^{\langle \xi,x\rangle}\,\mathrm{d}_F(x).
\end{aligned}$$

Applying D_h to both sides,

$$\begin{aligned}
D_h S(P)(\xi) &= \sum_{F\in\mathcal{F}(P)} \int_F D(P,F)D_h e^{\langle \xi,x\rangle}\,\mathrm{d}_F(x)\\
\sum_{x\in P\cap\mathbb{Z}^d} h(x)e^{\langle \xi,x\rangle} &= \sum_{F\in\mathcal{F}(P)} \int_F D(P,F)h(x)e^{\langle \xi,x\rangle}\,\mathrm{d}_F(x).
\end{aligned}$$

Evaluating the latter identity at $\xi = 0$, we get (see [BV07, Theorem 26] and [GP12, Theorem 2]):

$$\sum_{x\in P\cap\mathbb{Z}^d} h(x) = \sum_{F\in\mathcal{F}(P)} \int_F D(P,F)h(x)\,\mathrm{d}_F(x). \tag{5.10}$$

Equation (5.10) is called an *Euler-Maclaurin summation formula* since the sum on the right is expressed in terms of integrals taken over the faces of P, of functions that depend only on local information along each face. Applying it to the constant function $h(x) = 1$ and noticing that the constant term of $D(P,F)$ is equal to $\mu\big(\mathrm{trcone}(P,F)\big)(0)$, we get a local formula for the number of integer points [BV07, Corollary 30]:

$$|P\cap\mathbb{Z}^d| = \sum_{F\in\mathcal{F}(P)} \mathrm{vol}^*(F)\mu\big(\mathrm{trcone}(P,F)\big)(0), \tag{5.11}$$

where $\mathrm{vol}^*(F)$ is the *relative volume* of the face F, which differs from the usual volume inherited from $\mathbb{R}^d$ by a scaling factor so that $\det(\mathrm{lin}(F)\cap\mathbb{Z}^d) = 1$. Considering a dilation

tP for some $t > 0$, noting that $\mathrm{vol}^*(tF) = t^{\dim(F)}\mathrm{vol}^*(F)$, and recalling that $\mu\big(\mathrm{trcone}(P,P)\big) = \mu(\{0\}) = 1$, we get

$$L_P(t) := |tP \cap \mathbb{Z}^d| = t^d \mathrm{vol}(P) + \sum_{k=0}^{d-1} t^k \sum_{\substack{F \in \mathcal{F}(P) \\ \dim(F)=k}} \mathrm{vol}^*(F)\mu\big(t\mathrm{trcone}(P,F)\big)(0). \tag{5.12}$$

By item (d) of Theorem 5.2.12, the function $\mu\big(t\mathrm{trcone}(P,F)\big)(0)$ is periodic in t, with period dividing the smallest q such that $q\mathrm{aff}(F)$ contains integer points (note that $\mu_{\mathrm{lin}(F)}$ is a function defined in terms of the lattice $\mathbb{Z}^d/\mathrm{lin}(F) \subset \mathrm{lin}(F)^\perp$ and $\mathrm{aff}(F)/\mathrm{lin}(F)$ is a rational point in $\mathrm{lin}(F)^\perp$). Expression (5.12) is a quasi-polynomial and the periodic terms multiplying the factors t^k are the quasi-coefficients. In the next chapter we see an alternative method to compute them.

Chapter 6

Coefficients of the solid angle and Ehrhart quasi-polynomials

This chapter is based on the publication "F.C. Machado, S. Robins, *Coefficients of the solid angle and Ehrhart quasi-polynomials*, preprint arXiv:1912.08017, 2019, 35 pages".

Abstract. Macdonald studied a discrete volume measure for a rational polytope P, called solid angle sum, that gives a natural discrete volume for P. We give a local formula for the codimension two quasi-coefficient of the solid angle sum of P. We also show how to recover the classical Ehrhart quasi-polynomial from the solid angle sum and in particular we find a similar local formula for the codimension one and codimension two quasi-coefficients. These local formulas are naturally valid for all positive real dilates of P.

An interesting open question is to determine necessary and sufficient conditions on a polytope P for which the discrete volume of P given by the solid angle sum equals its continuous volume: $A_P(t) = \text{vol}(P)t^d$. We prove that a sufficient condition is that P tiles $\mathbb{R}^d$ by translations, together with the Hyperoctahedral group.

6.1 Introduction

Given a polytope $P \subset \mathbb{R}^d$, the number of integer points within P can be regarded as a discrete analog of the volume of the body. For a *rational polytope*, meaning that the vertices of P have rational coordinates, Ehrhart [Ehr62] showed that the number of integer points in the integer dilates $tP := \{tx : x \in P\}$ can be written as a *quasi-polynomial* function of t, that is, as an expression of the form

$$L_P(t) := |tP \cap \mathbb{Z}^d| = \text{vol}(P)t^d + e_{d-1}(t)t^{d-1} + \cdots + e_0(t), \tag{6.1}$$

for $t \in \mathbb{Z}$, $t > 0$. Here, each *quasi-coefficient* $e_k(t)$ is a periodic function with period dividing the *denominator* of P, defined to be the smallest integer m such that mP in an integer polytope. The function $L_P(t)$ is called the *Ehrhart quasi-polynomial* of P (see e.g., Beck and Robins [BR15]).

The Ehrhart quasi-polynomial of P is not, however, the only discrete volume that we may define. It has a sister polynomial, which is another measure of discrete volume for polytopes. Namely, each integer point located on the boundary of the polytope is assigned a fractional weight, according to the proportion of the space around that point which the polytope occupies. Indeed, Ehrhart and Macdonald already defined this other discrete volume of P, calling it the solid angle sum, and we will adopt their notation, as follows.

At each point $x \in \mathbb{R}^d$, we define the *solid angle* with respect to P:

$$\omega_P(x) := \lim_{\epsilon \to 0^+} \frac{\mathrm{vol}(S^{d-1}(x,\epsilon) \cap P)}{\mathrm{vol}(S^{d-1}(x,\epsilon))}, \tag{6.2}$$

where $S^{d-1}(x,\epsilon)$ denotes the $(d-1)$-dimensional sphere centered at x with radius ϵ. Similarly to Ehrhart, Macdonald [Mac63; Mac71] showed that if P is a rational polytope and t is a positive integer, the sum of these fractionally-weighted integer points inside tP is a quasi-polynomial of t. We define the *solid angle sum*

$$A_P(t) := \sum_{x \in \mathbb{Z}^d} \omega_{tP}(x) = \mathrm{vol}(P)t^d + a_{d-1}(t)t^{d-1} + \cdots + a_0(t), \tag{6.3}$$

and similarly to (6.1), we call $a_k(t)$ the quasi-coefficients of $A_P(t)$.

One of the motivations for studying these coefficients is that they capture geometric information about the polytope. Denote by $\mathrm{vol}^*(F)$ the *relative volume* of a face F, which differs from the usual volume inherited from $\mathbb{R}^d$ by a scaling factor such that the fundamental domain of the lattice of integer points on the linear space parallel to the face has volume 1. Assuming that P is full-dimensional, it is an easy fact e_d is the volume of P and, if we further assume that P is an integer polytope, then it is also fairly easy to show that e_{d-1} is half the sum of the relative volumes of the facets of P, and $e_0 = 1$ (see [BR15]). Analogous "simple" geometric interpretations for the other coefficients e_k are not yet known. On the other hand, one strong advantage that the solid angle sum has over the Ehrhart polynomial is that it is a better approximation to the volume of tP, in the following sense. For a full-dimensional integer polytope $P \subset \mathbb{R}^d$, restricting attention to integer dilates t gives:

$$A_P(t) := \sum_{x \in \mathbb{Z}^d} \omega_{tP}(x) = \mathrm{vol}(P)t^d + a_{d-2}t^{d-2} + a_{d-4}t^{d-4} + \dots, \tag{6.4}$$

a polynomial function of t, which is an even polynomial in even dimensions, and an odd polynomial in odd dimensions, and also $a_0 = 0$. This was already proved by Macdonald [Mac71], using the purely combinatorial technique of the Möbius μ-function of the face poset of P.

In this chapter, our main focus is on the coefficients of the solid angle quasi-polynomial, as in equation (6.3). One strong advantage that these quasi-polynomials have over their Ehrhart quasi-polynomial siblings is that the solid angle quasi-polynomials are a *simple valuation* (also called *solid*) on the polytope algebra. This means that for any given two rational polytopes $P, Q \subset R^d$ whose interiors are disjoint, we have $A_{P\cup Q}(t) = A_P(t) + A_Q(t)$, hence we never have to compute these valuations over intersections of such polytopes. However, for the Ehrhart polynomials, we have $L_{P\cup Q}(t) = L_P(t) + L_Q(t) - L_{P\cap Q}(t)$, so that in principle one has to compute these latter valuations over lower-dimensional intersections.

To state the main results of the literature, as well as our results here, we need to use the following definitions and data, associated to any polytope P. Let $\mathcal{F}(P)$ be the collection of all faces of P. Given any face $F \in \mathcal{F}(P)$, we define the *affine hull* $\mathrm{aff}(F)$ as the smallest affine space containing F and $\mathrm{lin}(F)$ as the linear subspace parallel to $\mathrm{aff}(F)$. We also define the *cone of feasible directions* of P at F as

$$\mathrm{fcone}(P, F) := \{\lambda(y - x) : x \in F, y \in P, \lambda \geq 0\}$$

and, picking any point x_F in the relative interior of the face F, we define the *tangent cone* of P at F

$$\mathrm{tcone}(P, F) := x_F + \mathrm{fcone}(P, F),$$

as the cone of feasible directions translated to its original position.

McMullen [McM79] (see also Barvinok [Bar08, Chapter 20]) proved the existence of functions μ such that for rational P,

$$|P \cap \mathbb{Z}^d| = \sum_{F\in\mathcal{F}(P)} \mathrm{vol}^*(F)\mu(P, F), \tag{6.5}$$

where $\mathcal{F}(P)$ is the collection of all faces of P and μ depends only on "local" geometric data associated to the face F, namely the cone $\mathrm{fcone}(P, F)$ and the translation class of $\mathrm{aff}(F)$ modulo $\mathbb{Z}^d$. Since the volume is homogeneous with degree $\dim(F)$, applying (6.5) to tP for integer t, we see that this expression implies a formula of the type

$$e_k(t) = \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=k}} \mathrm{vol}^*(F)\mu(tP, tF). \tag{6.6}$$

Such formula is called a *local formula* for the quasi-coefficients. Since $\mathrm{fcone}(P, F)$ doesn't change under dilations and, taking m as the denominator of P, $\mathrm{aff}(mF)$ has integer points, we see that indeed $e_k(t) = e_k(t + m)$.

These formulas (6.6) are not unique. Indeed, when P is an integer polytope, Pommersheim and Thomas [PT04] constructed infinite classes of such formulas based on an expression for the Todd class of a toric variety; For the case that P is a rational polytope, Barvinok [Bar06; Bar08] studied the algorithmic complexity of computing these coefficients, showing that fixing the codimension $\dim(P) - \dim(F)$, $\mu(P, F)$ is indeed computable in polynomial time and Berline and Vergne [BV07] computed a local formula based on a valuation that associates an analytic function to the tangent cone at each face. Garoufalidis and Pommersheim [GP12] showed that there exists such valuation (and hence a local formula) uniquely for each given "rigid complement map" of the vector space, which is a systematic way to extend functions initialy defined on subspaces to the entire space. Recently, Ring and Schürmann [RS19] also produced a method to build local formulas based on the choice of fundamental domains on sublattices. For simplicity, in this chapter we assume a fixed inner product on $\mathbb{R}^d$, which we also use to identify the space with its dual, and in this way these complement maps are simply given by orthogonal projection.

A simple way to see that the solid angle sum is indeed a quasi-polynomial and enjoys a lot of the same properties of the Ehrhart function follows by using a simple relation [BR15, Lemma 13.2] followed by the Ehrhart reciprocity law [BR15, Theorem 4.1]:

$$A_P(t) = \sum_{F \in \mathcal{F}(P)} \omega_P(F) L_{\mathrm{int}(F)}(t) = \sum_{F \in \mathcal{F}(P)} \omega_P(F)(-1)^{\dim(F)} L_F(-t), \tag{6.7}$$

where the sum is taken over all faces of P and $\omega_P(F)$ is defined as the solid angle of any point in the relative interior of the face F. In Section 6.8 we show how the relation (6.7) can be used to derive $a_k(t)$, given the coefficients $e_k(t)$. But we proceed in the opposite direction: first give formulations for the solid angle polynomial using Fourier analytic methods, then show how the Ehrhart coefficients can be recovered from them.

We make one more remark concerning the domain of the dilation parameter. Linke [Lin11] has shown that the Ehrhart function still preserves its quasi-polynomial structure when considered with positive real dilations instead only integer dilations. One of her main observations was that for a rational polytope P and $p, q \in \mathbb{Z}_{>0}$, one may use $L_P(p/q) = L_{\frac{1}{q}P}(p)$ and this relation indeed extends to the quasi-coefficients. Letting $e_k(P; t) := e_k(t)$, Linke showed that

$$e_k(P; p/q) = e_k\big((1/q)P; p\big)\, q^k. \tag{6.8}$$

Assuming further that P is full-dimensional, Linke showed that the quasi-coefficients $e_k(P; t)$ are piecewise polynomials of degree $d - k$ with discontinuities only at rational points, which makes the extension to real dilates straightforward.

Taking this observation into account together with the fact that our methods enable the consideration of real dilations quite naturally, we state our results for all positive real dilations. We do note, however, that as long as we retrict attention to the class of *all* rational polytopes, the main content of the theorems relies only on the integer dilations due to the reduction (6.8) above.

A subtle but important difference occurs when one fixes a single polytope P and compares its Ehrhart function $L_P(t)$ for integer versus real dilations, the latter carrying much more information. In the case where integer translations $P + w$ are considered, we note that the invariance $L_{P+w}(t) = L_P(t)$ is only guaranteed for integer dilations. Recently, Royer has carried out a detailed and extended study of precisely such an analysis. (Royer [Roy17a; Roy17b]).

The chapter is organized as follows. In Section 6.2 we state our main results. Section 6.3 contains a summary of the main results from Diaz, Le and Robins [DLR16]. Section 6.4 has a proof of the longest theorem of this chapter, a local formula for the quasi-coefficient $a_{d-2}(t)$. Section 6.5 shows how the formula for the solid angle sum quasi-coefficients can be used to determine the Ehrhart quasi-coefficients and we use this to obtain formulas for $e_{d-1}(t)$ and $e_{d-2}(t)$. Section 6.6 has examples of applications of these formulas to some three dimensional polytopes.

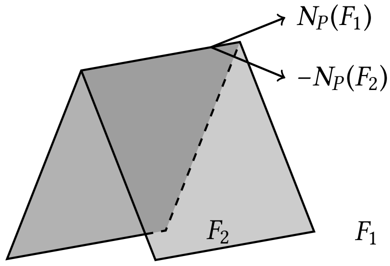

Figure 6.1: *The normal vectors of two facets, used in the computation of c_G.*

Finally, in Section 6.7 we define some interesting families of polytopes called 'concrete polytopes', for which the solid angle sum is trivial, in the sense that $A_P(t) = \mathrm{vol}(P)t^d$ for all positive integers t. We prove that a sufficient condition for such a phenomenon is that the polytope tiles Euclidean space by the Hyperoctahedral group, together with translations. It is still an open question to determine necessary and sufficient conditions for the occurrence of concrete polytopes.

6.2 Main results

The first main result is an explicit, local formula for the codimension two coefficient $a_{d-2}(t)$ of the solid angle sum $A_P(t)$ of any rational polytope P. We begin defining some local parameters at each face of P, which appear in the statements of our results. Let P be a d-dimensional rational polytope in $\mathbb{R}^d$. For each face F of P, let Λ_F be the lattice of integer vectors orthogonal to $\mathrm{lin}(F)$,

$$\Lambda_F := \mathrm{lin}(F)^\perp \cap \mathbb{Z}^d.$$

If F is a face of P and G is a facet of F, denote by $N_F(G)$ the unit normal vector in $\mathrm{lin}(F)$ pointing outward to G. For a $(d-2)$-dimensional face G of P, let $F_1 = F_1(G)$ and $F_2 = F_2(G)$ be the two facets whose intersection defines G. The solid angle of G, also called the *dihedral angle* of the edge when $d = 3$, can be computed as the angle between the normal vectors $N_P(F_1)$ and $-N_P(F_2)$ (see Figure 6.1). We let c_G denotes the cosine of this angle,

$$c_G := -\langle N_P(F_1), N_P(F_2)\rangle,$$

so that $\omega_P(G) = \arccos(c_G)/(2\pi)$. Let v_{F_1}, v_{F_2} be the primitive integer vectors in the directions of $N_P(F_1)$ and $N_P(F_2)$ and let $v_{F_1,G}$, $v_{F_2,G}$ be the Λ_G^*-primitive vectors in the directions of $N_{F_1}(G)$ and $N_{F_2}(G)$ (Λ_G^* stands for the dual lattice, see definition in Section 2.4.1). Let $\bar{x}_G$ be the projection of G onto $\mathrm{lin}(G)^\perp$,

$$\bar{x}_G := \mathrm{Proj}_{\mathrm{lin}(G)^\perp}(G),$$

and x_1, x_2 be the coordinates of $\bar{x}_G$ in terms of $v_{F_1,G}$ and $v_{F_2,G}$,

$$\bar{x}_G = x_1 v_{F_1,G} + x_2 v_{F_2,G}.$$

We can't assume that $v_{F_1,G}$ and $v_{F_2,G}$ form a basis for the lattice Λ_G^*, however since $v_{F_1,G}$

is a Λ_G^*-primitive vector, we can set $v_1 := v_{F_1,G}$ and find $v_2 \in \Lambda_G^*$ such that $\{v_1, v_2\}$ is a basis for the lattice Λ_G^*. Let h and k be the coprime integers such that

$$v_{F_2,G} = hv_1 + kv_2$$

(they are coprime since $v_{F_2,G}$ is Λ_G^*-primitive). Substituting v_2 by $-v_2$ if necessary, we may assume that k is positive and considering the basis operation $v_2 \mapsto v_2 + av_1$ with $a \in \mathbb{Z}$, we see that we may also choose v_2 such that $0 \le h < k$ (we are essentially using lattice basis reduction, for just dimension 2). Adapting an equivalent definition given by Pommersheim [Pom93, Section 6], we will say that the cone $\mathrm{fcone}(P, G)$ has *type* (h, k). We defined h and k in terms of the primitive vectors from Λ_G^*, however the same values could also have been obtained in terms of a similar relation between the primitive vectors from Λ_G, see Lemma 6.4.1

In order to describe more precisely the building blocks of the quasi-coefficients for both Ehrhart and solid angle polynomials, we consider the usual r'th Bernoulli polynomial, defined by the generating function

$$\frac{ze^{xz}}{e^z - 1} = \sum_{r\ge 0} \frac{B_r(x)}{r!} z^r,$$

so that the first couple are given by $B_1(x) = x - 1/2$ and $B_2(x) = x^2 - x + 1/6$. But here we truncate it, so that it is now supported on the unit interval: $B_r(x) := 0$, for $x \notin [0, 1]$. Now we may define the *periodized Bernoulli polynomials* as:

$$\overline{B}_1(x) := \begin{cases} B_1(x - \lfloor x \rfloor) & \text{when } x \notin \mathbb{Z}, \\ 0 & \text{when } x \in \mathbb{Z}, \end{cases}$$

and

$$\overline{B}_r(x) := B_r(x - \lfloor x \rfloor)$$

for all $r > 1$.

The parameters h and k from $\mathrm{fcone}(P, G)$ play an important role in the following sums. For any h, k coprime positive integers and $x, y \in \mathbb{R}$ the *Dedekind-Rademacher sum*, introduced by Rademacher [Rad64], is defined as

$$s(h, k; x, y) := \sum_{r \bmod k} \overline{B}_1\left(h\frac{r + y}{k} + x\right) \overline{B}_1\left(\frac{r + y}{k}\right). \tag{6.9}$$

Note that when x and y are both integers, this sum reduces to the classical *Dedekind sum*

$$s(h, k) := \sum_{r \bmod k} \overline{B}_1\left(\frac{rh}{k}\right) \overline{B}_1\left(\frac{r}{k}\right).$$

With these local parameters, we obtain the following formula for $a_{d-2}(t)$. We remark that in Theorem 6.2.1, each codimension two face G in the summation has its own local geometric data, namely: the type (h, k), and the parameters x_1, x_2, F_1, F_2.

Theorem 6.2.1. *Let $P \subset \mathbb{R}^d$ be a full-dimensional rational polytope. Then for positive real values of t, the codimension two quasi-coefficient of the solid angle sum $A_P(t)$ has the following finite form:*

$$a_{d-2}(t) = \sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G) \Bigg[\frac{c_G}{2k} \left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|} \overline{B}_2\big(\langle v_{F_1}, \bar{x}_G \rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|} \overline{B}_2\big(\langle v_{F_2}, \bar{x}_G \rangle t\big) \right)$$
$$+ \left(\omega_P(G) - \frac{1}{4} \right) \mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) - s\big(h, k; (x_1 + hx_2)t, -kx_2 t\big) \Bigg].$$

An important special case of Theorem 6.2.1 is the collection of integer polytopes, and the restriction to integer dilations t, as follows.

Corollary 6.2.2. *Let $P \subset \mathbb{R}^d$ be a full-dimensional integer polytope. Then for positive integer values of t, the codimension two coefficient of the solid angle sum $A_P(t)$ has the following finite form:*

$$a_{d-2} = \sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G) \left[\frac{c_G}{12k} \left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|} \right) + \omega_P(G) - \frac{1}{4} - s(h,k) \right].$$

In particular, for $d = 3$ or 4, let P be a full-dimensional integer polytope in $\mathbb{R}^d$. Then for positive integer values of t its solid angle sum is:

$$A_P(t) = \mathrm{vol}(P)t^d + \sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G) \left[\frac{c_G}{12k} \left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|} \right) + \omega_P(G) - \frac{1}{4} - s(h,k) \right] t^{d-2}.$$

In the last section, we study the question of which rational polytopes $P \subset \mathbb{R}^d$ have the special property that their discrete volumes are equal to their continuous volume. Namely, we would like to know when

$$A_P(t) = \mathrm{vol}(P)t^d, \tag{6.10}$$

for all integer dilations t. We exhibit a general family of polytopes that obey such a discrete-continuous property. In particular, suppose we begin with a rational polytope $P \subset \mathbb{R}^d$, and symmetrize it with respect to the hyperoctahedral group, obtaining an element Q of the polytope group (defined in Section 6.7). If Q multi-tiles (see Equation (6.26)) $\mathbb{R}^d$ by translations, then we prove in Theorem 6.7.4 that the original polytope P enjoys property (6.10). Previously known families of such polytopes arose from tiling (and multi-tiling) $\mathbb{R}^d$ by translations only. Here Theorem 6.7.4 extends the known families by introducing a non-abelian group.

Returning to Ehrhart quasi-polynomials, in Section 6.5 we adapt a technique from Barvinok [Bar06] to prove Theorem 6.5.1, showing how the solid angle sum quasi-polynomial of a rational polytope gives the Ehrhart quasi-polynomial, for all positive real t. This might seem counter-intuitive at first, because the solid angle sum polynomials are built up from a local metric at each integer point, while the Ehrhart polynomials are purely combinatorial objects. In particular, we obtain the following finite form for the codimension two quasi-coefficient. To state the result, we define the one-sided limits

$$\overline{B}_1^+(x) := \lim_{\epsilon \to 0^+} \overline{B}_1(x+\epsilon) \quad \text{and} \quad \overline{B}_1^-(x) := \lim_{\epsilon \to 0^+} \overline{B}_1(x-\epsilon),$$

which differ from $\overline{B}_1(x)$ only at the integers: $\overline{B}_1^+(n) = -1/2$ and $\overline{B}_1^-(n) = 1/2$ for $n \in \mathbb{Z}$.

Theorem 6.2.3. *Let $P \subset \mathbb{R}^d$ be a full-dimensional rational polytope. Then for all positive real values of t, the codimension two quasi-coefficient of the Ehrhart function $L_P(t)$ has the following finite form:*

$$e_{d-2}(t) = \sum_{\substack{G \in \mathcal{F}(P), \\ \dim(G)=d-2}} \mathrm{vol}^*(G) \Bigg[\frac{c_G}{2k} \left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|} \overline{B}_2\big(\langle v_{F_1}, \bar{x}_G \rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|} \overline{B}_2\big(\langle v_{F_2}, \bar{x}_G \rangle t\big) \right)$$

$$- s\big(h, k; (x_1 + hx_2)t, -kx_2 t\big) - \frac{1}{2} \mathbb{1}_{\mathbb{Z}}(kx_1 t)\, \overline{B}_1\big((h^{-1}x_1 + x_2)t\big) - \frac{1}{2} \mathbb{1}_{\mathbb{Z}}(kx_2 t) \overline{B}_1^+\big((x_1 + hx_2)t\big) \Bigg],$$

where h^{-1} denotes an integer satisfying $h^{-1}h \equiv 1 \mod k$ if $h \neq 0$ and $h^{-1} := 1$ in case $h = 0$ and $k = 1$.

We note that if P is an integer polytope and t is an integer, then $\langle v_F, x_F \rangle\, t \in \mathbb{Z}$, and the formula from Theorem 6.2.3 simplifies as follows.

Corollary 6.2.4. *Let $P \subset \mathbb{R}^d$ be a full-dimensional integer polytope. For positive integer values of t, the codimension two coefficient of the Ehrhart polynomial $L_P(t)$ is the following:*

$$e_{d-2} = \sum_{\substack{G \in \mathcal{F}(P), \\ \dim(G)=d-2}} \mathrm{vol}^*(G) \left[\frac{c_G}{12k} \left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|} \right) - s(h,k) + \frac{1}{4} \right].$$

We note that it is possible to obtain the latter formulas for the Ehrhart quasi-coefficients using the methods of Berline and Vergne [BV07] (see [BV07, Proposition 31] pertaining to a formula corresponding to Theorem 6.2.3, although the correspondence is a nontrivial notational task). We expand on their approach in Section 5.2.2.

6.2.1 Comments about algorithmic aspects

In this section we show how to compute the local parameters in the formula from Theorem 6.2.1, provided we are given the hyperplane description of the polytope. This formula uses the volumes of the faces of P, and we recall that the theoretical complexity of computing volumes of polytopes, from their facet description, is known to be $\#P$-hard (see [DF88]). In addition, the formula (Theorem 6.2.1) also uses solid-angles, which may be irrational. We therefore don't make statements about the theoretical complexity of computing with such formula. However we remark that in practice such computations can be approximated (for the solid-angles), especially if the dimension of the polytope is fixed (see [DF88]).

For an integer vector $x \in \mathbb{Z}^d$, denote by $\gcd(x)$ the greatest common divisor of its entries. Let the defining inequalities of the two facets F_1 and F_2 incident to a $(d-2)$-dimensional face G be $\langle a_1, x\rangle \le b_1$ and $\langle a_2, x\rangle \le b_2$, with $a_1, a_2 \in \mathbb{Z}^d$ and $b_1, b_2 \in \mathbb{Z}$. Since a_j is an outward-pointing normal vector to F_j, we can compute $v_{F_j} = \frac{1}{\gcd(a_j)} a_j$. Hence $c_G := -\langle N_P(F_1), N_P(F_2)\rangle = -\frac{\langle v_{F_1}, v_{F_2}\rangle}{\|v_{F_1}\|\|v_{F_2}\|}$.

Next we show how a lattice basis for Λ_G^* can be computed. We observe that by Lemma 2.4.3 below, Λ_G^* corresponds to the orthogonal projection of $\mathbb{Z}^d$ onto $\mathrm{lin}(G)^\perp$. Denoting the $d \times 2$ matrix with columns v_{F_1} and v_{F_2} by U, we have that $P = U(U^\top U)^{-1}U^\top$ is the orthogonal projection onto $\mathrm{lin}(G)^\perp$. Indeed, one can check directly that $PU = U$, $P^2 = P$ and $Pv = 0$ for any $v \in \mathrm{lin}(G)$. Therefore the columns of P generate Λ_G^*. From a set of generating vectors, one can compute a lattice basis by an application of the LLL-algorithm (as described by Buchmann and Pohst [BP89]).

Let $m = 1$ and $j = 2$, or $m = 2$ and $j = 1$. We now proceed to compute $v_{F_m,G}$, the Λ_G^*-primitive vector in the direction of $N_{F_m}(G)$. Let

$$f_{m,j} := \langle v_{F_m}, v_{F_m}\rangle v_{F_j} - \langle v_{F_m}, v_{F_j}\rangle v_{F_m}. \tag{6.11}$$

It is an integer vector in $\mathrm{lin}(G)^\perp$ orthogonal to v_{F_m} and since $\langle f_{m,j}, v_{F_j}\rangle > 0$ (by Cauchy-Schwarz), it is a vector in the same direction of $N_{F_m}(G)$. Since $f_{m,j} \in \mathbb{Z}^d \cap \mathrm{lin}(G)^\perp \subseteq \Lambda_G^*$, it has integral coordinates in the computed basis for Λ_G^*. Computing them and dividing by their gcd, we get $v_{F_m,G}$.

Having a lattice basis for Λ_G^*, its determinant $\det(\Lambda_G^*)$ can be computed directly. Also, using $v_{F_1,G}$ and $v_{F_2,G}$, we can compute v_2 such that $v_1 := v_{F_1,G}$ and v_2 is a lattice basis. Hence we can also compute h and k. To compute x_1 and x_2, we can use $\bar{x}_G = Px_G$ if we already know a point $x_G \in G$ and then write $\bar{x}_G$ in terms of $v_{F_1,G}$ and $v_{F_2,G}$. More generally, we observe that for any point $x_G \in G$ we must have $\langle a_1, x_G\rangle = b_1$ and $\langle a_2, x_G\rangle = b_2$, so:

$$\begin{aligned}
b_2 = \langle a_2, \bar{x}_G\rangle &= \|a_2\| \left\langle N_P(F_2), x_1 v_{F_1,G} + x_2 v_{F_2,G}\right\rangle \\
&= x_1\|a_2\|\|v_{F_1,G}\| \left\langle N_P(F_2), N_{F_1}(G)\right\rangle = x_1\|a_2\|\|v_{F_1,G}\|\sqrt{1-c_G^2} \\
&= x_1\|a_2\|\,|\det(v_{F_1,G}, v_{F_2,G})|/\|v_{F_2,G}\| = x_1\|a_2\|k/\|v_{F_2}\|,
\end{aligned}$$

(see the proof of Lemma 6.4.1) thus

$$x_1 = \frac{b_2}{k\gcd(a_2)}, \quad \text{and analogously,} \quad x_2 = \frac{b_1}{k\gcd(a_1)}.$$

For the Dedekind-Rademacher sums, Rademacher [Rad64] proves the following theorem that allows one to compute them efficiently, by proceeding as in the Euclidean algorithm.

Theorem 6.2.5. *If h and k are both relatively prime, and x and y are any real numbers, then*

$$s(h,k;x,y) + s(k,h;y,x) = -\frac{1}{4}\mathbb{1}_{\mathbb{Z}}(x)\mathbb{1}_{\mathbb{Z}}(y) + \overline{B}_1(x)\overline{B}_1(y)$$

$$+\frac{1}{2}\left(\frac{h}{k}\overline{B}_2(y)+\frac{1}{hk}\overline{B}_2(kx+hy)+\frac{k}{h}\overline{B}_2(x)\right).$$

We note that there exists the following periodicity, when m is an integer:

$$s(h,k;x,y)=s(h-mk,k;x+my,y),$$

and the following special cases:

$$s(1,k;0,0)=\frac{k}{12}+\frac{1}{6k}-\frac{1}{4},\quad s(1,k;0,y)=\frac{k}{12}+\frac{1}{k}\overline{B}_2(y).$$

6.3 Fourier transforms of polytopes and solid angle sums

In this section we present a summary of the main results from Diaz, Le, and Robins [DLR16]. The method from Diaz, Le, and Robins consists of two steps: First, the solid angles are written with convolutions and the solid angle sum is represented with the series from Lemma 2.5.2, next the Poisson summation formula is applied to represent $A_P(t)$ as a series with the Fourier transform of P, leading to (cf. Diaz, Le, and Robins [DLR16, Lemma 2]):

Lemma 6.3.1. *Let P be a full-dimensional polytope P in $\mathbb{R}^d$ and t any positive real number. Then the solid angle sum of P can be written as follows:*

$$A_P(t)=t^d\lim_{\epsilon\to 0^+}\sum_{\xi\in\mathbb{Z}^d}\hat{\mathbb{1}}_P(t\xi)e^{-\pi\epsilon\|\xi\|^2}.$$

Using the method described in Section 5.1, through successive applications of Stokes formula (in the frequency space of Poisson summation), the Fourier transform of P is then written as a sum over the faces of P [DLR16, Theorem 1]. By treating these terms carefully, keeping track of 'generic' and 'nongeneric' frequency vectors on the right-hand-side of Poissson summation, one can find local formulas for the coefficients $a_{d-k}(t)$. Recall that the Gaussian function $\phi_{d,\epsilon} := e^{-d/2}e^{-\pi\|x\|^2/\epsilon}$, has Fourier transform $\hat{\phi}_{d,\epsilon}(\xi)=e^{-\epsilon\pi\|\xi\|^2}$ (see e.g., [SW71, Chapter I, Theorem 1.13]), which we also denote by $\hat{\phi}_\epsilon(\xi)$. The next result from Diaz, Le, and Robins gives a formula for $a_k(t)$, for any positive real t:

Theorem 6.3.2. *[DLR16, Theorem 2] Let P be a full-dimensional rational polytope in $\mathbb{R}^d$, and t be a positive real number. Then we have $A_P(t)=\sum_{k=0}^d a_k(t)t^k$, where, for $0\le k\le d$,*

$$a_k(t)=\lim_{\epsilon\to 0^+}\sum_{\substack{T\in\mathfrak{C}(P):\\ l(T)=d-k}}\sum_{\xi\in\mathbb{Z}^d\cap S(T)}\mathcal{R}_T(\xi)\mathcal{E}_T(t\xi)\hat{\phi}_\epsilon(\xi).$$

Using this theorem one can get more explicit formulas for the coefficients, although their complexity increases with the length of the chains considered. For the quasi-coefficient $a_{d-1}(t)$, we have the following known formula, given in terms of the facets of P

and the periodized Bernoulli polynomial $\overline{B}_1$:

Theorem 6.3.3. *[DLR16, Theorem 3] Let P be a full-dimensional rational polytope. Then the codimension one quasi-coefficient of the solid angle sum $A_P(t)$ has the following local formula for all positive real values of t:*

$$a_{d-1}(t) = -\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \mathrm{vol}^*(F)\overline{B}_1\big(\langle v_F, x_F\rangle\, t\big),$$

where x_F is any point in F and v_F is the primitive integer vector in the direction of $N_P(F)$.

6.4 Proofs of Theorem 6.2.1 and Corollary 6.2.2

We start with a lemma that shows how the 'type (h,k)' simultaneously describes the relation of $\mathrm{fcone}(P,G)$ with respect to Λ_G and with Λ_G^*.

Lemma 6.4.1. *If h and k are such that $v_1 := v_{F_1,G}$ and $v_2 := (v_{F_2,G} - h v_{F_1,G})/k$ form a lattice basis for Λ_G^* (as defined above), then*

$$u_1 := v_{F_1} \text{ and } u_2 := (v_{F_2} + h v_{F_1})/k$$

form a lattice basis for Λ_G. In particular,

$$k = \frac{|\det(v_{F_1,G}, v_{F_2,G})|}{\det(\Lambda_G^*)} = \frac{|\det(v_{F_1}, v_{F_2})|}{\det(\Lambda_G)}.$$

Proof. We have to prove that $\langle v_{F_1,G}, v_{F_2}\rangle = \langle v_{F_2,G}, v_{F_1}\rangle = k$. Using this, the lemma follows directly from the following computation:

$$\begin{aligned}(v_2, v_1)^\mathsf{T}(u_1,u_2) &= \begin{pmatrix} -h/k & 1/k \\ 1 & 0\end{pmatrix}(v_{F_1,G}, v_{F_2,G})^\mathsf{T}(v_{F_1}, v_{F_2})\begin{pmatrix} 1 & h/k \\ 0 & 1/k\end{pmatrix} \\ &= \begin{pmatrix} -h/k & 1/k \\ 1 & 0\end{pmatrix}\begin{pmatrix} 0 & k \\ k & 0\end{pmatrix}\begin{pmatrix} 1 & h/k \\ 0 & 1/k\end{pmatrix} = k\begin{pmatrix} -h/k & 1/k \\ 1 & 0\end{pmatrix}\begin{pmatrix} 0 & 1/k \\ 1 & h/k\end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1\end{pmatrix}.\end{aligned}$$

Since we work simultaneously with two orthonormal basis $\{N_P(F_1), N_{F_1}(G)\}$ and $\{N_P(F_2), N_{F_2}(G)\}$ for $\mathrm{lin}(G)^\perp$, it is useful to know how they are related. From the outward orientation of the normal vectors (see Figure 6.2), we have

$$\begin{aligned} N_P(F_2) &= -c_G N_P(F_1) + \sqrt{1-c_G^2}N_{F_1}(G), \text{ and} \\ N_{F_2}(G) &= \sqrt{1-c_G^2}N_P(F_1) + c_G N_{F_1}(G). \end{aligned} \tag{6.12}$$

We prove $\langle v_{F_1,G}, v_{F_2}\rangle = k$, since the proof for the other inner product is the same. The Λ_G-primitive vector v_{F_2} along $N_P(F_2)$ and the Λ_G^*-primitive vector $v_{F_2,G}$ along $N_{F_2}(G)$ have a special relation. Using Lemma 2.4.1 with $\Lambda := \Lambda_G$ and L as the one dimensional lattice spanned by v_{F_2}, we get

$$\|v_{F_2}\| = \det(\Lambda_G)\|v_{F_2,G}\|. \tag{6.13}$$

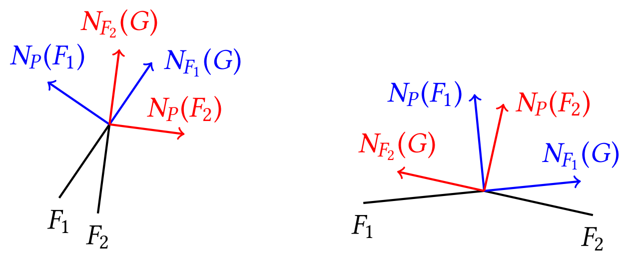

Figure 6.2: *Relative orientations between the normal vectors of each facet.*

Next we establish an identity developing $\det(v_{F_1,G}, v_{F_2,G})$ in two ways:

$$\begin{aligned}\det(v_{F_1,G}, v_{F_2,G})^2 &= \det\left((v_{F_1,G}, v_{F_2,G})^{\mathsf{T}}(v_{F_1,G}, v_{F_2,G})\right)\\ &= \|v_{F_1,G}\|^2\|v_{F_2,G}\|^2 - \langle v_{F_1,G}, v_{F_2,G}\rangle^2 = \|v_{F_1,G}\|^2\|v_{F_2,G}\|^2(1-c_G^2),\end{aligned}$$

and

$$\begin{aligned}\det(v_{F_1,G}, v_{F_2,G})^2 &= \det\left((v_{F_1,G}, v_{F_2,G})^{\mathsf{T}}(v_{F_1,G}, v_{F_2,G})\right)\\ &= \det\left(\left(\begin{smallmatrix}1 & h\\ 0 & k\end{smallmatrix}\right)^{\mathsf{T}}(v_1, v_2)^{\mathsf{T}}(v_1, v_2)\left(\begin{smallmatrix}1 & h\\ 0 & k\end{smallmatrix}\right)\right) = k^2\det(\Lambda_G^*)^2 = k^2/\det(\Lambda_G)^2.\end{aligned}$$

Finally,

$$\left\langle v_{F_1,G}, v_{F_2}\right\rangle = \|v_{F_1,G}\|\|v_{F_2}\|\left\langle N_{F_1}(G), N_P(F_2)\right\rangle = \|v_{F_1,G}\|\|v_{F_2,G}\|\det(\Lambda_G)\sqrt{1-c_G^2} = k. \qquad \square$$

We now proceed to the main result of the chapter, whose proof is somewhat longer, and is subdivided into several sections.

Theorem 6.2.1. *Let $P \subset \mathbb{R}^d$ be a full-dimensional rational polytope. Then for positive real values of t, the codimension two quasi-coefficient of the solid angle sum $A_P(t)$ has the following finite form:*

$$\begin{aligned}a_{d-2}(t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G)\Bigg[&\frac{c_G}{2k}\left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|}\overline{B}_2\big(\langle v_{F_1}, \bar{x}_G\rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|}\overline{B}_2\big(\langle v_{F_2}, \bar{x}_G\rangle t\big)\right)\\ &+\left(\omega_P(G) - \frac{1}{4}\right)\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) - s\big(h, k; (x_1 + hx_2)t, -kx_2t\big)\Bigg].\end{aligned}$$

6.4.1 Proof of Theorem 6.2.1

We start with the formula from Theorem 6.3.2 and consider all chains $(P \longrightarrow F \longrightarrow G)$ of length 2:

$$a_{d-2}(t) = \lim_{\epsilon\to 0^+}\frac{1}{(-2\pi i)^2}\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}}\ \sum_{\substack{G\in\mathcal{F}(F)\\ \dim(G)=d-2}} \mathrm{vol}(G)$$

$$\sum_{\xi \in \Lambda_G \setminus \Lambda_F} \frac{\langle \xi, N_P(F) \rangle \left\langle \mathrm{Proj}_F(\xi), N_F(G) \right\rangle}{\langle \xi, \xi \rangle \left\langle \mathrm{Proj}_F(\xi), \mathrm{Proj}_F(\xi) \right\rangle} e^{-2\pi i \langle \xi, t\bar{x}_G \rangle} \hat{\phi}_\epsilon(\xi).$$

Since $N_P(F)$ and $N_F(G)$ form an orthonormal basis for $\mathrm{lin}(G)^\perp$, for $\xi \in \mathrm{lin}(G)^\perp$, we have $\mathrm{Proj}_F(\xi) = \langle \xi, N_F(G) \rangle N_F(G)$ and we can simplify the expression above with

$$\frac{\langle \xi, N_P(F) \rangle \left\langle \mathrm{Proj}_F(\xi), N_F(G) \right\rangle}{\langle \xi, \xi \rangle \left\langle \mathrm{Proj}_F(\xi), \mathrm{Proj}_F(\xi) \right\rangle} = \frac{\langle \xi, N_P(F) \rangle}{\langle \xi, N_F(G) \rangle \langle \xi, \xi \rangle}.$$

Denoting by F_1 and F_2 the two facets incident to a face G of dimension $d-2$, we switch the order of the sums to obtain

$$a_{d-2}(t) = \sum_{\substack{G \in \mathcal{F}(P), \\ \dim(G) = d-2}} \lim_{\epsilon \to 0^+} \frac{\mathrm{vol}(G)}{(-2\pi i)^2} \sum_{j=1}^{2} \sum_{\xi \in \Lambda_G \setminus \Lambda_{F_j}} \frac{\langle \xi, N_P(F_j) \rangle e^{-2\pi i \langle \xi, t\bar{x}_G \rangle}}{\langle \xi, N_{F_j}(G) \rangle \langle \xi, \xi \rangle} \hat{\phi}_\epsilon(\xi).$$

It follows from Lemma 2.4.1 that $\det(\mathrm{lin}(G) \cap \mathbb{Z}^d) = \det(\mathrm{lin}(G)^\perp \cap \mathbb{Z}^d) =: \det(\Lambda_G)$. We note that we are using here the property that P is a rational d-dimensional polytope, so that $(\mathrm{lin}(G) \cap \mathbb{Z}^d)^\perp = \mathrm{lin}(G)^\perp \cap \mathbb{Z}^d$. We therefore conclude that

$$\mathrm{vol}^*(G) := \frac{\mathrm{vol}(G)}{\det(\mathrm{lin}(G) \cap \mathbb{Z}^d)} = \frac{\mathrm{vol}(G)}{\det(\Lambda_G)}.$$

We decompose the expression into three distinct sums:

$$a_{d-2}(t) = \sum_{\substack{G \in \mathcal{F}(P), \\ \dim(G) = d-2}} \mathrm{vol}^*(G) \big(b_1(G;t) + b_2(G;t) + c(G;t) \big), \tag{6.14}$$

where for $j = 1$ and $m = 2$, or for $j = 2$ and $m = 1$, we define

$$b_j(G;t) := \lim_{\epsilon \to 0^+} \frac{\det(\Lambda_G)}{(-2\pi i)^2} \sum_{\xi \in \Lambda_{F_m} \setminus \{0\}} \frac{\langle \xi, N_P(F_j) \rangle e^{-2\pi i \langle \xi, t\bar{x}_G \rangle}}{\langle \xi, N_{F_j}(G) \rangle \langle \xi, \xi \rangle} \hat{\phi}_\epsilon(\xi),$$

and

$$c(G;t) := \lim_{\epsilon \to 0^+} \frac{\det(\Lambda_G)}{(-2\pi i)^2} \sum_{\xi \in \Lambda_G \setminus (\Lambda_{F_1} \cup \Lambda_{F_2})} \left(\frac{\langle \xi, N_P(F_1) \rangle}{\langle \xi, N_{F_1}(G) \rangle} + \frac{\langle \xi, N_P(F_2) \rangle}{\langle \xi, N_{F_2}(G) \rangle} \right) \frac{e^{-2\pi i \langle \xi, t\bar{x}_G \rangle}}{\langle \xi, \xi \rangle} \hat{\phi}_\epsilon(\xi).$$

Next we treat each of these terms separately. The sum in $b_j(G;t)$ is simpler and is dealt with a direct application of Theorem 2.5.3, which is in fact an application of Poisson summation. The sum in $c(G;t)$ takes more work and, after some preparation, is also dealt with the help of Theorem 2.5.3 (this time it is a 2-dimensional lattice sum minus two lines) and in the end we recognize the occurrence of a Dedekind-Rademacher sum on each $(d-2)$-dimensional face of P.

Computation of $b_j(G;t)$

Let $j=1$ and $m=2$, or $j=2$ and $m=1$. To compute $b_j(G;t)$, write $\xi \in \Lambda_{F_m}$ as $\xi = r v_{F_m}$ with $r \in \mathbb{Z}$:

$$b_j(G;t) = \lim_{\epsilon \to 0^+} \frac{\det(\Lambda_G)}{(-2\pi i)^2} \sum_{r \in \mathbb{Z}\setminus\{0\}} \frac{\langle v_{F_m}, N_P(F_j)\rangle e^{-2\pi i r \langle v_{F_m}, t\bar{x}_G\rangle}}{\langle v_{F_m}, N_{F_j}(G)\rangle \|v_{F_m}\|^2 r^2} \hat{\phi}_\epsilon(r),$$

where we use that $\hat{\phi}_\epsilon(r v_{F_m}) = \hat{\phi}_{\epsilon\|v_{F_m}\|^2}(r)$ and note that this can be replaced by $\hat{\phi}_\epsilon(r)$ due to the limit in ϵ.

Next, note that $\langle v_{F_m}, N_P(F_j)\rangle = \|v_{F_m}\|\langle N_P(F_m), N_P(F_j)\rangle = -\|v_{F_m}\| c_G$ and that $\langle v_{F_m}, N_{F_j}(G)\rangle = \|v_{F_m}\|\langle N_P(F_m), N_{F_j}(G)\rangle = \|v_{F_m}\|\sqrt{1-c_G^2}$, so

$$\frac{\langle v_{F_m}, N_P(F_j)\rangle}{\langle v_{F_m}, N_{F_j}(G)\rangle} = \frac{-c_G}{\sqrt{1-c_G^2}}.$$

We substitute this and recognize the 1-dimensional sum $L_{\mathbb{Z}}((1),(2);\langle v_{F_m}, t\bar{x}_G\rangle)$:

$$b_j(G;t) = \frac{-c_G \det(\Lambda_G)}{\sqrt{1-c_G^2}\|v_{F_m}\|^2} \lim_{\epsilon \to 0^+} \frac{1}{(2\pi i)^2} \sum_{r \in \mathbb{Z}\setminus\{0\}} \frac{e^{-2\pi i r \langle v_{F_m}, t\bar{x}_G\rangle}}{r^2} \hat{\phi}_\epsilon(r).$$

Let I be the interval $I := [\langle v_{F_m}, t\bar{x}_G\rangle, \langle v_{F_m}, t\bar{x}_G\rangle + 1]$ and apply Theorem 2.5.3:

$$b_j(G;t) = \frac{c_G \det(\Lambda_G)}{2\sqrt{1-c_G^2}\|v_{F_m}\|^2} \sum_{n \in \mathbb{Z}\cap I} B_2\big(n - \langle v_{F_m}, t\bar{x}_G\rangle\big)\omega_I(n).$$

Depending on $\langle v_{F_m}, t\bar{x}_G\rangle$ being an integer or not, the sum may have one or two terms. In either case, since $B_2(0) = B_2(1)$ and since $\overline{B}_2$ is an even function,

$$b_j(G;t) = \frac{c_G \det(\Lambda_G)}{2\sqrt{1-c_G^2}\|v_{F_m}\|^2} \overline{B}_2\big(\langle v_{F_m}, \bar{x}_G\rangle t\big).$$

Recalling $\det(\Lambda_G) = |\det(v_{F_1}, v_{F_2})|/k$ (Lemma 6.4.1), we get

$$b_j(G;t) = \frac{c_G\|v_{F_j}\|}{2k\|v_{F_m}\|} \overline{B}_2\big(\langle v_{F_m}, \bar{x}_G\rangle t\big). \tag{6.15}$$

Computation of $c(G;t)$

The expression

$$\frac{1}{\langle \xi, \xi\rangle}\left(\frac{\langle \xi, N_P(F_1)\rangle}{\langle \xi, N_{F_1}(G)\rangle} + \frac{\langle \xi, N_P(F_2)\rangle}{\langle \xi, N_{F_2}(G)\rangle}\right)$$

becomes simpler if we write $N_P(F_1)$, $N_P(F_2)$, and ξ in terms of $N_{F_1}(G)$ and $N_{F_2}(G)$.

From (6.12), we obtain

$$\begin{aligned} N_P(F_1) &= \frac{-c_G}{\sqrt{1-c_G^2}} N_{F_1}(G) + \frac{1}{\sqrt{1-c_G^2}} N_{F_2}(G), \text{ and} \\ N_P(F_2) &= \frac{1}{\sqrt{1-c_G^2}} N_{F_1}(G) + \frac{-c_G}{\sqrt{1-c_G^2}} N_{F_2}(G). \end{aligned} \tag{6.16}$$

To write $\xi \in \Lambda_G$ as a combination of $N_{F_1}(G)$ and $N_{F_2}(G)$, write $\xi = AN_{F_1}(G) + BN_{F_2}(G)$, take inner-products with $N_{F_1}(G)$ and $N_{F_2}(G)$ and solve a linear system to obtain:

$$\xi = \left(\frac{\langle \xi, N_{F_1}(G)\rangle - c_G\langle \xi, N_{F_2}(G)\rangle}{1-c_G^2}\right) N_{F_1}(G) + \left(\frac{-c_G\langle \xi, N_{F_1}(G)\rangle + \langle \xi, N_{F_2}(G)\rangle}{1-c_G^2}\right) N_{F_2}(G). \tag{6.17}$$

Next we add the two fractions

$$\frac{\langle \xi, N_P(F_1)\rangle}{\langle \xi, N_{F_1}(G)\rangle} + \frac{\langle \xi, N_P(F_2)\rangle}{\langle \xi, N_{F_2}(G)\rangle} = \frac{\langle \xi, N_{F_2}(G)\rangle\langle \xi, N_P(F_1)\rangle + \langle \xi, N_{F_1}(G)\rangle\langle \xi, N_P(F_2)\rangle}{\langle \xi, N_{F_1}(G)\rangle\langle \xi, N_{F_2}(G)\rangle},$$

and substitute (6.16),

$$= \frac{\langle \xi, N_{F_1}(G)\rangle^2 + 2c_G\langle \xi, N_{F_1}(G)\rangle\langle \xi, N_{F_2}(G)\rangle + \langle \xi, N_{F_2}(G)\rangle^2}{\sqrt{1-c_G^2}\langle \xi, N_{F_1}(G)\rangle\langle \xi, N_{F_2}(G)\rangle}.$$

Substituting (6.17) into $\langle \xi, \xi\rangle$, we get that the numerator of the last expression is $(1-c_G^2)\langle \xi, \xi\rangle$, hence

$$\frac{1}{\langle \xi, \xi\rangle}\left(\frac{\langle \xi, N_P(F_1)\rangle}{\langle \xi, N_{F_1}(G)\rangle} + \frac{\langle \xi, N_P(F_2)\rangle}{\langle \xi, N_{F_2}(G)\rangle}\right) = \frac{\sqrt{1-c_G^2}}{\langle \xi, N_{F_1}(G)\rangle\langle \xi, N_{F_2}(G)\rangle}.$$

Substituting this into the definition of $c(G;t)$,

$$c(G;t) = \lim_{\epsilon \to 0^+} \frac{\sqrt{1-c_G^2}\det(\Lambda_G)}{(-2\pi i)^2} \sum_{\xi \in \Lambda_G \setminus (\Lambda_{F_1} \cup \Lambda_{F_2})} \frac{e^{-2\pi i \langle \xi, t\bar{x}_G\rangle}}{\langle \xi, N_{F_1}(G)\rangle\langle \xi, N_{F_2}(G)\rangle} \hat{\phi}_\epsilon(\xi).$$

This expression is similar to $L_\Lambda(W, e; x)$, that was considered in Section 2.5, however to use it we scale $N_{F_1}(G)$ and $N_{F_2}(G)$ to $v_{F_1,G}$ and $v_{F_2,G}$ to have vectors in the lattice Λ_G^*. Let W be the matrix with $v_{F_1,G}$ and $v_{F_2,G}$ as columns. Then

$$c(G;t) = \sqrt{1-c_G^2}\det(\Lambda_G)\|v_{F_1,G}\|\|v_{F_2,G}\| L_{\Lambda_G}(W, (1,1); t\bar{x}_G).$$

Applying Theorem 2.5.4, we get

$$c(G;t) = \frac{\sqrt{1-c_G^2}\|v_{F_1,G}\|\|v_{F_2,G}\|}{\det(W^\top W)^{1/2}} \sum_{n \in \Lambda_G^* \cap P_{W,t\bar{x}_G}} \mathcal{B}_{1,1}\left(W^+(n - t\bar{x}_G)\right)\omega_{P_{W,t\bar{x}_G}}(n),$$

where $P_{W,t\bar{x}_G} := t\bar{x}_G + W[0,1]^2$ and $W^+ := (W^\top W)^{-1}W^\top$ is the pseudoinverse of W. Noting

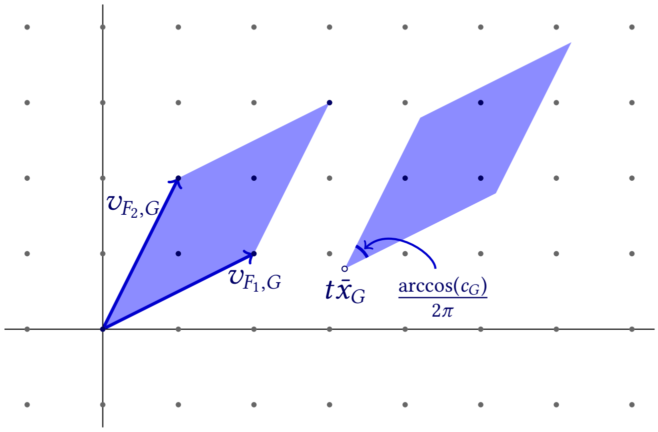

Figure 6.3: *The parallelepiped $P_{W,t\bar{x}_G}$ and the solid angle at its vertex.*

that

$$\det(W^\top W) = \|v_{F_1,G}\|^2\|v_{F_2,G}\|^2 - \langle v_{F_1,G}, v_{F_2,G}\rangle^2 = \|v_{F_1,G}\|^2\|v_{F_2,G}\|^2(1 - c_G^2),$$

we get

$$c(G;t) = \sum_{n\in\Lambda_G^*\cap P_{W,t\bar{x}_G}} \mathcal{B}_{1,1}\left(W^+(n - t\bar{x}_G)\right)\omega_{P_{W,t\bar{x}_G}}(n). \tag{6.18}$$

We now treat separately the terms in the boundary and in the interior of $P_{W,t\bar{x}_G}$.

Terms in the boundary of $P_{W,t\bar{x}_G}$

Since $P_{W,t\bar{x}_G}$ is a 2-dimensional parallelepiped, if $n \in \Lambda_G^* \cap \partial P_{W,t\bar{x}_G}$, then n is either in an edge or is a vertex of it.

If it is in an edge, say $n = t\bar{x}_G + pv_{F_1,G}$, with $0 < p < 1$, then since $v_{F_2,G} \in \Lambda_G^*$, we have that $n + v_{F_2,G}$ is in the middle of the opposite edge. Since both solid angles are equal to 1/2, n contributes to the sum with $B_1(p)B_1(0)/2$ and $n + v_{F_2,G}$ contributes with $B_1(p)B_1(1)/2$. Since $B_1(0) = -B_1(1)$, both terms cancel each other in the sum. The same situation happens in the edges spanned by $v_{F_2,G}$. Hence there is no contribution from the points in the edges.

If n is a vertex of $P_{t\bar{x}_G}$, then, since $v_{F_1,G}, v_{F_2,G} \in \Lambda_G^*$, all four vertices are points from Λ_G^* and contribute to the sum. Since $B_1(0)B_1(0) = B_1(1)B_1(1) = 1/4$ and $B_1(0)B_1(1) = -1/4$, it rests to compute the solid angles at the vertices.

Since the unit vectors in the directions of $v_{F_1,G}, v_{F_2,G}$ are $N_{F_1}(G)$ and $N_{F_2}(G)$ and $\langle N_{F_1}(G), N_{F_2}(G)\rangle = c_G$, we have that $\omega_{P_{W,t\bar{x}_G}}(t\bar{x}_G) = \arccos(c_G)/(2\pi)$ and the solid angle at the other vertex is $(\pi - \arccos(c_G))/(2\pi)$.

The contribution of the four vertices becomes

$$\frac{2}{4}\frac{\arccos(c_G) - (\pi - \arccos(c_G))}{2\pi} = \frac{\arccos(c_G)}{2\pi} - \frac{1}{4} = \omega_P(G) - \frac{1}{4}.$$

Since the condition for having the four vertices in Λ_G^* is $t\bar{x}_G \in \Lambda_G^*$, the boundary lattice points of $P_{W,t\bar{x}_G}$ contributes with

$$\sum_{n\in\Lambda_G^*\cap\partial P_{W,t\bar{x}_G}} \mathcal{B}_{1,1}(W^+(n-t\bar{x}_G))\omega_{P_{W,t\bar{x}_G}}(n) = \left(\omega_P(G)-\frac{1}{4}\right)\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) \tag{6.19}$$

to the sum (6.18). Note that this is the only term where nontrivial solid angles actually appear.

Terms in the interior of $P_{W,t\bar{x}_G}$

For the terms in sum (6.18) that are in the interior of $P_{W,t\bar{x}_G}$, we introduce a basis for the lattice Λ_G^* and write n in terms of it to recognize a Dedekind-Rademacher sum, as defined in (6.9).

Since $v_{F_1,G}$ is a Λ_G^*-primitive vector, we can set $v_1 := v_{F_1,G}$ and find $v_2\in\Lambda_G^*$ such that $\{v_1,v_2\}$ is a basis for the lattice Λ_G^*. Letting V be the matrix with v_1 and v_2 as columns, we have that $W = VA$ with $A = \left(\begin{smallmatrix}1 & h\\ 0 & k\end{smallmatrix}\right)$ and h,k coprime integers. By the choice of v_2, we may assume that k is positive and $0\le h<k$.

Now make the change of variables $n\mapsto Vn'$, so that n' lies in $V^+\Lambda_G^* = \mathbb{Z}^2$:

$$\sum_{n\in\Lambda_G^*\cap\operatorname{int}(P_{W,t\bar{x}_G})} \mathcal{B}_{1,1}(W^+(n-t\bar{x}_G)) = \sum_{n\in\mathbb{Z}^2\cap\operatorname{int}(V^+P_{W,t\bar{x}_G})} \mathcal{B}_{1,1}(A^{-1}n - tW^+\bar{x}_G).$$

We compute $A^{-1} = \left(\begin{smallmatrix}1 & -h/k\\ 0 & 1/k\end{smallmatrix}\right)$. Also recalling that $W^+\bar{x}_G =: \left(\begin{smallmatrix}x_1\\ x_2\end{smallmatrix}\right)$ and noting that $n = \left(\begin{smallmatrix}n_1\\ n_2\end{smallmatrix}\right)\in\operatorname{int}(V^+P_{W,t\bar{x}_G}) \iff A^{-1}n - tW^+\bar{x}_G\in(0,1)^2$, we have:

$$\begin{cases} 0 < n_1 - \frac{h}{k}n_2 - tx_1 < 1,\\ \quad 0 < \frac{n_2}{k} - tx_2 < 1\end{cases} \iff \begin{cases} tx_1 + \frac{h}{k}n_2 < n_1 < tx_1 + \frac{h}{k}n_2 + 1,\\ \qquad tx_2k < n_2 < tx_2k + k.\end{cases}$$

Therefore n_2 varies over all residues modulo k and for each n_2 we have only one integer n_1 (except in the boundary cases $tx_2k\in\mathbb{Z}$ and $tx_1 + \frac{h}{k}n_2\in\mathbb{Z}$, however the following stays true, since $\overline{B}_1(x) = 0$ for $x\in\mathbb{Z}$). Thus,

$$\begin{aligned}
\sum_{n\in\mathbb{Z}^2\cap\operatorname{int}(V^+P_{W,t\bar{x}_G})} \mathcal{B}_{1,1}(A^{-1}n - tW^+\bar{x}_G) &= -\sum_{r \bmod k} \overline{B}_1\left(\frac{r}{k} - tx_2\right)\overline{B}_1\left(\frac{h}{k}r + tx_1\right)\\
&= -\sum_{r \bmod k} \overline{B}_1\left(\frac{r-tkx_2}{k}\right)\overline{B}_1\left(h\frac{r-tkx_2}{k} + t(x_1+hx_2)\right)\\
&= -s\big(h,k;t(x_1+hx_2),-tkx_2\big),
\end{aligned}$$

where in the first equality we use that $\overline{B}_1(x)$ is periodic and odd. In the last equality we recognize (6.9). Hence the interior lattice points of $P_{W,t\bar{x}_G}$ contributes with

$$\sum_{n\in\Lambda_G^*\cap\operatorname{int}(P_{W,t\bar{x}_G})} \mathcal{B}_{1,1}(W^+(n-t\bar{x}_G))\omega_{P_{W,t\bar{x}_G}}(n) = -s\big(h,k;(x_1+hx_2)t,-kx_2t\big) \tag{6.20}$$

to the sum (6.18). Finally, substituting (6.15), (6.19), and (6.20) into (6.14), we obtain the expression in the statement of Theorem 6.2.1. $\square$

Next, we prove Corollary 6.2.2.

Corollary 6.2.2. *Let $P \subset \mathbb{R}^d$ be a full-dimensional integer polytope. Then for positive integer values of t, the codimension two coefficient of the solid angle sum $A_P(t)$ has the following finite form:*

$$a_{d-2} = \sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G)\left[\frac{c_G}{12k}\left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|}\right) + \omega_P(G) - \frac{1}{4} - s(h,k)\right].$$

In particular, for $d = 3$ or 4, let P be a full-dimensional integer polytope in $\mathbb{R}^d$. Then for positive integer values of t its solid angle sum is:

$$A_P(t) = \mathrm{vol}(P)t^d + \sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \mathrm{vol}^*(G)\left[\frac{c_G}{12k}\left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|}\right) + \omega_P(G) - \frac{1}{4} - s(h,k)\right]t^{d-2}.$$

Proof. The formula from Theorem 6.2.1 for $a_{d-2}(t)$ is:

$$a_{d-2}(t) = \sum_{\substack{G \in \mathcal{F}(P),\\ \dim G=d-2}} \mathrm{vol}^*(G)\left[\frac{c_G}{2k}\left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|}\overline{B}_2\big(\left\langle v_{F_1}, \bar{x}_G\right\rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|}\overline{B}_2\big(\left\langle v_{F_2}, \bar{x}_G\right\rangle t\big)\right)\right.$$
$$\left. + \left(\omega_P(G) - \frac{1}{4}\right)\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) - s\big(h,k;(x_1+hx_2)t, -kx_2t\big)\right].$$

Since now we are assuming that P is an integer polytope, all its faces have integer points and since t is an integer, we have that $\langle v_F, \bar{x}_G\rangle\, t$ is an integer and thus both occurrences of $\overline{B}_2$ evaluate to 1/6. The first term becomes

$$\frac{c_G}{12k}\left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|} + \frac{\|v_{F_1}\|}{\|v_{F_2}\|}\right).$$

Letting W be the matrix with $v_{F_1,G}$ and $v_{F_2,G}$ as columns and V being the matrix with the lattice basis v_1, v_2 of Λ_G^* as columns, recall that $\binom{x_1}{x_2} := W^+\bar{x}_G$ and $W^+ = A^{-1}V^+$, where $A^{-1} = \left(\begin{smallmatrix}1 & -h/k\\ 0 & 1/k\end{smallmatrix}\right)$. Since $\bar{x}_G = \mathrm{Proj}_{\mathrm{lin}(G)^\perp}(x_G)$ and x_G can be chosen as an integer vector in the face G, $\bar{x}_G \in \Lambda_G^*$ (by Lemma 2.4.3) and $V^+\bar{x}_G \in \mathbb{Z}^2$. Hence $\binom{x_1}{x_2} = \left(\begin{smallmatrix}1 & -h/k\\ 0 & 1/k\end{smallmatrix}\right)\binom{n_1}{n_2} = \binom{n_1 - hn_2/k}{n_2/k}$. Thus $x_1 + hx_2 = n_1 \in \mathbb{Z}$ and $kx_2 = n_2 \in \mathbb{Z}$ so the Dedekind-Radamacher sum $s\big(h,k;(x_1+hx_2)t, -kx_2t\big)$ becomes the Dedekind sum $s(h,k)$. Similarly, since $t\bar{x}_G \in \Lambda_G^*$, $\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G)$ evaluates to 1. □

6.5 Obtaining the Ehrhart quasi-coefficients $e_{d-1}(t)$ and $e_{d-2}(t)$

In this section we show how the Ehrhart quasi-polynomial can be obtained from the solid angle sum quasi-polynomial by means of a limit process and we show that this relation also extends to the quasi-coefficients. As a result we obtain local formulas for the quasi-coefficients $e_{d-1}(t)$ and $e_{d-2}(t)$ for all positive real values of t. The technique used here is an adaptation of a method used by Barvinok [Bar06] for a similar purpose, but instead of giving finite formulas, he focuses in determining the algorithmic complexity of computing $e_{d-k}(t)$ for a fixed k.

Since we are dealing with different polytopes in this section, we modify the notation and write $e_k(P;t)$ and $a_k(P;t)$ in place of $e_k(t)$ and $a_k(t)$ for the quasi-coefficients of $L_P(t)$ and $A_P(t)$ respectively.

Let $P, R \subset \mathbb{R}^d$ be d-dimensional rational polytopes. We introduce the *shifted solid angle sum*

$$A_{P,R}(t) := \sum_{x \in \mathbb{Z}^d} \omega_{tP+R}(x),$$

where the "+" stands for the Minkowski sum $P + R := \{x + y : x \in P, y \in R\}$. Since the function $\varphi(P) := \sum_{x\in\mathbb{Z}^d} \omega_{P+R}(x)$ is a valuation[1] on rational polytopes, McMullen [McM79] shows that this shifted solid angle sum can also be expressed as a quasi-polynomial

$$A_{P,R}(t) = a_d(P,R;t)t^d + a_{d-1}(P,R;t)t^{d-1} + \cdots + a_0(P,R;t),$$

with period dividing the denominator of P, and hence *does not depending* on R, for integer values of t. Moreover, this expression can be extended to real values of t in the same manner than with the Ehrhart and solid angle sum expressions (c.f. Linke [Lin11, Theorem 1.2]). Thus, if m is the denominator of P, we have $a_k(P,R;t+m) = a_k(P,R;t)$ for all $0 \le k \le d$ and $t \in \mathbb{R}$, $t > 0$.

Theorem 6.5.1. *Let $P \subset \mathbb{R}^d$ be a d-dimensional rational polytope and $a \in \operatorname{int}(P)$ be a rational vector. Then pointwise for any positive real t,*

$$L_P(t) = \lim_{\tau \to 0^+} A_{P,\tau(P-a)}(t).$$

Furthermore,

$$e_k(P;t) = \lim_{\tau\to 0^+} a_k(P, \tau(P-a); t)$$

pointwise for all $0 \le k \le d$ and positive real t.

Proof. Since $P - a$ is a polytope with the origin in its interior, for any t, $\tau > 0$ we have that $tP \subset tP + \tau(P-a)$. Further, since $\mathbb{Z}^d$ is discrete, for any fixed positive real t and all sufficiently small τ,

$$|(tP + \tau(P-a)) \cap \mathbb{Z}^d| = |tP \cap \mathbb{Z}^d| \quad \text{and} \quad \partial(tP + \tau(P-a)) \cap \mathbb{Z}^d = \emptyset.$$

This establishes the first claim.

To see how the limit also holds for the quasi-coefficients, let m be the denominator of P. Since m is a period for both the Ehrhart and the shifted solid angle sum quasi-coefficients,

[1] I.e., satisfies $\varphi(P) + \varphi(Q) = \varphi(P \cup Q) + \varphi(P \cap Q)$ whenever $P \cup Q$ is a polytope.

we have

$$e_k(P, t + jm) = e_k(P, t) \quad \text{and} \quad a_k(P, \tau(P - a); t + jm) = a_k(P, \tau(P - a); t),$$

for any integer $j \geq 0$ and $0 \leq k \leq d$. Evaluating the equality for quasi-polynomials with $t, t + m, \ldots, t + dm$, we get the $d + 1$ equations

$$\sum_{k=0}^{d} e_k(P, t)(t + jm)^k = \lim_{\tau \longrightarrow 0^+} \sum_{k=0}^{d} a_k(P, \tau(P - a); t)(t + jm)^k, \quad \text{for } j = 0, \ldots, d.$$

Since the Vandermonde matrix $\left((t + jm)^k\right)_{j,k=0}^{d}$ is invertible, these equations imply the equality for the quasi-coefficients. □

Theorem 6.5.1 gives a formula for $e_k(t)$ in terms of the quasi-coefficients of the shifted solid angle sum, however in Theorems 6.3.3 and 6.2.1 we have formulas for the solid angle sum quasi-coefficients without the shift. Next we adapt the proof of Theorem 6.3.2 (from Diaz, Le, and Robins [DLR16]) where instead of considering the solid angle sum of the polytope P, we now consider the solid angle sum of the perturbed polytope $P + \tau(P - a)$ and we show that in the limit as $\tau \longrightarrow 0^+$ both $\lim_{\tau \longrightarrow 0^+} a_k(P, \tau(P - a); t)$ and $\lim_{\tau \longrightarrow 0^+} a_k(P + \tau(P - a); t)$ are in fact the same.

Lemma 6.5.2. *Let $P \subset \mathbb{R}^d$ be a d-dimensional rational polytope and $a \in \operatorname{int}(P)$ be a rational vector. Then pointwise for any positive real t,*

$$\lim_{\tau \longrightarrow 0^+} a_k(P, \tau(P - a); t) = \lim_{\tau \longrightarrow 0^+} a_k(P + \tau(P - a); t).$$

Hence by Theorem 6.5.1 both expressions are equal to the Ehrhart quasi-coefficient $e_k(P; t)$.

Proof. In this proof we follow closely the procedure from Diaz, Le, and Robins [DLR16], revised in Section 6.3. For any $t, \tau > 0$ we write the shifted solid angle sum $A_{P,\tau(P-a)}(t)$ using Lemma 2.5.2, followed by Poisson summation (Theorem 2.4.16):

$$\begin{aligned}
A_{P,\tau(P-a)}(t) &= \sum_{x \in \mathbb{Z}^d} \omega_{tP+\tau(P-a)}(x) \\
&= \lim_{\epsilon \longrightarrow 0^+} \sum_{x \in \mathbb{Z}^d} (\mathbb{1}_{tP+\tau(P-a)} * \phi_{d,\epsilon})(x) \\
&= \lim_{\epsilon \longrightarrow 0^+} \sum_{\xi \in \mathbb{Z}^d} \hat{\mathbb{1}}_{tP+\tau(P-a)}(\xi)\hat{\phi}_\epsilon(\xi) \\
&= (t + \tau)^d \lim_{\epsilon \longrightarrow 0^+} \sum_{\xi \in \mathbb{Z}^d} e^{-2\pi i \langle \xi, -\tau a \rangle} \hat{\mathbb{1}}_P((t + \tau)\xi)\hat{\phi}_\epsilon(\xi),
\end{aligned}$$

in the last line we use $\hat{\mathbb{1}}_{tP+\tau(P-a)}(\xi) = (t + \tau)^d e^{-2\pi i \langle \xi, -\tau a \rangle} \hat{\mathbb{1}}_P\left((t + \tau)\xi\right)$, which can be proven by the change of variables $x \mapsto (t + \tau)x - \tau a$ in the integral.

Next we apply the combinatorial Stokes formula [DLR16, Theorem 1] for P and use the rational weights $\mathcal{R}_T(\xi)$ defined in Section 6.3.

$$A_{P,\tau(P-a)}(t) = (t+\tau)^d \lim_{\epsilon \longrightarrow 0^+} \sum_T \sum_{\xi \in \mathbb{Z}^d \cap S(T)} (t+\tau)^{-l(T)} \mathcal{R}_T(\xi) e^{-2\pi i \langle \xi, (t+\tau)x_T - \tau a\rangle} \hat{\phi}_\epsilon(\xi),$$

where the outer sum is taken over all chains of G_P and x_T is any point from the last face of chain T. Similarly as in Theorem 6.3.2, this leads to a formula for the coefficients of $A_{P,-\tau a}(t+\tau)$:

$$A_{P,\tau(P-a)}(t) := \sum_{x \in \mathbb{Z}^d} \omega_{tP+\tau(P-a)}(x) = A_{P,-\tau a}(t+\tau) = \sum_{k=0}^d a_k(P, -\tau a; t+\tau)(t+\tau)^k,$$

where

$$a_k(P,-\tau a; t+\tau) = \lim_{\epsilon \longrightarrow 0^+} \sum_{\substack{T \in \mathfrak{C}(P),\\ l(T)=d-k}} \sum_{\xi \in \mathbb{Z}^d \cap S(T)} \mathcal{R}_T(\xi) e^{-2\pi i \langle \xi, (t+\tau)x_T - \tau a\rangle} \hat{\phi}_\epsilon(\xi).$$

To get the quasi-coefficients $a_k(P, \tau(P-a); t)$, we expand $(t+\tau)^k$ and rearrange the terms:

$$\begin{aligned} A_{P,\tau(P-a)}(t) &= \sum_{l=0}^d a_l(P,-\tau a; t+\tau)(t+\tau)^l = \sum_{l=0}^d a_l(P,-\tau a; t+\tau) \sum_{k=0}^l \binom{l}{k} t^k \tau^{l-k} \\ &= \sum_{k=0}^d \left(\sum_{l=k}^d \binom{l}{k} a_l(P,-\tau a; t+\tau)\tau^{l-k} \right) t^k. \end{aligned}$$

Hence

$$a_k(P, \tau(P-a); t) = \sum_{l=k}^d \binom{l}{k} a_l(P,-\tau a; t+\tau)\tau^{l-k}. \tag{6.21}$$

Before considering the limit $\tau \longrightarrow 0^+$, next we show that the quasi-coefficients $a_l(P,-\tau a; t+\tau)$ can be bounded for all $\tau < 1$ and $t > 0$. Indeed, let $0 < \tau < 1$ and replace t by $t-\tau$ so that we just have t in the argument. Let m be the period of P, since $A_{P,-\tau a}(t)$ is a quasi-polynomial with period m, we may assume $0 < t \leq m$. Evaluate $A_{P,-\tau a}(t)$ replacing t by $t, t+m, \ldots, t+dm$ to obtain $d+1$ equations

$$A_{P,-\tau a}(t+jm) = \sum_{l=0}^d a_l(P,-\tau a; t)(t+jm)^l \quad \text{for } 0 \leq j \leq d.$$

Since the interpolation which sends the $d+1$ values $\left(A_{P,-\tau a}(t+jm)\right)_{j=0}^d$ to the coefficients $\left(a_l(P,-\tau a; t)\right)_{l=0}^d$ is a linear transformation with matrix equal to the inverse of $\left((t+jm)^l\right)_{j,l=0}^d$ and since its norm is a continuous function on t, it can be bounded for $0 \leq t \leq m$. Furthermore, the value $A_{P,-\tau a}(t+dm)$ is bounded for $\tau < 1$ and $0 < t \leq m$, thus the coefficients $a_l(P,-\tau a; t)$ are also bounded, as we claimed.

Now we fix a $t > 0$ and consider the limit $\tau \longrightarrow 0^+$ in (6.21). Since $|a_l(P,-\tau a; t+\tau)|$ is bounded independently on t and $\tau < 1$, all terms with $l > k$ vanish as $\tau \longrightarrow 0^+$ and we get

$$\lim_{\tau \longrightarrow 0^+} a_k(P, \tau(P-a); t) = \lim_{\tau \longrightarrow 0^+} a_k(P,-\tau a; t+\tau)$$

$$= \lim_{\tau \to 0^+} \lim_{\epsilon \to 0^+} \sum_{\substack{T \in \mathfrak{C}(P), \\ l(T)=d-k}} \sum_{\xi \in \mathbb{Z}^d \cap S(T)} \mathcal{R}_T(\xi) e^{-2\pi i \langle \xi, (t+\tau)x_T - \tau a \rangle} \hat{\phi}_\epsilon(\xi)$$

$$= \lim_{\tau \to 0^+} \lim_{\epsilon \to 0^+} \sum_{\substack{T \in \mathfrak{C}(P), \\ l(T)=d-k}} \sum_{\xi \in \mathbb{Z}^d \cap S(T)} \mathcal{R}_T(\xi) e^{-2\pi i \langle t\xi, (1+\tau)x_T - \tau a \rangle} \hat{\phi}_\epsilon(\xi),$$

where in the last step we make the change of variables $\tau \mapsto t\tau$ in the limit.

On the other hand, we may compute a expression for $a_k(P + \tau(P - a); t)$ using the original formula from Theorem 6.3.2, but with the polytope $P + \tau(P - a)$ instead of the polytope P. The chains of both polytopes can be identified, since the transformation $P \mapsto P + \tau(P - a)$ is a dilation followed by a translation. The rational weight gets multiplied by $(1 + \tau)^{d-l(T)}$ due to the dilation of the faces and the fact that the weights $W_{(F_{j-1}, F_j)}(\xi)$ only depend on the cone of feasible directions $\mathrm{fcone}(F_{j-1}, F_j)$. The exponential weight becomes $e^{-2\pi i \langle \xi, x_T + \tau(x_T - a) \rangle}$, thus

$$\lim_{\tau \to 0^+} a_k(P + \tau(P - a); t) = \lim_{\tau \to 0^+} \lim_{\epsilon \to 0^+} \sum_{\substack{T \in \mathfrak{C}(P), \\ l(T)=d-k}} \sum_{\xi \in \mathbb{Z}^d \cap S(T)} (1 + \tau)^{d-k} \mathcal{R}_T(\xi) e^{-2\pi i \langle t\xi, (1+\tau)x_T - \tau a \rangle} \hat{\phi}_\epsilon(\xi)$$

$$= \lim_{\tau \to 0^+} \lim_{\epsilon \to 0^+} \sum_{\substack{T \in \mathfrak{C}(P), \\ l(T)=d-k}} \sum_{\xi \in \mathbb{Z}^d \cap S(T)} \mathcal{R}_T(\xi) e^{-2\pi i \langle t\xi, (1+\tau)x_T - \tau a \rangle} \hat{\phi}_\epsilon(\xi),$$

where we simply have taken the factor $(1 + \tau)^{d-k}$ out and used the product rule of limits. The lemma follows since we obtained the same formula for both limits. □

With Lemma 6.5.2 and Theorems 6.3.3 and 6.2.1, we can produce formulas for $e_{d-1}(t)$ and $e_{d-2}(t)$ for all real $t > 0$. We recall the one-sided limits

$$\overline{B}_1^+(x) := \lim_{\epsilon \to 0^+} \overline{B}_1(x + \epsilon) \quad \text{and} \quad \overline{B}_1^-(x) := \lim_{\epsilon \to 0^+} \overline{B}_1(x - \epsilon),$$

that differ from $\overline{B}_1(x)$ only at integer points ($\overline{B}_1^+(x) = -1/2$ and $\overline{B}_1^-(x) = 1/2$ for $x \in \mathbb{Z}$).

Theorem 6.5.3. *Let P be a full-dimensional rational polytope in $\mathbb{R}^d$. Then for all positive real values of t, the codimension one quasi-coefficient of the Ehrhart function $L_P(t)$ has the following finite form:*

$$e_{d-1}(t) = -\sum_{\substack{F \in \mathcal{F}(P), \\ \dim(F)=d-1}} \mathrm{vol}^*(F) \overline{B}_1^+\big(\langle v_F, x_F \rangle \, t \big),$$

where x_F is any point in F and v_F is the primitive integer vector in the direction of $N_P(F)$.

Proof. We have from Theorem 6.3.3 the formula for $a_{d-1}(t)$,

$$a_{d-1}(P; t) = -\sum_{\substack{F \in \mathcal{F}(P), \\ \dim(F)=d-1}} \mathrm{vol}^*(F) \overline{B}_1\big(\langle v_F, x_F \rangle \, t \big).$$

We use the formula from Lemma 6.5.2 for $e_{d-1}(P; t)$ and observe that the effect of replacing the polytope P by $P + \tau(P - a)$ is replace F by $(1 + \tau)F$ inside the relative volume and replace

x_F by $x_F + \tau(x_F - a)$. We get

$$\begin{aligned} e_{d-1}(P;t) &= \lim_{\tau\to 0^+} a_{d-1}(P+\tau(P-a);t) \\ &= -\lim_{\tau\to 0^+} \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \operatorname{vol}^*\big((1+\tau)F\big)\overline{B}_1\big(\langle v_F, x_F + \tau(x_F - a)\rangle\, t\big) \\ &= -\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \operatorname{vol}^*(F)\overline{B}_1^+\big(\langle v_F, x_F\rangle\, t\big), \end{aligned}$$

where we have used that vol^* is continuous and $\langle v_F, x_F - a\rangle > 0$, since v_F points outwards to F and $a \in \operatorname{int}(P)$. □

When P is an integer polytope and t is an integer, the formula from Theorem 6.5.3 simplifies to the classical formula

$$e_{d-1} = \frac{1}{2}\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \operatorname{vol}^*(F).$$

The same technique can be applied to the computation of $e_{d-2}(t)$.

Theorem 6.2.3. *Let $P \subset \mathbb{R}^d$ be a full-dimensional rational polytope. Then for all positive real values of t, the codimension two quasi-coefficient of the Ehrhart function $L_P(t)$ has the following finite form:*

$$\begin{aligned} e_{d-2}(t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \operatorname{vol}^*(G)\Bigg[&\frac{c_G}{2k}\left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|}\overline{B}_2\big(\langle v_{F_1}, \bar{x}_G\rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|}\overline{B}_2\big(\langle v_{F_2}, \bar{x}_G\rangle t\big)\right) \\ &- s\big(h,k;(x_1+hx_2)t,-kx_2t\big) - \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_1t)\,\overline{B}_1\big((h^{-1}x_1+x_2)t\big) - \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_2t)\overline{B}_1^+\big((x_1+hx_2)t\big)\Bigg], \end{aligned}$$

where h^{-1} denotes an integer satisfying $h^{-1}h \equiv 1 \mod k$ if $h \neq 0$ and $h^{-1} := 1$ in case $h = 0$ and $k = 1$.

Proof. Once more we use the formula from Lemma 6.5.2, this time with the formula from Theorem 6.2.1 for $a_{d-2}(t)$:

$$\begin{aligned} a_{d-2}(P;t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \operatorname{vol}^*(G)\Bigg[&\frac{c_G}{2k}\left(\frac{\|v_{F_2}\|}{\|v_{F_1}\|}\overline{B}_2\big(\langle v_{F_1}, \bar{x}_G\rangle t\big) + \frac{\|v_{F_1}\|}{\|v_{F_2}\|}\overline{B}_2\big(\langle v_{F_2}, \bar{x}_G\rangle t\big)\right) \\ &+ \left(\omega_P(G) - \frac{1}{4}\right)\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) - s\big(h,k;(x_1+hx_2)t,-kx_2t\big)\Bigg]. \end{aligned}$$

The effect of replacing the polytope P by $P + \tau(P-a)$ is scaling the relative volume of G by $(1+\tau)^{d-2}$ and replace $\bar{x}_G$ by $\bar{x}_G + \tau(\bar{x}_G - \bar{a})$, where $\bar{a} = \operatorname{Proj}_{\operatorname{lin}(G)^\perp}(a)$. Recall that x_1 and x_2 are defined as the coordinates of $\bar{x}_G$ as a linear combination of $v_{F_1,G}$ and $v_{F_2,G}$, so letting W be the matrix with $v_{F_1,G}$ and $v_{F_2,G}$ as columns and $W^+ := (W^\top W)^{-1}W^\top$ being its pseudoinverse, we have $\binom{x_1}{x_2} = W^+\bar{x}_G$ and we replace it by $\binom{x_1}{x_2} + \tau W^+(\bar{x}_G - \bar{a})$. Note that by the orientation of $v_{F_1,G}$, $v_{F_2,G}$, and $\bar{x}_G - \bar{a}$, the vector $W^+(\bar{x}_G - \bar{a})$ has positive entries (see Figure 6.2).

To compute $\lim_{\tau\to 0^+} a_{d-2}(P + \tau(P - a); t)$, note that $\overline{B}_2$ is continuous, so we can replace τ by 0 in it. Λ_G^* is discrete and $\bar{x}_G - \bar{a} \neq 0$, so $\mathbb{1}_{\Lambda_G^*}\big(t(\bar{x}_G + \tau(\bar{x}_G - \bar{a}))\big) = 0$ for all sufficiently small τ. To analyze the limit in the Dedekind-Rademacher sum, denote $\binom{a_1}{a_2} := W^+(\bar{x}_G - \bar{a})$ so:

$$\begin{aligned}
&\lim_{\tau\to 0^+} s\big(h, k; (x_1+\tau a_1)t + h(x_2 + \tau a_2)t, -k(x_2 + \tau a_2)t\big) \\
&\qquad = \lim_{\tau\to 0^+} \sum_{r \bmod k} \overline{B}_1\left(\frac{r}{k} - tx_2 - t\tau a_2\right)\overline{B}_1\left(\frac{h}{k}r + tx_1 + t\tau a_1\right) \\
&\qquad = \sum_{r \bmod k} \overline{B}_1^-\left(\frac{r}{k} - tx_2\right)\overline{B}_1^+\left(\frac{h}{k}r + tx_1\right).
\end{aligned}$$

Using the identities $\overline{B}_1^+(x) = \overline{B}_1(x) - \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(x)$ and $\overline{B}_1^-(x) = \overline{B}_1(x) + \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(x)$, we may rewrite it as

$$\begin{aligned}
= s(h, k; (x_1 + hx_2)t, -kx_2t) &- \frac{1}{2}\sum_{r \bmod k} \mathbb{1}_{\mathbb{Z}}\left(\frac{h}{k}r + tx_1\right)\overline{B}_1\left(\frac{r}{k} - tx_2\right) \\
&+ \frac{1}{2}\sum_{r \bmod k} \mathbb{1}_{\mathbb{Z}}\left(\frac{r}{k} - tx_2\right)\overline{B}_1^+\left(\frac{h}{k}r + tx_1\right).
\end{aligned}$$

Note that $hr/k + tx_1$ is an integer if and only if tkx_1 is an integer and $r \equiv -h^{-1}kx_1t \mod k$, where h^{-1} denotes an integer satisfying $h^{-1}h \equiv 1 \mod k$ (in case $k = 1$ and $h = 0$, we take $h^{-1} = 1$). So the first sum becomes $\frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_1t)\,\overline{B}_1\big((h^{-1}x_1 + x_2)t\big)$. Similarly, $r/k - tx_2$ is an integer if and only if tkx_2 is an integer and $r \equiv tkx_2 \mod k$, so the second sum becomes $\frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_2t)\overline{B}_1^+\big((x_1 + hx_2)t\big)$.

Putting all this together, we get the desired formula for $e_{d-2}(t)$. □

When P is an integer polytope and t is an integer, the formula from Theorem 6.2.3 simplifies. Similarly to Corollary 6.2.2, we have:

Corollary 6.2.4. *Let $P \subset \mathbb{R}^d$ be a full-dimensional integer polytope. For positive integer values of t, the codimension two coefficient of the Ehrhart polynomial $L_P(t)$ is the following:*

$$e_{d-2} = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \operatorname{vol}^*(G)\left[\frac{c_G}{12k}\left(\frac{\|v_{F_1}\|}{\|v_{F_2}\|} + \frac{\|v_{F_2}\|}{\|v_{F_1}\|}\right) - s(h,k) + \frac{1}{4}\right].$$

Pommersheim found a very similar formula for e_{d-2} [Pom93, Theorem 4], where it is assumed $d = 3$ and P an integer tetrahedra. The formula there is not a local formula though, since it is given in terms of the relative volumes of the facets of P. The direct comparison of both formulas immediately gives an identity valid for tetrahedra, as follows.

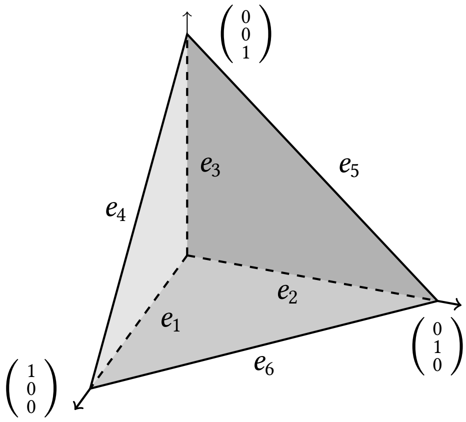

Figure 6.4: *The standard simplex* $\Delta := \operatorname{conv}\{(0,0,0)^\mathsf{T}, (1,0,0)^\mathsf{T}, (0,1,0)^\mathsf{T}, (0,0,1)^\mathsf{T}\}$ *and its edges.*

Corollary 6.5.4. *Let $P \subset \mathbb{R}^3$ be an integer tetrahedra. Then the following identity holds*

$$\sum_{\substack{G \in \mathcal{F}(P),\\ \dim(G)=d-2}} \frac{\operatorname{vol}^*(G)}{k}\left[\frac{\|v_{F_1}\|}{\|v_{F_2}\|}\left(c_G - \frac{\operatorname{vol}(F_1)}{3\operatorname{vol}(F_2)}\right) + \frac{\|v_{F_2}\|}{\|v_{F_1}\|}\left(c_G - \frac{\operatorname{vol}(F_2)}{3\operatorname{vol}(F_1)}\right)\right] = 0.$$

6.6 Two examples in three dimensions

In this section we consider two examples to show how the computations described in Section 6.2.1 are performed in practice. With Theorems 6.3.3 and 6.5.3 we also have a formula for the codimension one quasi-coefficients and even without having a general formula for the codimension three quasi-coefficients, in these examples we fully compute the quasi-polynomials for all positive real t using the knowledge of $A_P(t)$ and $L_P(t)$ in the interval $0 < t < 1$. We also make use of the third periodized Bernoulli polynomial $\overline{B}_3(t) := (t - \lfloor t \rfloor)^3 - \frac{3}{2}(t - \lfloor t \rfloor)^2 + \frac{1}{2}(t - \lfloor t \rfloor)$.

Example 6.6.1. *The first example is the standard simplex* $\Delta := \operatorname{conv}\{(0,0,0)^\mathsf{T}, (1,0,0)^\mathsf{T}, (0,1,0)^\mathsf{T}, (0,0,1)^\mathsf{T}\}$, *whose solid angle polynomial was computed by Beck and Robins [BR15, Example 13.3] for integer values of t. Here we show that for all positive real values of t,*

$$A_\Delta(t) = \frac{1}{6}t^3 - \frac{1}{2}\overline{B}_1(t)t^2 + \left(\frac{1}{2}\overline{B}_2(t) + \left(\frac{3}{2\pi}\arccos\left(\frac{1}{\sqrt{3}}\right) - \frac{3}{4}\right)\mathbb{1}_{\mathbb{Z}}(t) + \frac{1}{4}\right)t - \overline{B}_1(t)\left(\frac{1}{6}\overline{B}_2(t) + \frac{2}{9}\right),$$

and

$$L_\Delta(t) = \frac{1}{6}t^3 + \left(-\frac{1}{2}\overline{B}_1^+(t) + \frac{3}{4}\right)t^2 + \left(\frac{1}{2}\overline{B}_2(t) - \frac{3}{2}\overline{B}_1^+(t) + 1\right)t - \frac{1}{6}\overline{B}_3(t) + \frac{3}{4}\overline{B}_2(t) - \overline{B}_1^+(t) + \frac{3}{8}.$$

Proof. This polytope has four facets with corresponding supporting inequalities $F_1 : x_1 \geq 0$, $F_2 : x_2 \geq 0$, $F_3 : x_3 \geq 0$, and $F_4 : x_1 + x_2 + x_3 \leq 1$.

We know that $A_\Delta(t)$ and $L_\Delta(t)$ have quasi-polynomial expressions

$$A_\Delta(t) = \mathrm{vol}(\Delta)t^3 + a_2(t)t^2 + a_1(t)t + a_0(t),$$
$$L_\Delta(t) = \mathrm{vol}(\Delta)t^3 + e_2(t)t^2 + e_1(t)t + e_0(t),$$

with quasi-coefficients having period 1, $a_0(0) = a_2(0) = 0$ (due to the Macdonald's Reciprocity Theorem [BR15, Theorem 13.7]) and $e_0(0) = 1$ (due to [BR15, Corollary 3.15]).

We have that $\mathrm{vol}(\Delta) = 1/6$ and we can compute $a_2(t)$ and $e_2(t)$ with Theorems 6.3.3 and 6.5.3. Since $\overline{B}_1(0) = 0$ and $0 \in F_1, F_2, F_3$, using that $\mathrm{vol}^*(F_4) = 1/2$ and $v_{F_4} = (1,1,1)^\intercal$, we get

$$a_2(t) = -\frac{1}{2}\overline{B}_1(t).$$

Since $\overline{B}_1^+(0) = -1/2$ and $\mathrm{vol}^*(F_1) = \mathrm{vol}^*(F_2) = \mathrm{vol}^*(F_3) = 1/2$, we get

$$e_2(t) = -\frac{1}{2}\overline{B}_1^+(t) + \frac{3}{4}.$$

We use Theorems 6.2.1 and 6.2.3 together with the procedure described in Section 6.2.1 to compute $a_1(t)$ and $e_1(t)$. Due to the symmetry of Δ, we only have to consider two edges.

The edge e_1 has incident facets F_2 and F_3 and relative volume $\mathrm{vol}^*(e_1) = 1$. From the inequalities, we get $v_{F_2} = (0,-1,0)^\intercal$ and $v_{F_3} = (0,0,-1)^\intercal$. From their inner product, we have $c_{e_1} = 0$ and $\omega_\Delta(e_1) = 1/4$. Next we write $U = (v_{F_2}, v_{F_3}) = \begin{pmatrix} 0 & 0 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}$ and compute the projection onto $\mathrm{lin}(e_1)^\perp$, $P = U(U^\intercal U)^{-1}U^\intercal = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$. Inspecting its columns, we get the lattice basis $\{(0,0,1)^\intercal, (0,1,0)^\intercal\}$ for $\Lambda^*_{e_1}$. Computing $f_{2,3}$ with formula (6.11) we obtain $(0,0,-1)^\intercal$ and thus $v_{F_2,e_1} = (0,0,-1)^\intercal$, also $f_{3,2} = (0,-1,0)^\intercal$, so $v_{F_3,e_1} = (0,-1,0)^\intercal$. Hence we can make $v_1 = v_{F_2,e_1}$ and $v_2 = v_{F_3,e_1}$ so that $h = 0$ and $k = 1$. Letting $V = (v_1, v_2)$, we compute $\det(\Lambda_{e_1}) = \det(V^\intercal V)^{-1/2} = 1$. Since $(0,0,0)^\intercal \in e_1$, we get $\bar{x}_{e_1} = P(0,0,0)^\intercal = (0,0,0)^\intercal$, so $x_1 = x_2 = 0$. With this information, the contribution from edge e_1 (and also from e_2 and e_3) to the sum in Theorem 6.2.1 is $-s(0,1;0,0) = 0$ and to the sum in Theorem 6.2.3 is 1/4.

The edge e_4 has incident facets F_2 and F_4 and relative volume $\mathrm{vol}^*(e_4) = 1$. From the inequalities, we get $v_{F_2} = (0,-1,0)^\intercal$ and $v_{F_4} = (1,1,1)^\intercal$. From their inner product, we have $c_{e_4} = 1/\sqrt{3}$ and $\omega_\Delta(e_4) = \arccos\left(1/\sqrt{3}\right)/(2\pi)$. Next we write $U = (v_{F_2}, v_{F_4}) = \begin{pmatrix} 0 & 1 \\ -1 & 1 \\ 0 & 1 \end{pmatrix}$ and compute the projection onto $\mathrm{lin}(e_4)^\perp$, $P = U(U^\intercal U)^{-1}U^\intercal = \begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}$. Inspecting its columns, we get the lattice basis $\{(1/2,0,1/2)^\intercal, (0,1,0)^\intercal\}$ for $\Lambda^*_{e_4}$. Computing $f_{2,4}$ with formula (6.11) we obtain $(1,1,1)^\intercal + (0,-1,0)^\intercal = (1,0,1)^\intercal$ and thus $v_{F_2,e_4} = (1/2,0,1/2)^\intercal$, also $f_{4,2} = (0,-3,0)^\intercal + (1,1,1)^\intercal = (1,-2,1)^\intercal$, so $v_{F_4,e_4} = (1/2,-1,1/2)^\intercal$. Hence we can make $v_1 = v_{F_2,e_4}$ and $v_2 = v_{F_4,e_4}$ (check that all columns from P can be obtained as integer combinations of v_1 and v_2) so that $h = 0$ and $k = 1$. Letting $V = (v_1, v_2)$, we compute $\det(\Lambda_{e_4}) = \det(V^\intercal V)^{-1/2} = \sqrt{2}$. Since $(1,0,0)^\intercal \in e_4$, we get $\bar{x}_{e_4} = P(1,0,0)^\intercal = (1/2,0,1/2)^\intercal$ and $x_1 = 1$, $x_2 = 0$. With this information, the contribution from edge e_4 (and also from e_5

and e_6) to the sum in Theorem 6.2.1 is

$$\begin{aligned}\frac{1}{2\sqrt{3}}\left(\frac{\sqrt{3}}{1}\overline{B}_2(0)+\frac{1}{\sqrt{3}}\overline{B}_2(t)\right)+\left(\frac{1}{2\pi}\arccos\left(\frac{1}{\sqrt{3}}\right)-\frac{1}{4}\right)\mathbb{1}_{\mathbb{Z}}(t)-s(0,1;t,0)\\=\frac{1}{12}+\frac{1}{6}\overline{B}_2(t)+\left(\frac{1}{2\pi}\arccos\left(\frac{1}{\sqrt{3}}\right)-\frac{1}{4}\right)\mathbb{1}_{\mathbb{Z}}(t),\end{aligned}$$

and to the sum in Theorem 6.2.3,

$$\begin{aligned}\frac{1}{2\sqrt{3}}\left(\frac{\sqrt{3}}{1}\overline{B}_2(0)+\frac{1}{\sqrt{3}}\overline{B}_2(t)\right)-s(0,1;t,0)-\frac{1}{2}\mathbb{1}_{\mathbb{Z}}(t)\overline{B}_1(t)-\frac{1}{2}\overline{B}_1^+(t)\\=\frac{1}{12}+\frac{1}{6}\overline{B}_2(t)-\frac{1}{2}\overline{B}_1^+(t).\end{aligned}$$

Multiplying by three to take into account the three similar edges, the coefficient $a_1(t)$ of $A_\Delta(t)$, for all positive $t\in\mathbb{R}$, is

$$a_1(t)=\frac{1}{2}\overline{B}_2(t)+\left(\frac{3}{2\pi}\arccos\left(\frac{1}{\sqrt{3}}\right)-\frac{3}{4}\right)\mathbb{1}_{\mathbb{Z}}(t)+\frac{1}{4}.$$

When $t\in\mathbb{Z}$, this becomes $3\arccos\left(1/\sqrt{3}\right)/(2\pi)-5/12$, as computed in Example 13.3 of Beck and Robins [BR15]. Similarly, the coefficient $e_1(t)$ of $L_\Delta(t)$, for all positive $t\in\mathbb{R}$, is

$$e_1(t)=\frac{1}{2}\overline{B}_2(t)-\frac{3}{2}\overline{B}_1^+(t)+1.$$

To compute $a_0(t)$, we observe that for $0<t<1$, the only integer point in $t\Delta$ is $(0,0,0)^\intercal$ and its solid angle is $1/8$, so $A_\Delta(t)=1/8$. Hence, for $0<t<1$,

$$\begin{aligned}a_0(t)&=\frac{1}{8}-\frac{1}{6}t^3-a_2(t)t^2-a_1(t)t=\frac{1}{8}-\frac{1}{6}t^3+\frac{1}{2}\overline{B}_1(t)t^2-\left(\frac{1}{4}+\frac{1}{2}\overline{B}_2(t)\right)t\\&=-\overline{B}_1(t)\left(\frac{1}{6}\overline{B}_2(t)+\frac{2}{9}\right).\end{aligned}$$

Similarly for $e_0(t)$, we have $L_\Delta(t)=1$ for $0<t<1$, so

$$\begin{aligned}e_0(t)&=1-\frac{1}{6}t^3-e_2(t)t^2-e_1(t)t\\&=1-\frac{1}{6}t^3-\left(-\frac{1}{2}\overline{B}_1^+(t)+\frac{3}{4}\right)t^2-\left(1+\frac{1}{2}\overline{B}_2(t)-\frac{3}{2}\overline{B}_1^+(t)\right)t\\&=-\frac{1}{6}\overline{B}_3(t)+\frac{3}{4}\overline{B}_2(t)-\overline{B}_1^+(t)+\frac{3}{8}.\end{aligned}$$ □

Example 6.6.2. *The second example is the order simplex* $\triangleleft := \operatorname{conv}\{(0,0,0)^\intercal,(1,0,0)^\intercal,(1,1,0)^\intercal,(1,1,1)^\intercal\}$, *that receives this name since it corresponds to the linear ordering* $x_3\le x_2\le x_1$ *and is interesting since it tiles the cube together with the reflections corresponding to the six permutations of its coordinates. Here we show that for all positive real values of t,*

$$A_\triangleleft(t)=\frac{1}{6}t^3-\frac{1}{2}\overline{B}_1(t)t^2+\left(\frac{1}{24}+\frac{1}{2}\overline{B}_2(t)-\frac{1}{8}\mathbb{1}_{\mathbb{Z}}(t)\right)t-\overline{B}_1(t)\left(\frac{1}{6}\overline{B}_2(t)+\frac{1}{72}\right),$$

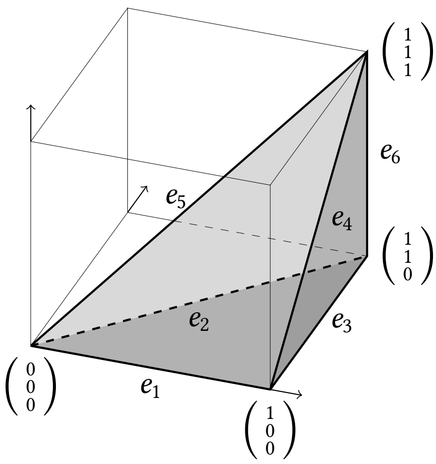

Figure 6.5: *The order simplex* $\triangleleft := \operatorname{conv}\{(0,0,0)^{\mathsf{T}}, (1,0,0)^{\mathsf{T}}, (1,1,0)^{\mathsf{T}}, (1,1,1)^{\mathsf{T}}\}$ *from Example 6.6.2 and its edges.*

and,

$$L_{\triangleleft}(t) = \frac{1}{6}t^3 + \left(-\frac{1}{2}\overline{B}_1^{+}(t) + \frac{3}{4}\right)t^2 + \left(\frac{1}{2}\overline{B}_2(t) - \frac{3}{2}\overline{B}_1^{+}(t) + 1\right)t - \frac{1}{6}\overline{B}_3(t) + \frac{3}{4}\overline{B}_2(t) - \overline{B}_1^{+}(t) + \frac{3}{8}.$$

Proof. This polytope has four facets with corresponding supporting inequalities $F_1 : x_3 \geq 0$, $F_2 : x_3 - x_2 \leq 0$, $F_3 : x_2 - x_1 \leq 0$, and $F_4 : x_1 \leq 1$.

Again, we know that $A_{\triangleleft}(t)$ and $L_{\triangleleft}(t)$ have quasi-polynomial expressions

$$A_{\triangleleft}(t) = \operatorname{vol}(\triangleleft)t^3 + a_2(t)t^2 + a_1(t)t + a_0(t),$$
$$L_{\triangleleft}(t) = \operatorname{vol}(\triangleleft)t^3 + e_2(t)t^2 + e_1(t)t + e_0(t),$$

with quasi-coefficients having period 1, $a_0(0) = a_2(0) = 0$ (due to the Macdonald's Reciprocity Theorem [BR15, Theorem 13.7]) and $e_0(0) = 1$ (due to [BR15, Corollary 3.15]).

We have that $\operatorname{vol}(\triangleleft) = 1/6$ and we can compute $a_2(t)$ and $e_2(t)$ with Theorems 6.3.3 and 6.5.3. Obtaining

$$a_2(t) = -\frac{1}{2}\overline{B}_1(t),$$

and

$$e_2(t) = -\frac{1}{2}\overline{B}_1^{+}(t) + \frac{3}{4}.$$

We use Theorems 6.2.1 and 6.2.3 together with the procedure described in Section 6.2.1 to compute $a_1(t)$ and $e_1(t)$. To avoid repetition, we skip the computation of the contribution from edges e_1, e_2, e_3, and e_4. All them contribute with 0 to $a_1(t)$ and they contribute with $\frac{3}{8}$, $\frac{1}{4}$, $-\frac{1}{2}\overline{B}_1^{+}(t)$, and $-\frac{1}{2}\overline{B}_1^{+}(t)$ respectively to $e_1(t)$.

The edge e_5 has incident facets F_2 and F_3 and relative volume $\operatorname{vol}^*(e_5) = 1$. From the inequalities, we get $v_{F_2} = (0,-1,1)^{\mathsf{T}}$ and $v_{F_3} = (-1,1,0)^{\mathsf{T}}$. From their inner-product, we have $c_{e_5} = 1/2$ and $\omega_{\triangleleft}(e_5) = 1/6$. Next we write $U = (v_{F_2}, v_{F_3}) = \begin{pmatrix} 0 & -1 \\ -1 & 1 \\ 1 & 0 \end{pmatrix}$ and compute the projection onto $\mathrm{lin}(e_5)^\perp$, $P = U(U^\top U)^{-1}U^\top = \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ -1/3 & 2/3 & -1/3 \\ -1/3 & -1/3 & 2/3 \end{pmatrix}$. Inspecting its columns, we get the lattice basis $\{(2/3, -1/3, -1/3)^\top, (-1/3, 2/3, -1/3)^\top\}$ for $\Lambda^*_{e_5}$. Computing $f_{2,3}$ with (6.11) we obtain $(-2, 1, 1)^\top$ and thus $v_{F_2,e_5} = (-2/3, 1/3, 1/3)^\top$, also $f_{3,2} = (-1, -1, 2)^\top$, so $v_{F_3,e_5} = (-1/3, -1/3, 2/3)^\top$. Hence we can make $v_1 = v_{F_2,e_5}$ and $v_2 = v_{F_3,e_5}$ so that $h = 0$ and $k = 1$. Letting $V = (v_1, v_2)$, we compute $\det(\Lambda_{e_5}) = \det(V^\top V)^{-1/2} = \sqrt{3}$. Since $(0,0,0)^\top \in e_5$, we get $\bar{x}_{e_5} = P(0,0,0)^\top = (0,0,0)^\top$, so $x_1 = x_2 = 0$. With this information, the contribution from edge e_5 to the sum in Theorem 6.2.1 is

$$\frac{1}{4}\left(\frac{1}{6} + \frac{1}{6}\right) - \frac{1}{12} - s(0, 1; 0, 0) = 0,$$

and to the sum in Theorem 6.2.3 is

$$\frac{1}{4}\left(\frac{1}{6} + \frac{1}{6}\right) - s(0, 1; 0, 0) + \frac{1}{4} = \frac{1}{3}.$$

The edge e_6 has incident facets F_3 and F_4 and relative volume $\mathrm{vol}^*(e_6) = 1$. From the inequalities, we get $v_{F_3} = (-1, 1, 0)^\top$ and $v_{F_4} = (1, 0, 0)^\top$. From their inner-product, we have $c_{e_6} = 1/\sqrt{2}$ and $\omega_\triangleleft(e_6) = 1/8$. Next we write $U = (v_{F_3}, v_{F_4}) = \begin{pmatrix} -1 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}$ and compute the projection onto $\mathrm{lin}(e_6)^\perp$, $P = U(U^\top U)^{-1}U^\top = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. Inspecting its columns, we get the lattice basis $\{(1, 1, 0)^\top, (0, 1, 0)^\top\}$ for $\Lambda^*_{e_6}$. Computing $f_{3,4}$ with (6.11) we obtain $(1, 1, 0)^\top$ and thus $v_{F_3,e_6} = (1, 1, 0)^\top$, also $f_{4,3} = (0, 1, 0)^\top$, so $v_{F_4,e_6} = (0, 1, 0)^\top$. Hence we can make $v_1 = v_{F_3,e_6}$ and $v_2 = v_{F_4,e_6}$ so that $h = 0$ and $k = 1$. Letting $V = (v_1, v_2)$, we compute $\det(\Lambda_{e_6}) = \det(V^\top V)^{-1/2} = 1$. Since $(1, 1, 0)^\top \in e_6$, we get $\bar{x}_{e_6} = P(1, 1, 0)^\top = (1, 1, 0)^\top$, so $x_1 = 1$ and $x_2 = 0$. With this information, the contribution from edge e_6 to the sum in Theorem 6.2.1 is

$$\frac{1}{2\sqrt{2}}\left(\sqrt{2}\,\overline{B}_2(t) + \frac{1}{6\sqrt{2}}\right) - \frac{1}{8}\mathbb{1}_{\mathbb{Z}}(t) - s(0, 1; t, 0) = \frac{1}{2}\overline{B}_2(t) - \frac{1}{8}\mathbb{1}_{\mathbb{Z}}(t) + \frac{1}{24},$$

and to the sum in Theorem 6.2.3 is

$$\frac{1}{2\sqrt{2}}\left(\sqrt{2}\,\overline{B}_2(t) + \frac{1}{6\sqrt{2}}\right) - s(0, 1; t, 0) - \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(t)\overline{B}_1(t) - \frac{1}{2}\overline{B}_1^+(t) = \frac{1}{2}\overline{B}_2(t) - \frac{1}{2}\overline{B}_1^+(t) + \frac{1}{24}.$$

Therefore the coefficient $a_1(t)$ of $A_\triangleleft(t)$, for all positive $t \in \mathbb{R}$, is

$$a_1(t) = \frac{1}{2}\overline{B}_2(t) - \frac{1}{8}\mathbb{1}_{\mathbb{Z}}(t) + \frac{1}{24}.$$

When $t \in \mathbb{Z}$, this becomes 0, as expected due to the fact that $\triangleleft$ tiles the space together with the simplices obtained by reflections across its facets. Similarly, the coefficient $e_1(t)$ of $A_\triangleleft(t)$, for all positive $t \in \mathbb{R}$, is

$$e_1(t) = \frac{3}{8} + \frac{1}{4} - \overline{B}_1^+(t) + \frac{1}{3} + \frac{1}{2}\overline{B}_2(t) - \frac{1}{2}\overline{B}_1^+(t) + \frac{1}{24} = \frac{1}{2}\overline{B}_2(t) - \frac{3}{2}\overline{B}_1^+(t) + 1.$$

To compute $a_0(t)$, we observe that for $0 < t < 1$, the only integer point in $(t\triangleleft)$ is $(0,0,0)^\intercal$ and its solid angle is 1/6.1/8 (to see this, we use again that $\triangleleft$ together with six reflections tiles the cube), so $A_\triangleleft(t) = 1/48$. Hence, for $0 < t < 1$,

$$\begin{aligned} a_0(t) &= \frac{1}{48} - \frac{1}{6}t^3 - a_2(t)t^2 - a_1(t)t = \frac{1}{48} - \frac{1}{6}t^3 + \frac{1}{2}\overline{B}_1(t)t^2 - \left(\frac{1}{24} + \frac{1}{2}\overline{B}_2(t)\right)t \\ &= -\overline{B}_1(t)\left(\frac{1}{6}\overline{B}_2(t) + \frac{1}{72}\right). \end{aligned}$$

Similarly for $e_0(t)$, we have $L_\triangleleft(t) = 1$ for $0 < t < 1$, so

$$\begin{aligned} e_0(t) &= 1 - \frac{1}{6}t^3 - e_2(t)t^2 - e_1(t)t \\ &= 1 - \frac{1}{6}t^3 - \left(-\frac{1}{2}\overline{B}_1^+(t) + \frac{3}{4}\right)t^2 - \left(\frac{1}{2}\overline{B}_2(t) - \frac{3}{2}\overline{B}_1^+(t) + 1\right)t \\ &= -\frac{1}{6}\overline{B}_3(t) + \frac{3}{4}\overline{B}_2(t) - \overline{B}_1^+(t) + \frac{3}{8}. \end{aligned}$$

□

Remark 6.6.3. Notice that albeit the polytopes in both examples have very different solid angle sum functions, they have the same Ehrhart function. This is not a surprise since the unimodular transformation $U = \left(\begin{smallmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{smallmatrix}\right)$ sends the standard simplex to the order simplex and since it maps $\mathbb{Z}^3$ to $\mathbb{Z}^3$, we indeed have $|(t\Delta) \cap \mathbb{Z}^3| = |(t\triangleleft) \cap \mathbb{Z}^3|$ for all positive real t. Since the transformation given by matrix U is not orthogonal, it doesn't preserve solid angles though.

6.7 Concrete polytopes and further remarks

We introduce a family of polytopes, called concrete polytopes, which come up naturally in our context, and in the context of multi-tiling. Consider Example 6.6.2, where we had a polytope P whose solid angle sum was $A_P(t) = \mathrm{vol}(P)t^d$, for all positive integer values of t. More generally, as done by Brandolini, Colzani, Robins, and Travaglini [Bra+19], we say that a polytope P is *concrete* if:

$$A_P(t) = \mathrm{vol}(P)t^d, \tag{6.22}$$

for all positive integer values of t. Such polytopes are very special, because their discrete volume $A_P(t)$ matches exactly their continuous (Lebesgue) volume.

As another example, consider any integer polygon P in $\mathbb{R}^2$. It is then always true that $A_P(t) = \mathrm{vol}(P)t^2$, for all positive integer values of t, which is an equivalent formulation of *Pick's Theorem.*

The motivation for using the word 'concrete' is borrowed from the title of the book "Concrete Mathematics", where Graham, Knuth, and Patashnik mention that the word 'concrete', which uses the first 3 letters of 'continuous', and the last 5 letters of 'discrete', embodies objects that are both "continuous" and "discrete".

Another special family of concrete polytopes is the collection of *integer zonotopes* (see Lemma 6.7.2 below). Integer zonotopes are projections of cubes or, equivalently, integer polytopes whose faces (of all dimensions) are centrally symmetric (see e.g. Ziegler [Zie95, Section 7.3]). Alexandrov [Ale33], and independently Shephard [She67], proved the following fact.

Lemma 6.7.1 (Alexandrov, Shephard)**.** *Let P be any real, d-dimensional polytope, with $d \geq 3$. If the facets of P are centrally symmetric, then P is centrally symmetric.*

The following statement appeared in [BP99, Corollary 7.7], but we offer a proof here that is in the spirit of the current work.

Lemma 6.7.2 (Barvinok)**.** *Suppose P is a d-dimensional integer polytope in $\mathbb{R}^d$ all of whose facets are centrally symmetric. Then P is a concrete polytope.*

Proof. We recall the formula for the solid angle polynomial $A_P(t)$ from Lemma 6.3.1:

$$A_P(t) = \lim_{\epsilon \to 0^+} \sum_{\xi \in \mathbb{Z}^d} \hat{\mathbb{1}}_{tP}(\xi) e^{-\pi\epsilon\|\xi\|^2}. \tag{6.23}$$

The Fourier transform of the indicator function of a polytope may be written as follows, after one application of the 'combinatorial Stokes' formula (see [DLR16], equation (26)):

$$\hat{\mathbb{1}}_{tP}(\xi) = t^d \mathrm{vol}(P)[\xi = 0] + \left(\frac{-1}{2\pi i}\right) t^{d-1} \sum_{\substack{F \in \mathcal{F}(P), \\ \dim(F) = d-1}} \frac{\langle \xi, N_P(F) \rangle}{\|\xi\|^2} \hat{\mathbb{1}}_F(t\xi)[\xi \neq 0], \tag{6.24}$$

where we sum over all facets F of P. Plugging this into (6.23) we get

$$A_P(t) - t^d \mathrm{vol}(P) = \left(\frac{-1}{2\pi i}\right) t^{d-1} \lim_{\epsilon \to 0^+} \sum_{\xi \in \mathbb{Z}^d \setminus \{0\}} \frac{e^{-\pi\epsilon\|\xi\|^2}}{\|\xi\|^2} \sum_{\substack{F \in \mathcal{F}(P), \\ \dim(F) = d-1}} \langle \xi, N_P(F) \rangle \hat{\mathbb{1}}_F(t\xi) \tag{6.25}$$

Thus, if we show that the latter sum over the facets vanishes, then we are done.

The assumption that all facets of P are centrally symmetric implies that P itself is also centrally symmetric, by Lemma 6.7.1. We may therefore combine the facets of P in pairs of opposite facets F and F'. We know that $F' = F + c$, where c is an integer vector, using the fact that the facets are centrally symmetric.

Therefore, since $N_P(F') = -N_P(F)$, we have

$$\begin{aligned} \langle \xi, N_P(F) \rangle \hat{\mathbb{1}}_F(t\xi) + \langle \xi, -N_P(F) \rangle \hat{\mathbb{1}}_{F+c}(t\xi) &= \langle \xi, N_P(F) \rangle \hat{\mathbb{1}}_F(t\xi) - \langle \xi, N_P(F) \rangle \hat{\mathbb{1}}_F(t\xi) e^{-2\pi i \langle t\xi, c \rangle} \\ &= \langle \xi, N_P(F) \hat{\mathbb{1}}_F(t\xi) \left(1 - e^{-2\pi i \langle t\xi, c \rangle}\right) = 0, \end{aligned}$$

because $\langle t\xi, c \rangle \in \mathbb{Z}$ for $\xi \in \mathbb{Z}^d$ and $t \in \mathbb{Z}$. We conclude that the entire right-hand side of (6.25) vanishes, proving the lemma. □

Fourier analysis can also be used to give more general classes of polytopes that satisfy the formula $A_P(t) = \mathrm{vol}(P) t^d$, for positive integer values of t. A polytope P is said to *k-tile*

$\mathbb{R}^d$ (or *multi-tile* $\mathbb{R}^d$ *at level* k) by integer translations, if

$$\sum_{\lambda\in\mathbb{Z}^d} \mathbb{1}_P(x-\lambda) = k \tag{6.26}$$

for every $x \notin \partial P + \mathbb{Z}^d$. Gravin, Robins, and Shiryaev [GRS12, Theorem 6.1] gave a characterization of these polytopes in terms of solid angles.

Theorem 6.7.3 (Gravin, Robins, Shiryaev)**.** *A polytope P k-tiles $\mathbb{R}^d$ by integer translations if and only if*

$$\sum_{\lambda\in\mathbb{Z}^d} \omega_{P+v}(\lambda) = k,$$

for every $v \in \mathbb{R}^d$.

Note that the sum on the left is equal to $A_{P+v}(1)$, so this condition can be rephrased as asking for the function $P \mapsto A_P(1)$ to be invariant under all real translates of P. To see how multi-tiling implies the concrete polytope property, note that since $f(x) := \sum_{\lambda\in\mathbb{Z}^d} \mathbb{1}_P(x-\lambda)$ is periodic modulo $\mathbb{Z}^d$, it has a Fourier series (see e.g., [SW71, Chapter VII, Theorem 2.4]) $f(x) = \sum_{\xi\in\mathbb{Z}^d} \hat{\mathbb{1}}_P(\xi)e^{2\pi i\langle\xi,x\rangle}$, and so P k-tiles by integer translations if and only if $\hat{\mathbb{1}}_P(\xi) = 0$ for all $\xi \in \mathbb{Z}^d \setminus \{0\}$, and $\hat{\mathbb{1}}_P(0) = k = \mathrm{vol}(P)$. By Lemma 6.3.1, we see that this implies $A_P(t) = \mathrm{vol}(P)t^d$ for all $t \in \mathbb{Z}$, $t > 0$.

Note that the order simplex in Example 6.6.2 doesn't k-tile $\mathbb{R}^3$ by integer translations; however, this simplex is still concrete. To produce more general concrete polytopes, we introduce two new concepts:

The *Hyperoctahedral group* B_d is the group of symmetries of the hypercube $[-1,1]^d$; all of its $2^d d!$ elements are simultaneously unimodular and orthogonal transformations, hence when an element of this group is applied to a polytope it preserves its solid angle polynomial.

The *polytope group* $\mathscr{P}^d$ (cf. [LL19a, Section 3.2]) is the abelian group formally generated by the elements $[A]$ where A runs through all sets in $\mathbb{R}^d$ which can be represented as the union of a finite number of polytopes with disjoint interiors and subject to the relations $[A]+[B] = [A\cup B]$ whenever A and B are two sets with disjoint interiors. Since any element $P \in \mathscr{P}^d$ can be uniquely represented as a finite sum $Q = \sum_j m_j[A_j]$ where m_j are distinct nonzero integers and A_j are sets with pairwise disjoint interiors, any additive function φ defined on the set of polytopes in $\mathbb{R}^d$ (such as the volume $A \mapsto \mathrm{vol}(A)$ or the indicator function $A \mapsto \mathbb{1}_A$ viewed as a function in $L^1(\mathbb{R}^d)$) can be uniquely extended to a function in $\mathscr{P}^d$ by linearity, that is, $\varphi(Q) := \sum_j m_j\varphi(A_j)$ for an element Q written as above. With this extension, the definition of multi-tiling can also be extended to $\mathscr{P}^d$.

With these definitions, we may adapt the proof of (the forward direction of) [LL19a, Theorem 4.1] and prove the following more general sufficiency condition for the concrete polytope property.

Theorem 6.7.4. *If P is a rational polytope in $\mathbb{R}^d$ such that $Q := \sum_{\gamma\in\mathsf{B}_d}[\gamma P]$ multi-tiles $\mathbb{R}^d$ by integer translations, then $A_P(t) = \mathrm{vol}(P)t^d$ for all positive integers t.*

Proof. If P is a rational polytope such that $Q = \sum_{\gamma\in\mathsf{B}_d}[\gamma P]$ k-tiles $\mathbb{R}^d$ by integer translations, then for a positive integer t we also have that $Q_t := \sum_{\gamma\in \mathsf{B}_d}[\gamma(tP)]$ $(t^d k)$-tiles $\mathbb{R}^d$. Let $D := [0,1]^d$, then $Q_t - (t^d k)[D]$ tiles at level zero by integer translations and by [LL19a, Proposition 3.4] we can represent it as a finite sum $Q_t - (t^d k)[D] = \sum_j([B_j] - [B_j'])$ where for each j, B_j, B_j' are polytopes such that B_j' is obtained from B_j by a translation along an integer vector, thus $A_{B_j}(1) = A_{B_j'}(1)$. Hence

$$A_{Q_t}(1) = t^d k A_D(1) = t^d k = \mathrm{vol}(Q)t^d = |\mathsf{B}_d|\mathrm{vol}(P)t^d,$$

where we have used that if Q k-tiles $\mathbb{R}^d$ by integer translations, then $k = \mathrm{vol}(Q)$ and that the action of B_d preserves volumes, thus $\mathrm{vol}(\gamma P) = \mathrm{vol}(P)$ for all $\gamma \in \mathsf{B}_d$. Also,

$$A_{Q_t}(1) = \sum_{\gamma\in\mathsf{B}_d} A_{\gamma(tP)}(1) = \sum_{\gamma\in\mathsf{B}_d} A_{tP}(1) = |\mathsf{B}_d| A_P(t). \qquad \square$$

Example 6.7.5. *The simplex $\triangleleft$, which we used in Example 6.6.2, is now seen to satisfy the condition of Theorem 6.7.4, because it tiles the cube together with the reflections corresponding to the six permutations of coordinates and these reflections are a subgroup of B_3. Further, the simplex $\frac{1}{2}\triangleleft$ also satisfies the hypothesis of Theorem 6.7.4 (because the orbit of $\frac{1}{2}\triangleleft$ under the action of B_3 produces the cube $[-\frac{1}{2},\frac{1}{2}]^3$ that tiles the space by integer translations) and this is an example of a rational (and non-integer) polytope that has the concrete polytope property.*

As a side-note, this fact can also be seen in the expression given for $A_\triangleleft(t)$ in Example 6.6.2, verifying the fact that $a_2(1/2) = a_1(1/2) = a_0(1/2) = 0$, and using the fact that all coefficients of the quasi-polynomial have period 1.

It seems natural to ask whether multi-tiling is a necessary and sufficient condition for a polytope to be concrete, as follows.

Question. Is a rational polytope $P \subset \mathbb{R}^d$ concrete if and only if

$$Q := \sum_{\gamma\in\mathsf{B}_d}[\gamma P]$$

multi-tiles $\mathbb{R}^d$ by integer translations?

This question has a negative answer, however, as very recently shown by Garber and Pak [GP20]. They produced a counterexample in $\mathbb{R}^3$, based on the Dehn invariant of the direct sum of some tetrahedra and then extended it to $\mathbb{R}^d$. It remains an open question to give necessary and sufficient conditions for which P is concrete. Perhaps a more general type of tiling is required.

Question. Suppose we know the solid angle quasi-polynomial $A_P(t)$, for all positive t, but we also know that it is associated to a rational polytope P. Can we recover P completely, up to the action of the finite hyperoctahedral group B_d?

Question. Can the current theory be extended to all real polytopes?

6.8 Appendix: Obtaining the solid angle quasi-coefficients from the Ehrhart quasi-coefficients

Complementing the process described in this chapter, we reverse the order of things and show that the solid angle sum of a polytope can also be obtained from the Ehrhart function of its faces. This can be naturally done with the following well known formula

$$A_P(t) = \sum_{F\in\mathcal{F}(P)} \omega_P(F) L_{\mathrm{int}(F)}(t) = \sum_{F\in\mathcal{F}(P)} \omega_P(F)(-1)^{\dim(F)} L_F(-t).$$

In this appendix we take the formulas from Theorems 6.5.3 and 6.2.3 as given and use them to recover Theorems 6.3.3 and 6.2.1. This point of view is justifiable since the formulas for the Ehrhart coefficients can be obtained by other means, as done by Berline and Vergne [BV07] and summarized in Section 5.2.2.

Expanding the Ehrhart quasi-polynomials of each face and comparing quasi-coefficients, we get:

$$\begin{aligned}
&\mathrm{vol}(P)t^d + a_{d-1}(P;t)t^{d-1} + a_{d-2}(P;t)t^{d-2} + \dots \\
&\qquad = \mathrm{vol}(P)t^d + \Big(- e_{d-1}(P;-t) + \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \frac{1}{2} e_{d-1}(F;-t) \Big) t^{d-1} \\
&\qquad\quad + \Big(e_{d-2}(P;-t) - \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \frac{1}{2} e_{d-2}(F;-t) + \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \omega_P(G) e_{d-2}(G;-t) \Big) t^{d-2} + \dots
\end{aligned}$$

Great care has to be taken before using Theorems 6.5.3 and 6.2.3, because these theorems assume the polytopes to be full-dimensional, while to use the expressions above we must consider all of the lower dimensional faces F.

The main difference is that when $0 \notin \mathrm{aff}(F)$, then $L_F(t) = 0$ for all t such that $\mathrm{aff}(tF)$ has no integer points. Letting $\bar{x}_F$ be the projection of $\mathrm{aff}(F)$ onto $\mathrm{lin}(F)^\perp$, we may express this condition equivalently as $t\bar{x}_F \notin \Lambda_F^* = \mathrm{Proj}_{\mathrm{lin}(F)^\perp}(\mathbb{Z}^d)$. Therefore we have to multiply the formulas from Theorems 6.5.3 and 6.2.3 by $\mathbb{1}_{\Lambda_F^*}(t\bar{x}_F)$ to take into account this effect.

Thus for $a_{d-1}(P;t)$ we obtain:

$$\begin{aligned}
a_{d-1}(P;t) &= -e_{d-1}(P;-t) + \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \frac{1}{2} e_{d-1}(F;-t) = \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \mathrm{vol}^*(F)\Big(\overline{B}_1^+\big(-\langle v_F, \bar{x}_F\rangle\, t\big) + \frac{1}{2}\mathbb{1}_{\Lambda_F^*}(-t\bar{x}_F)\Big) \\
&= \sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \mathrm{vol}^*(F)\Big(\overline{B}_1\big(-\langle v_F, \bar{x}_F\rangle\, t\big)\Big) = -\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \mathrm{vol}^*(F)\overline{B}_1\big(\langle v_F, \bar{x}_F\rangle\, t\big),
\end{aligned}$$

where we have used that v_F is Λ_F-primitive and hence $t\bar{x}_F \in \Lambda_F^*$ exactly when $\langle v_F, \bar{x}_F\rangle\, t \in \mathbb{Z}$.

For $a_{d-2}(P;t)$ we obtain:

$$\begin{aligned} a_{d-2}(P;t) - e_{d-2}(P;-t) &= -\sum_{\substack{F\in\mathcal{F}(P),\\ \dim(F)=d-1}} \frac{1}{2} e_{d-2}(F;-t) + \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(G)=d-2}} \omega_P(G) e_{d-2}(G;-t) \\ &= \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(F)=d-2}} \operatorname{vol}^*(G)\Bigg[\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G)\omega_P(G) + \frac{1}{2}\mathbb{1}_{\Lambda_{F_1}^*}(t\bar{x}_{F_1})\overline{B}_1^+\Big(\Big\langle \frac{v_{F_1,G}}{\|v_{F_1,G}\|^2}, -t\bar{x}_G\Big\rangle\Big) \\ &\quad + \frac{1}{2}\mathbb{1}_{\Lambda_{F_2}^*}(t\bar{x}_{F_2})\overline{B}_1^+\Big(\Big\langle \frac{v_{F_2,G}}{\|v_{F_2,G}\|^2}, -t\bar{x}_G\Big\rangle\Big)\Bigg], \end{aligned}$$

where we have used that each codimension two face is a facet of exactly two codimension one faces and $v_{F_i,G}/\|v_{F_i,G}\|^2$ is the Λ_G-primitive vector in the direction of $N_{F_i}(G)$.

Next, since $\operatorname{aff}(G) \subset \operatorname{aff}(F)$, we may take $x_G \in \operatorname{aff}(G)$ as a representative of both $\operatorname{aff}(F_1)$ and $\operatorname{aff}(F_2)$. Using the expression $\bar{x}_G = x_1 v_{F_1,G} + x_2 v_{F_2,G}$ together with $\langle v_{F_1}, t\bar{x}_G\rangle = tkx_2$ (see the proof of Lemma 6.4.1) we conclude that $t\bar{x}_{F_1} \in \Lambda_{F_1}^*$ if and only if $tkx_2 \in \mathbb{Z}$. Similarly, $t\bar{x}_{F_2} \in \Lambda_{F_2}^*$ if and only if $tkx_1 \in \mathbb{Z}$, so:

$$\begin{aligned} a_{d-2}(P;t) - e_{d-2}(P;-t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(F)=d-2}} \operatorname{vol}^*(G)\Bigg[&\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G)\omega_P(G) + \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_2t)\overline{B}_1^+\Big(\Big\langle \frac{v_{F_1,G}}{\|v_{F_1,G}\|^2}, -t\bar{x}_G\Big\rangle\Big) \\ &+ \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_1t)\overline{B}_1^+\Big(\Big\langle \frac{v_{F_2,G}}{\|v_{F_2,G}\|^2}, -t\bar{x}_G\Big\rangle\Big)\Bigg]. \end{aligned}$$

Using $v_{F_2,G} = hv_{F_1,G} + kv_2$ and since $v_{F_1,G}/\|v_{F_1,G}\|^2 \in \Lambda_G$ and $v_2 \in \Lambda_G^*$, when $kx_2t \in \mathbb{Z}$,

$$\begin{aligned} \Big\langle \frac{v_{F_1,G}}{\|v_{F_1,G}\|^2}, -t\bar{x}_G\Big\rangle &= -tx_1 - \frac{tx_2}{\|v_{F_1,G}\|^2}\big\langle v_{F_1,G}, v_{F_2,G}\big\rangle \\ &= -tx_1 - thx_2 - tkx_2\frac{\langle v_{F_1,G}, v_2\rangle}{\|v_{F_1,G}\|^2} = -tx_1 - thx_2 \pmod 1. \end{aligned}$$

Similarly, let h^{-1} be an integer such that $hh^{-1} = 1 \pmod k$. Using $hv_{F_1,G} = v_{F_2,G} - kv_2$, $h^{-1} \in \mathbb{Z}$, $v_{F_2,G}/\|v_{F_2,G}\|^2 \in \Lambda_G$, and $v_2 \in \Lambda_G^*$, when $kx_1t \in \mathbb{Z}$, we get

$$\begin{aligned} \Big\langle \frac{v_{F_2,G}}{\|v_{F_2,G}\|^2}, -t\bar{x}_G\Big\rangle &= -tx_2 - tx_1\Big\langle \frac{v_{F_2,G}}{\|v_{F_2,G}\|^2}, v_{F_1,G}\Big\rangle \\ &= -tx_2 - tx_1h^{-1}\Big(1 - k\Big\langle \frac{v_{F_2,G}}{\|v_{F_2,G}\|^2}, v_2\Big\rangle\Big) \pmod 1 = -t(h^{-1}x_1 + x_2) \pmod 1. \end{aligned}$$

Applying these relations to the main expression,

$$\begin{aligned} a_{d-2}(P;t) - e_{d-2}(P;-t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(F)=d-2}} \operatorname{vol}^*(G)\Big[&\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G)\omega_P(G) + \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_2t)\overline{B}_1^+\big(-(x_1+hx_2)t\big) \\ &- \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_1t)\overline{B}_1\big((h^{-1}x_1+x_2)t\big) - \frac{1}{4}\mathbb{1}_{\mathbb{Z}}(kx_1t)\mathbb{1}_{\mathbb{Z}}\big((h^{-1}x_1+x_2)t\big)\Big]. \end{aligned}$$

Next we use $\mathbb{1}_{\mathbb{Z}}(kx_1 t)\mathbb{1}_{\mathbb{Z}}\big((h^{-1}x_1 + x_2)t\big) = \mathbb{1}_{\Lambda_G^*}(t\bar{x}_G)$. To see why this is true, from $\bar{x}_G = x_1 v_{F_1,G} + x_2 v_{F_2,G} = (x_1 + hx_2)v_1 + kx_2 v_2$, we see that $\bar{x}_G \in \Lambda_G^*$ if and only if $kx_2 \in \mathbb{Z}$ and $x_1 + hx_2 \in \mathbb{Z}$. Hence, if $kx_1 \in \mathbb{Z}$ and $h^{-1}x_1 + x_2 \in \mathbb{Z}$, multiplying the second item by h we conclude that $x_1 + hx_2 \in \mathbb{Z}$ while multiplying it by k gives $h^{-1}kx_1 + kx_2 \in \mathbb{Z}$, so $kx_2 \in \mathbb{Z}$ and then $\bar{x}_G \in \Lambda_G^*$. The other direction is also easy.

Returning to the main expression,

$$
\begin{aligned}
a_{d-2}(P;t) - e_{d-2}(P;-t) = \sum_{\substack{G\in\mathcal{F}(P),\\ \dim(F)=d-2}} \operatorname{vol}^*(G)\bigg[\Big(\omega_P(G) - \frac{1}{4}\Big)\mathbb{1}_{\Lambda_G^*}(t\bar{x}_G) \\
+ \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_2 t)\overline{B}_1^{+}\big(-(x_1 + hx_2)t\big) - \frac{1}{2}\mathbb{1}_{\mathbb{Z}}(kx_1 t)\overline{B}_1\big((h^{-1}x_1 + x_2)t\big)\bigg].
\end{aligned}
$$

To finish the verification of formula $a_{d-2}(P;t)$ from Theorem 6.2.1, we must also take into account $e_{d-2}(P;-t)$ using the formula from Theorem 6.2.3. For that, notice that the functions $\overline{B}_2$ are even while the Dedekind-Rademacher sum satisfies $s(h,k;-x,-y) = s(h,k;x,y)$. The other two terms with $\overline{B}_1$ cancels exactly the terms we got from the computation above, which completes the verification of Theorem 6.2.1, given Theorem 6.2.3.

Chapter 7

The null set of a polytope and the Pompeiu property for polytopes

This chapter is based on the publication *"F.C. Machado, S. Robins,* The null set of a polytope, and the Pompeiu property for polytopes, *preprint arXiv:2104.01957, 2021, 9 pages."*

Abstract. We study the null set $N(P)$ of the Fourier-Laplace transform of a polytope $P \subset \mathbb{R}^d$, and we find that $N(P)$ does not contain (almost all) circles in $\mathbb{R}^d$. As a consequence, the null set does not contain the algebraic varieties $\{z \in \mathbb{C}^d \mid z_1^2 + \cdots + z_d^2 = \alpha^2\}$ for each fixed $\alpha \in \mathbb{C}$, and hence we get an explicit proof that the Pompeiu property is true for all polytopes. Our proof uses the Brion-Barvinok theorem, which gives a concrete formulation for the Fourier-Laplace transform of a polytope, and it also uses properties of Bessel functions.

The original proof that polytopes (as well as other bodies) possess the Pompeiu property was given by Brown, Schreiber, and Taylor [BST73] for dimension 2. Williams [Wil76, p. 184] later observed that the same proof also works for $d > 2$ and, using eigenvalues of the Laplacian, gave another proof valid for $d \geq 2$ that polytopes have the Pompeiu property.

7.1 Introduction

The Pompeiu problem is a fundamental problem that initially arose by intertwining the basic theory of convex bodies with harmonic analysis. To describe it precisely, consider the group $M(d)$ of all rigid motions of $\mathbb{R}^d$, including translations, and fix any bounded set with positive measure $P \subset \mathbb{R}^d$ with $\dim(P) = d$. In 1929, Pompeiu [Pom29a; Pom29b] asked the following question. Suppose that all of the following integrals vanish:

$$\int_{\sigma(P)} f(x)\,\mathrm{d}x = 0, \tag{7.1}$$

taken over all rigid motions $\sigma \in M(d)$. Does it necessarily follow that $f = 0$?

If the answer is affirmative, then the set $P \subset \mathbb{R}^d$ is said to have the Pompeiu property. It is a conjecture that in every dimension, balls are the only sets with a boundary homeomorphic to the sphere that do not have the Pompeiu property [Wil76]. As is immediately apparent, the Pompeiu property is equivalent to the claim that the integral of f over P, as well as the integrals of f over all the rigid motions of P, uniquely determine the function f.

It is rather surprising that after almost 100 years, the Pompeiu problem remains unsolved for general sets in $\mathbb{R}^d$. There are, however, infinite families of sets which are known to have the Pompeiu property, and we recall some of these results.

More attention has been devoted to dimension $d = 2$, and a breakthrough occurred with the results of Brown, Schreiber, and Taylor [BST73], who showed that the Pompeiu problem is very closely related to mean periodic functions, developed by L. Schwartz [Sch47]. In [BST73, Theorem 5.11] the authors prove that any Lipschitz curve in the plane with a 'corner' has the Pompeiu property, and consequently all polygons have the Pompeiu property. Williams [Wil76] mentions that the proof of Theorem 5.11 in [BST73] generalizes directly to d-dimensions, though such a proof is not explicitly given there. Moreover, Williams [Wil76] also proves that if a set homemorphic to the sphere does not have the Pompeiu property and has a portion of a real analytic surface on its boundary, then any connected real analytic extension of this surface also lies on the boundary of the set, and as a consequence large infinite families of bodies have the Pompeiu property, including polytopes.

Despite these advances, even in dimension 2 the Pompeiu problem remains open for general sets. On the other hand, there has been a lot of interesting work that relates the Pompeiu problem to other branches of Mathematics, such as the recent work of Kiss, Malikiosis, Somlai, and Vizer [Kis+20], where a discretized version of the Pompeiu problem is shown to be closely tied to the (unsolved) Fuglede conjecture over finite abelian groups.

It turns out that the Pompeiu problem is equivalent to a few other long-standing problems. One of these equivalences is the celebrated conjecture of Schiffer in pde's, relating the Pompeiu problem directly to eigenvalues of the Laplacian (see e.g., Section 3 of Berenstein [Ber80]).

When we consider the Fourier-Laplace transform of the body P, a very useful necessary and sufficient condition arises. To describe it precisely, suppose we are given the indicator function $\mathbb{1}_P$ of a polytope P. Recall the definition of the Fourier-Laplace transform of P for all $z \in \mathbb{C}^d$,

$$\hat{\mathbb{1}}_P(z) := \int_P e^{-2\pi i \langle x, z \rangle} \, \mathrm{d}x,$$

with the inner product $\langle x, z \rangle := x_1 z_1 + \cdots x_d z_d$ (we note that this is not the Hermitian inner product). The null set of the Fourier-Laplace transform of a polytope P is defined by

$$N(P) := \{\xi \in \mathbb{C}^d \mid \hat{\mathbb{1}}_P(\xi) = 0\},$$

which we also refer to simply as the *null set of P*. It is an interesting problem how the null set determines the characteristics of a bounded domain Ω, see the lecture notes from Kobayashi [Kob91] for a long study on this topic and in particular on asymptotic properties of $N(\Omega)$ in the case where the boundary of Ω is infinitely smooth and has positive curvature. Bianchi [Bia16] proves similar results weakening the smoothing assumptions on the boundary of Ω and Benguria, Levitin, and Parnovski [BLP09] make some conjectures and theorems about the shortest vector in $N(\Omega)$.

We define the complex algebraic variety

$$S_{\mathbb{C}}(\alpha) := \{z \in \mathbb{C}^d \mid z_1^2 + \cdots + z_d^2 = \alpha^2\},$$

for each fixed $\alpha \in \mathbb{C}$.

Theorem 7.1.1 (Brown, Shreiber, and Taylor [BST73]). *A bounded set with positive measure $P \subset \mathbb{R}^d$ has the Pompeiu property if and only if the Fourier-Laplace transform of P, namely $\hat{\mathbb{1}}_P(z)$, does not vanish identically on any of the complex varieties $S_{\mathbb{C}}(\alpha)$, for any $\alpha \in \mathbb{C} \setminus \{0\}$.*

In other words, Pompeiu's problem is equivalent to the claim that the null set $N(P)$ does not contain any of the complex algebraic varieties $S_{\mathbb{C}}(\alpha)$. The authors of [BST73] prove this condition for dimension $d = 2$, and they mention that the same proof works in general dimension. Bagchi and Sitaram [BS90, p. 74–75] reprove Theorem 7.1.1, for $d = 2$, and they also mention that the same proof works for general dimension. Berenstein comments (Section 3 of [Ber80]), that the condition '$\alpha \in \mathbb{C} \setminus \{0\}$' from Theorem 7.1.1 can be replaced by '$\alpha > 0$' (possibly under the condition that P is simply-connected). We do not use this restriction in our proof, however, since our arguments work for any complex '$\alpha \in \mathbb{C} \setminus \{0\}$'.

One direction of Theorem 7.1.1 is easy to see. If $S_{\mathbb{C}}(\alpha) \subset N(P)$ for some $\alpha \in \mathbb{C} \setminus \{0\}$, then taking $\xi \in S_{\mathbb{C}}(\alpha)$ and letting $f(x) := e^{-2\pi i \langle x, \xi \rangle}$, we have $\int_{\sigma(P)} f(x)\, dx = 0$ for all $\sigma \in M(d)$. For the other direction, first we notice that it is apparent that $S_{\mathbb{C}}(0) \not\subset N(P)$, because the zero element $0 \in S_{\mathbb{C}}(0)$, yet $0 \notin N(P)$ since $\hat{1}_P(0) = \mathrm{vol}(P) \neq 0$. Berenstein [Ber80, p. 133] observes that in [BST73], Brown, Schreiber, and Taylor show that if P doesn't have the Pompeiu property, then $\hat{\mathbb{1}}_{\sigma(P)}$ has a common zero z for all $\sigma \in M(d)$. Next, using the fact that for a rotation $\sigma \in \mathrm{SO}(d, \mathbb{R}) \subset M(d)$ we get $\hat{\mathbb{1}}_{\sigma(P)}(z) = \hat{\mathbb{1}}_P(\sigma^{-1} z)$, we obtain that the orbit $\mathrm{SO}(d, \mathbb{R}) z \subset N(P)$. Letting $\alpha := z_1^2 + \cdots + z_d^2$, we have that $\mathrm{SO}(d, \mathbb{R}) z$ is a real submanifold of $S_{\mathbb{C}}(\alpha)$, on which the analytic function $\hat{\mathbb{1}}_P$ vanishes, hence it also vanishes on the rest of $S_{\mathbb{C}}(\alpha)$ (see e.g., Lemma 3.1.2 in [Leb20]).

Here we prove, in an explicit manner, that the Pompeiu property is true for all polytopes $\mathcal{P} \subset \mathbb{R}^d$, with $d \geq 2$. In other words, we give a new proof that all polytopes have the Pompeiu property, which is simple and is essentially self-contained. In addition, the present methods allow us to prove slightly more: 'most' circles in $\mathbb{R}^d$ are not contained in the null set $N(P)$ (stated precisely in Theorem 7.1.2).

By way of comparison, the machinery developed in [Wil76], from which it also follows that polytopes have the Pompeiu property, is highly non-trivial; the present proof uses an explicitly known form of the Fourier-Laplace transform of a polytope, and is much simpler. Our main result is as follows.

Theorem 7.1.2. *Let $P \subset \mathbb{R}^d$ be a d-dimensional polytope, $H \subset \mathbb{R}^d$ be a 2-dimensional real* *subspace that is not orthogonal to any edge from P, and fix an orthonormal basis $\{e, f\} \subset \mathbb{R}^d$ for H.*

Then the null set $N(P)$ does not contain the 'circle'

$$C_\alpha := \left\{ \alpha(\cos t)e + \alpha(\sin t)f \in \mathbb{C}^d \mid t \in [-\pi, \pi] \right\},$$

for any $\alpha \in \mathbb{C} \setminus \{0\}$.

As an immediate consequence of Theorem 7.1.2 and Theorem 7.1.1, we recover William's result [Wil76] for polytopes, as follows.

Corollary 7.1.3. *The null set $N(P)$ does not contain the complex variety $S_{\mathbb{C}}(\alpha)$, for any $\alpha \in \mathbb{C} \setminus \{0\}$. Consequently, all polytopes in $\mathbb{R}^d$ have the Pompeiu property, for each $d \geq 2$.*

Remark 7.1.4. We note that as a special case of Theorem 7.1.2, the null set $N(P)$ does not contain any real circle sitting in $\mathbb{R}^d$, except perhaps for those circles that lie in some two-dimensional hyperplane orthogonal to some edge of P. The reason we cannot yet exclude this (zero measure) set of circles is because of the singularities that come from the denominators in Brion's formula for the Fourier transform of a polytope. However, because these singularities are removable, we conjecture that no circle in $\mathbb{R}^d$ is contained in the null set $N(P)$.

7.2 Preliminaries

The proof of Theorem 7.1.2 uses the development of the Fourier-Laplace transform of a polytope via Brion's theorem, which we summarized in Section 5.2.1, and also some properties of the Bessel functions, which we see next.

7.2.1 Some properties of the Bessel functions

The Bessel functions are a very well known family of functions that appear in physical problems with spherical or cylindrical symmetry. One reason for their ubiquity is their appearance as solutions of the wave equation when put into spherical or cylindrical coordinate systems.

Here we collect some of their useful properties, all of which can be found e.g. in the Chapter 9 from the book of Temme [Tem96]. We will be interested in the Bessel functions of the first kind, called $J_n(z)$, which are defined for complex values of z, and integer order n (although they may also be defined for complex n). They appear in the present work since they have the following integral representation:

$$J_n(z) = \frac{1}{2\pi} \int_0^{2\pi} e^{iz \sin t} e^{-int} \, dt.$$

This identity implies that they are the coefficients of the Fourier series expansion of $e^{iz \sin t}$:

$$e^{iz \sin t} = \sum_{n \in \mathbb{Z}} J_n(z) e^{int}, \tag{7.2}$$

an identity that is also known as the Jacobi-Anger expansion. Another representation for $J_n(z)$ is the hypergeometric series

$$J_n(z) = \left(\frac{z}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{(n+k)!k!}\left(\frac{z}{2}\right)^{2k},$$

from which it easily follows that $J_n(-z) = (-1)^n J_n(z)$, and also that there is the following asymptotic behavior for large n and fixed z:

$$\lim_{n\to\infty} J_n(z)\left(\frac{1}{n!}\left(\frac{z}{2}\right)^n\right)^{-1} = 1. \tag{7.3}$$

7.3 Proof of Theorem 7.1.2

We divide the proof into two parts using the following lemma.

Lemma 7.3.1. *Let $P \subset \mathbb{R}^d$ be a polytope oriented in such a way that no edge vector has both of its first two coordinates zero. For each vertex $v \in V(P)$, represent its first two coordinates in polar form:*

$$v = (r_v \cos\phi_v, r_v \sin\phi_v, v_3, \dots, v_d).$$

Let Q be the intersection of the plane generated by the first two coordinates of $\mathbb{C}^d$, with the null set $N(P)$. If Q contains a 'circle'

$$C'_\alpha := \{(\alpha\cos t, \alpha\sin t, 0, \dots, 0) \mid t \in [-\pi, \pi]\}$$

for some $\alpha \in \mathbb{C}\setminus\{0\}$, then there exist N and coefficients $c_{v,k} \in \mathbb{C}$ for $-N \le k \le N$, not all of them zero, so that α satisfies the following identity for every $n \in \mathbb{Z}$:

$$\sum_{v\in V(P)} e^{-in\phi_v} \sum_{k=-N}^{N} c_{v,k} J_{n-k}(2\pi\alpha r_v) i^k e^{ik\phi_v} = 0. \tag{7.4}$$

Proof. As mentioned in Section 5.2.1, Brion's theorem gives us Equation (5.8), valid for any $z \in \mathbb{C}^d$ that doesn't annul some denominator:

$$\hat{\mathbb{1}}_P(z) = \sum_{v\in V(P)} \sum_{j=1}^{M_v} \frac{e^{-2\pi i\langle v,z\rangle}}{(2\pi i)^d} \frac{\det K_{v,j}}{\langle w^v_{j,1}, z\rangle \dots \langle w^v_{j,d}, z\rangle}. \tag{7.5}$$

We parameterize C'_α as $z(t) = (z_1, \dots, z_d) \in \mathbb{C}^d$, with

$$z_1 = \alpha\cos t, \quad z_2 = \alpha\sin t, \quad z_3 = \dots = z_d = 0, \tag{7.6}$$

for $t \in (-\pi, \pi]$.

Substituting $\cos t = (e^{it} + e^{-it})/2$, $\sin t = (e^{it} - e^{-it})/(2i)$ in (7.6) and using the assumption that the directions $w^v_{j,l}$ do not have both of their first two coordinates equal to zero, we may see each factor $\langle w^v_{j,l}, z(t)\rangle$ as a trigonometric polynomial of degree 1 (that is, a function of the form $c_{-1}e^{-it} + c_0 + c_1 e^{it}$, with $c_1 \in \mathbb{C} \setminus \{0\}$), as well the product of all these factors

$$p(t) := \prod_{v \in V(P)} \prod_{j=1}^{M_v} \prod_{l=1}^{d} \langle w_{j,l}^{v}, z(t) \rangle,$$

as a trigonometric polynomial. Multiplying (7.5) by $(2\pi i)^d p(t)$ and using the assumption that $\hat{\mathbb{1}}_P(z(t)) = 0$ for all $t \in (-\pi, \pi]$, we get

$$0 = \sum_{v \in V(P)} p_v(t) e^{-2\pi i \langle v, z(t) \rangle}, \tag{7.7}$$

where each $p_v(t)$ is also a trigonometric polynomial, since the factors in the denominators of (7.5) and in $p(t)$ cancel out. We denote the coefficients of $p_v(t)$ by $c_{v,k}$, as follows:

$$p_v(t) := p(t) \sum_{j=1}^{M_v} \frac{\det K_{v,j}}{\langle w_{j,1}^{v}, z(t) \rangle \ldots \langle w_{j,d}^{v}, z(t) \rangle} = \sum_{k=-N}^{N} c_{v,k} e^{ikt}. \tag{7.8}$$

Defining

$$q_v(t) := \prod_{y \in V(P) \setminus \{v\}} \prod_{j=1}^{M_y} \prod_{l=1}^{d} \langle w_{j,l}^{y}, z(t) \rangle,$$

we may write $p_v(t)$ as

$$p_v(t) = q_v(t) \sum_{j=1}^{M_v} \det K_{v,j} \prod_{\substack{k=1 \\ k \neq j}}^{M_v} \prod_{l=1}^{d} \langle w_{k,l}^{v}, z(t) \rangle.$$

To confirm that no cancellation happens and that in particular the functions $p_v(t)$ are not all identically zero, observe that because no edge has both of its first two coordinates equal to zero, the intersection between the subspace of $\mathbb{R}^d$ spanned by the first two coordinates and the spaces orthogonal to each edge is a finite set of lines. Letting $\alpha = re^{i\phi}$ with $r > 0$ and $\phi \in (-\pi, \pi]$, we may also observe that $e^{-i\phi} z(t) \in \mathbb{R}^d$. Thus we can choose $t_0 \in (-\pi, \pi]$ such that $e^{-i\phi} z(t_0)$ is not orthogonal to any edge. If we define

$$u := \operatorname{argmin}_{x \in V(P)} \langle x,\ e^{-i\phi} z(t_0) \rangle,$$

then $\langle w_{k,l}^{u}, e^{-i\phi} z(t_0) \rangle > 0$ for all k and l. Hence

$$\sum_{j=1}^{M_u} \det K_{u,j} \prod_{\substack{k=1 \\ k \neq j}}^{M_u} \prod_{l=1}^{d} \langle w_{k,l}^{u}, e^{-i\phi} z(t_0) \rangle = e^{-i\phi d(M_u - 1)} \sum_{j=1}^{M_u} \det K_{u,j} \prod_{\substack{k=1 \\ k \neq j}}^{M_u} \prod_{l=1}^{d} \langle w_{k,l}^{u}, z(t_0) \rangle > 0,$$

and therefore $p_u(t)$ is not identically zero.

Next, we use the generating functions for the Bessel functions (7.2). To adapt the formulas for our context, we write the first two coordinates of v in polar form: $v =$

$(r_v \cos\phi_v, r_v \sin\phi_v, v_3, \dots, v_d)$, so that

$$-\langle v, z(t)\rangle = -\alpha r_v \cos(t - \phi_v) = \alpha r_v \sin(t - \phi_v - \pi/2).$$

Hence from (7.2) follows

$$e^{-2\pi i\langle v, z(t)\rangle} = \sum_{n\in\mathbb{Z}} J_n(2\pi\alpha r_v) e^{int} e^{-in(\phi_v+\pi/2)}.$$

Substituting into (7.7),

$$0 = \sum_{n\in\mathbb{Z}} \sum_{v\in V(P)} p_v(t) e^{-in(\phi_v+\pi/2)} J_n(2\pi\alpha r_v) e^{int}.$$

Next we substitute formula (7.8) into $p_v(t)$ and then replace n by $n-k$ in the summation:

$$\begin{aligned} 0 &= \sum_{n\in\mathbb{Z}} \sum_{v\in V(P)} \sum_{k=-N}^{N} c_{v,k} e^{-in(\phi_v+\pi/2)} J_n(2\pi\alpha r_v) e^{i(n+k)t} \\ &= \sum_{n\in\mathbb{Z}} \sum_{v\in V(P)} \sum_{k=-N}^{N} c_{v,k} e^{-i(n-k)(\phi_v+\pi/2)} J_{n-k}(2\pi\alpha r_v) e^{int}. \end{aligned}$$

The last expression is the Fourier series of the resulting function in $t \in (-\pi, \pi]$, and therefore all of the coefficients must vanish:

$$\sum_{v\in V(P)} e^{-in\phi_v} \sum_{k=-N}^{N} c_{v,k} J_{n-k}(2\pi\alpha r_v) e^{ik(\phi_v+\pi/2)} = 0.$$

Using $e^{ik\pi/2} = i^k$, we get the formula from the statement. □

To prove Theorem 7.1.2 we will now analyze Equation (7.4) for large n and determine the asymptotically dominant terms.

Proof of Theorem 7.1.2. Let $P \subset \mathbb{R}^d$ be a d-dimensional polytope, H be a 2-dimensional subspace not orthogonal to any edge from P and $e, f \in \mathbb{R}^d$ which form an orthogonal basis for H. Suppose, by way of contradiction, that $N(P)$ does contain a 'circle' $C_\alpha := \{\alpha(\cos t)e + \alpha(\sin t)f \in \mathbb{C}^d \mid t \in (-\pi, \pi]\}$ for some $\alpha \in \mathbb{C} \setminus \{0\}$.

We may consider a rotation R that sends H to the plane spanned by the first two coordinates of $\mathbb{R}^d$ and observe that $N(P)$ contains C_α if and only if $N(RP)$ contains $C'_\alpha := \{(\alpha\cos t, \alpha\sin t, 0, \dots, 0) \mid t \in [-\pi, \pi]\}$. The assumption that H is not orthogonal to any edge gets translated to the assumption that no direction $Rw^v_{j,l}$ has both of its first two coordinates equal to zero, and hence we have satisfied the hypotheses of Lemma 7.3.1. For simplicity, we henceforth omit the rotation R and we assume that P and H already have this orientation, in particular $C_\alpha = C'_\alpha$.

By Lemma 7.3.1, we know that identity (7.4) must be true. Since not all of the coefficients $c_{v,k}$ are zero, we may assume that N is the highest degree of a nonzero coefficient and we let $u \in V(P)$ be such that $c_{u,N} \neq 0$. Because a translation of the polytope by a vector $c \in \mathbb{R}^d$

implies that $\hat{\mathbb{1}}_{P+c}(z) = \hat{\mathbb{1}}_P(z)e^{-2\pi i\langle z,c\rangle}$, we may translate the polytope while preserving the assumption that its null set contains C_α. By translating P in the direction of u, we may assume that $u = \arg\max_{v\in V} r_v$ and that u is the only vertex that attains this maximum.

Using the asymptotic (7.3) for $J_n(z)$, we have:

$$\begin{aligned}\lim_{n\to\infty} \frac{(n-N)!2^{n-N}}{(2\pi r_u\alpha)^{n-N}} J_{n-k}(2\pi r_v\alpha) &= \lim_{n\to\infty} \frac{(n-N)!2^{n-N}}{(2\pi r_u\alpha)^{n-N}} \frac{(2\pi r_v\alpha)^{n-k}}{(n-k)!2^{n-k}} \\ &= \begin{cases} 1 \text{ if } k = N \text{ and } u = v, \\ 0 \text{ if } k < N \text{ or } (k = N \text{ and } u \neq v). \end{cases}\end{aligned} \tag{7.9}$$

For any $n > N$, we would like to focus on the unique dominant term of (7.4), which grows with n as $\frac{1}{(n-N)!}\left(\frac{2\pi r_u\alpha}{2}\right)^{n-N}$. To be more precise, we multiply Equation (7.4) by $e^{in\phi_u}\frac{(n-N)!2^{n-N}}{(2\pi r_u\alpha)^{n-N}}$ to get:

$$\sum_{v\in V(P)} e^{-in(\phi_v-\phi_u)} \sum_{k=-N}^{N} c_{v,k} \frac{(n-N)!2^{n-N}}{(2\pi r_u\alpha)^{n-N}} J_{n-k}(2\pi r_v\alpha) i^k e^{ik\phi_v} = 0.$$

Taking the limit as $n \longrightarrow \infty$, (7.9) tells us that all terms with $k < N$ and $v \neq u$ tend to 0, leaving us with only the $k = N$ term:

$$c_{u,N}\, i^N\, e^{iN\phi_u} = 0,$$

implying that $c_{u,N} = 0$, a contradiction.

Therefore we conclude that no α can satisfy Equation (7.4) for every n and hence by Lemma 7.3.1, $N(P)$ cannot contain C_α for any plane H that is not orthogonal to any edge of P. □

References

[Ale33] A.D. Alexandrov. “A theorem on convex polyhedra”. In: *Trudy Mat. Int. Steklov, Sect. Math* 4 (1933), p. 87 (cit. on p. 131).

[Apo76] Tom M. Apostol. *Introduction to analytic number theory.* Undergraduate Texts in Mathematics. Springer-Verlag, New York-Heidelberg, 1976, pp. xii+338 (cit. on p. 35).

[Bac+09] Christine Bachoc et al. “Lower bounds for measurable chromatic numbers”. In: *Geom. Funct. Anal.* 19.3 (2009), pp. 645–661. ISSN: 1016-443X. DOI: 10.1007/s00039-009-0013-7 (cit. on pp. 58, 70).

[Bac+12] Christine Bachoc et al. “Invariant semidefinite programs”. In: *Handbook on semidefinite, conic and polynomial optimization.* Vol. 166. Internat. Ser. Oper. Res. Management Sci. Springer, New York, 2012, pp. 219–269. DOI: 10.1007/978-1-4614-0769-0_9 (cit. on pp. 10, 41, 48).

[Bar02] Alexander Barvinok. *A course in convexity.* Vol. 54. Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, 2002, pp. x+366. ISBN: 0-8218-2968-8. DOI: 10.1090/gsm/054 (cit. on pp. 61–63).

[Bar06] Alexander Barvinok. “Computing the Ehrhart quasi-polynomial of a rational simplex”. In: *Math. Comp.* 75.255 (2006), pp. 1449–1466. ISSN: 0025-5718. DOI: 10.1090/S0025-5718-06-01836-9 (cit. on pp. 91, 103, 107, 119).

[Bar08] Alexander Barvinok. *Integer points in polyhedra.* Zurich Lectures in Advanced Mathematics. European Mathematical Society (EMS), Zürich, 2008, pp. viii+191. ISBN: 978-3-03719-052-4. DOI: 10.4171/052 (cit. on pp. 92–94, 96, 103).

[Bar92] Alexander Barvinok. “Exponential integrals and sums over convex polyhedra”. In: *Funktsional. Anal. i Prilozhen.* 26.2 (1992), pp. 64–66. ISSN: 0374-1990. DOI: 10.1007/BF01075276 (cit. on pp. 90, 94).

[Bar93] Alexander I. Barvinok. “Computing the volume, counting integral points, and exponential sums”. In: *Discrete Comput. Geom.* 10.2 (1993), pp. 123–141. ISSN: 0179-5376. DOI: 10.1007/BF02573970 (cit. on p. 90).

[Bar94] Alexander I. Barvinok. “A polynomial time algorithm for counting integral points in polyhedra when the dimension is fixed”. In: *Math. Oper. Res.* 19.4 (1994), pp. 769–779. ISSN: 0364-765X. DOI: 10.1287/moor.19.4.769 (cit. on p. 2).

[Ber80] Carlos A. Berenstein. “An inverse spectral theorem and its relation to the Pompeiu problem”. In: *Journal d’Analyse Mathématique* 37.1 (1980), pp. 128–144. DOI: 10.1007/BF02797683 (cit. on pp. 138, 139).

[Bez+17] Jeff Bezanson et al. “Julia: a fresh approach to numerical computing”. In: *SIAM Rev.* 59.1 (2017), pp. 65–98. ISSN: 0036-1445. DOI: 10.1137/141000671 (cit. on pp. 70, 77).

[Bia16] Gabriele Bianchi. "The covariogram and Fourier-Laplace transform in $\mathbb{C}^n$". In: *Proc. Lond. Math. Soc. (3)* 113.1 (2016), pp. 1–23. ISSN: 0024-6115. DOI: 10.1112/plms/pdw020 (cit. on p. 139).

[BLP09] Rafael Benguria, Michael Levitin, and Leonid Parnovski. "Fourier transform, null variety, and Laplacian's eigenvalues". In: *J. Funct. Anal.* 257.7 (2009), pp. 2088–2123. ISSN: 0022-1236. DOI: 10.1016/j.jfa.2009.06.022 (cit. on p. 139).

[BMV04] Eiichi Bannai, Akihiro Munemasa, and Boris Venkov. "The nonexistence of certain tight spherical designs". In: *Algebra i Analiz* 16.4 (2004), pp. 1–23. ISSN: 0234-0852. DOI: 10.1090/S1061-0022-05-00868-X (cit. on p. 73).

[Boc41] Salomon Bochner. "Hilbert distances and positive definite functions". In: *Ann. of Math. (2)* 42 (1941), pp. 647–656. ISSN: 0003-486X. DOI: 10.2307/1969252 (cit. on pp. 10, 13).

[BP89] Johannes Buchmann and Michael Pohst. "Computing a lattice basis from a system of generating vectors". In: *EUROCAL '87 (Leipzig, 1987)*. Vol. 378. Lecture Notes in Comput. Sci. Springer, Berlin, 1989, pp. 54–63. DOI: 10.1007/3-540-51517-8_89 (cit. on p. 109).

[BP99] Alexander Barvinok and James E. Pommersheim. "An algorithmic theory of lattice points in polyhedra". In: *New perspectives in algebraic combinatorics (Berkeley, CA, 1996–97)*. Vol. 38. Math. Sci. Res. Inst. Publ. Cambridge Univ. Press, Cambridge, 1999, pp. 91–147 (cit. on pp. 2, 89, 92, 131).

[BR15] Matthias Beck and Sinai Robins. *Computing the continuous discretely*. Second. Undergraduate Texts in Mathematics. Integer-point enumeration in polyhedra, With illustrations by David Austin. Springer, New York, 2015, pp. xx+285. ISBN: 978-1-4939-2968-9; 978-1-4939-2969-6. DOI: 10.1007/978-1-4939-2969-6 (cit. on pp. 91, 95, 101, 102, 104, 125–128).

[Bra+19] Luca Brandolini et al. "Convergence of multiple Fourier series and Pick's theorem". In: *arXiv preprint arXiv:1909.03435* (2019) (cit. on p. 130).

[Bri88] Michel Brion. "Points entiers dans les polyèdres convexes". In: *Ann. Sci. École Norm. Sup. (4)* 21.4 (1988), pp. 653–663. ISSN: 0012-9593. URL: http://www.numdam.org/item?id=ASENS_1988_4_21_4_653_0 (cit. on p. 93).

[BS90] S. C. Bagchi and A. Sitaram. "The Pompeiu problem revisited". In: *Enseign. Math. (2)* 36.1-2 (1990), pp. 67–91. ISSN: 0013-8584 (cit. on p. 139).

[BST73] Leon Brown, Bertram M. Schreiber, and B. Alan Taylor. "Spectral synthesis and the Pompeiu problem". In: *Ann. Inst. Fourier (Grenoble)* 23.3 (1973), pp. 125–154. ISSN: 0373-0956. URL: http://www.numdam.org/item?id=AIF_1973__23_3_125_0 (cit. on pp. 137–139).

[Buk16] Boris Bukh. "Bounds on equiangular lines and on related spherical codes". In: *SIAM J. Discrete Math.* 30.1 (2016), pp. 549–554. ISSN: 0895-4801. DOI: 10.1137/15M1036920 (cit. on p. 76).

[BV07] Nicole Berline and Michèle Vergne. "Local Euler-Maclaurin formula for polytopes". In: *Mosc. Math. J.* 7.3 (2007), pp. 355–386, 573. ISSN: 1609-3321. DOI: 10.17323/1609-4514-2007-7-3-355-386 (cit. on pp. 2, 96–98, 103, 108, 134).

[BV08] Christine Bachoc and Frank Vallentin. "New upper bounds for kissing numbers from semidefinite programming". In: *J. Amer. Math. Soc.* 21.3 (2008), pp. 909–924. ISSN: 0894-0347. DOI: 10.1090/S0894-0347-07-00589-9 (cit. on pp. 13, 19, 21, 57, 58, 67, 70, 71).

[BY13] Alexander Barg and Wei-Hsuan Yu. "New bounds for spherical two-distance sets". In: *Exp. Math.* 22.2 (2013), pp. 187–194. ISSN: 1058-6458. DOI: 10.1080/10586458.2013.767725 (cit. on pp. 58, 59, 71, 77).

[BY14] Alexander Barg and Wei-Hsuan Yu. "New bounds for equiangular lines". In: *Discrete geometry and algebraic combinatorics.* Vol. 625. Contemp. Math. Amer. Math. Soc., Providence, RI, 2014, pp. 111–121. DOI: 10.1090/conm/625/12494 (cit. on pp. 71, 72, 74–77, 81–86).

[CE03] Henry Cohn and Noam Elkies. "New upper bounds on sphere packings. I". In: *Ann. of Math. (2)* 157.2 (2003), pp. 689–714. ISSN: 0003-486X. DOI: 10.4007/annals.2003.157.689 (cit. on pp. 50, 52, 55).

[CK07] Henry Cohn and Abhinav Kumar. "Universally optimal distribution of points on spheres". In: *J. Amer. Math. Soc.* 20.1 (2007), pp. 99–148. ISSN: 0894-0347. DOI: 10.1090/S0894-0347-06-00546-7 (cit. on p. 73).

[Coh+17] Henry Cohn et al. "The sphere packing problem in dimension 24". In: *Ann. of Math. (2)* 185.3 (2017), pp. 1017–1033. ISSN: 0003-486X. DOI: 10.4007/annals.2017.185.3.8 (cit. on p. 56).

[Del73] P. Delsarte. "An algebraic approach to the association schemes of coding theory". In: *Philips Res. Rep. Suppl.* 10 (1973), pp. vi+97 (cit. on p. 57).

[DF88] Martin E. Dyer and Alan M. Frieze. "On the complexity of computing the volume of a polyhedron". In: *SIAM J. Comput.* 17.5 (1988), pp. 967–974. ISSN: 0097-5397. DOI: 10.1137/0217060 (cit. on p. 108).

[DGS77] Philippe Delsarte, Jean-Marie Goethals, and Johan J. Seidel. "Spherical codes and designs". In: *Geometriae Dedicata* 6.3 (1977), pp. 363–388. ISSN: 0046-5755. DOI: 10.1007/BF03187604 (cit. on pp. 57, 58, 70, 71, 73).

[DLR16] Ricardo Diaz, Quang-Nhat Le, and Sinai Robins. "Fourier transforms of polytopes, solid angle sums, and discrete volume". In: *arXiv preprint* (2016). arXiv:1602.08593 (cit. on pp. 37, 40, 89, 104, 110, 111, 120, 131).

[Dos+17] Maria Dostert et al. "New upper bounds for the density of translative packings of three-dimensional convex bodies with tetrahedral symmetry". In: *Discrete Comput. Geom.* 58.2 (2017), pp. 449–481. ISSN: 0179-5376. DOI: 10.1007/s00454-017-9882-y (cit. on pp. 53, 77).

[Dos17] Maria M. Dostert. "Geometric Packings of Non-Spherical Shapes". PhD thesis. Universität zu Köln, 2017. URL: https://kups.ub.uni-koeln.de/7706/ (cit. on pp. 41, 53).

[Ehr62] Eugène Ehrhart. "Sur les polyèdres rationnels homothétiques à n dimensions". In: *C. R. Acad. Sci. Paris* 254 (1962), pp. 616–618. ISSN: 0001-4036 (cit. on p. 101).

[EW17] Manfred Einsiedler and Thomas Ward. *Functional analysis, spectral theory, and applications.* Vol. 276. Graduate Texts in Mathematics. Springer, Cham, 2017, pp. xiv+614. ISBN: 978-3-319-58539-0; 978-3-319-58540-6. DOI: 10.1007/978-3-319-58540-6 (cit. on pp. 26, 27).

[FH91] William Fulton and Joe Harris. *Representation theory.* Vol. 129. Graduate Texts in Mathematics. A first course, Readings in Mathematics. Springer-Verlag, New York, 1991, pp. xvi+551. ISBN: 0-387-97527-6; 0-387-97495-4. DOI: 10.1007/978-1-4612-0979-9 (cit. on p. 5).

[Fie+17] Claus Fieker et al. "Nemo/Hecke: computer algebra and number theory packages for the Julia programming language". In: *ISSAC'17—Proceedings of the 2017 ACM International Symposium on Symbolic and Algebraic Computation.* ACM, New York, 2017, pp. 157–164. DOI: 10.1145/3087604.3087611 (cit. on p. 77).

[Fol16] Gerald B. Folland. *A course in abstract harmonic analysis.* Second. Textbooks in Mathematics. CRC Press, Boca Raton, FL, 2016, xiii+305 pp.+loose errata. ISBN: 978-1-4987-2713-6. DOI: 10.1201/b19172 (cit. on pp. 5, 8, 9).

[FR13] Simon Foucart and Holger Rauhut. *A mathematical introduction to compressive sensing.* Applied and Numerical Harmonic Analysis. Birkhäuser/Springer, New York, 2013, pp. xviii+625. ISBN: 978-0-8176-4947-0; 978-0-8176-4948-7. DOI: 10.1007/978-0-8176-4948-7 (cit. on p. 59).

[GL17] Rachel Greenfeld and Nir Lev. "Fuglede's spectral set conjecture for convex polytopes". In: *Anal. PDE* 10.6 (2017), pp. 1497–1538. ISSN: 2157-5045. DOI: 10.2140/apde.2017.10.1497 (cit. on p. 91).

[GLS81] M. Grötschel, L. Lovász, and A. Schrijver. "The ellipsoid method and its consequences in combinatorial optimization". In: *Combinatorica* 1.2 (1981), pp. 169–197. ISSN: 0209-9683. DOI: 10.1007/BF02579273 (cit. on p. 45).

[GLV09] Nebojsa Gvozdenović, Monique Laurent, and Frank Vallentin. "Block-diagonal semidefinite programming hierarchies for 0/1 programming". In: *Oper. Res. Lett.* 37.1 (2009), pp. 27–31. ISSN: 0167-6377. DOI: 10.1016/j.orl.2008.10.003 (cit. on pp. 48, 61).

[GMS12] Dion C. Gijswijt, Hans D. Mittelmann, and Alexander Schrijver. "Semidefinite code bounds based on quadruple distances". In: *IEEE Trans. Inform. Theory* 58.5 (2012), pp. 2697–2705. ISSN: 0018-9448. DOI: 10.1109/TIT.2012.2184845 (cit. on p. 59).

[GP04] Karin Gatermann and Pablo A. Parrilo. "Symmetry groups, semidefinite programs, and sums of squares". In: *J. Pure Appl. Algebra* 192.1-3 (2004), pp. 95–128. ISSN: 0022-4049. DOI: 10.1016/j.jpaa.2003.12.011 (cit. on p. 54).

[GP12] Stavros Garoufalidis and James Pommersheim. "Sum-integral interpolators and the Euler-Maclaurin formula for polytopes". In: *Trans. Amer. Math. Soc.* 364.6 (2012), pp. 2933–2958. ISSN: 0002-9947. DOI: 10.1090/S0002-9947-2012-05381-5 (cit. on pp. 96–98, 103).

[GP20] Alexey Garber and Igor Pak. "Concrete polytopes may not tile the space". In: *arXiv preprint arXiv:2003.04667* (2020) (cit. on p. 133).

[Gre+16] Gary R.W. Greaves et al. "Equiangular lines in Euclidean spaces". In: *J. Combin. Theory Ser. A* 138 (2016), pp. 208–235. ISSN: 0097-3165. DOI: 10.1016/j.jcta.2015.09.008 (cit. on pp. 75, 76).

[Gre18] Gary R.W. Greaves. "Equiangular line systems and switching classes containing regular graphs". In: *Linear Algebra Appl.* 536 (2018), pp. 31–51. ISSN: 0024-3795. DOI: 10.1016/j.laa.2017.09.008 (cit. on p. 72).

[GRS12] Nick Gravin, Sinai Robins, and Dmitry Shiryaev. "Translational tilings by a polytope, with multiplicity". In: *Combinatorica* 32.6 (2012), pp. 629–649. ISSN: 0209-9683. DOI: 10.1007/s00493-012-2860-3 (cit. on p. 132).

[GS03] Paul E. Gunnells and Robert Sczech. "Evaluation of Dedekind sums, Eisenstein cocycles, and special values of L-functions". In: *Duke Math. J.* 118.2 (2003), pp. 229–260. ISSN: 0012-7094. DOI: 10.1215/S0012-7094-03-11822-0 (cit. on pp. 35, 39, 40).

[GSY20] Gary R.W. Greaves, Jeven Syatriadi, and Pavlo Yatsyna. "Equiangular lines in low dimensional Euclidean spaces". In: *arXiv preprint arXiv:2002.08085* (2020) (cit. on p. 72).

[GY18] Alexey Glazyrin and Wei-Hsuan Yu. "Upper bounds for s-distance sets and equiangular lines". In: *Adv. Math.* 330 (2018), pp. 810–833. ISSN: 0001-8708. DOI: 10.1016/j.aim.2018.03.024 (cit. on pp. 73–75, 81–86).

[GY19] Gary R.W. Greaves and Pavlo Yatsyna. "On equiangular lines in 17 dimensions and the characteristic polynomial of a Seidel matrix". In: *Math. Comp.* 88.320 (2019), pp. 3041–3061. ISSN: 0025-5718. DOI: 10.1090/mcom/3433 (cit. on p. 72).

[Haa48] J. Haantjes. "Equilateral point-sets in elliptic two- and three-dimensional spaces". In: *Nieuw Arch. Wiskunde (2)* 22 (1948), pp. 355–362 (cit. on pp. 59, 72).

[Hig96] John R Higgins. *Sampling Theory in Fourier and Signal Analysis*. First. Clarendon Press, Oxford, 1996, p. 222 (cit. on p. 89).

[Jia+19] Zilin Jiang et al. "Equiangular lines with a fixed angle". In: *arXiv preprint arXiv:1907.12466* (2019) (cit. on p. 76).

[Joh17] Fredrik Johansson. "Arb: efficient arbitrary-precision midpoint-radius interval arithmetic". In: *IEEE Transactions on Computers* 66 (8 2017), pp. 1281–1292. DOI: 10.1109/TC.2017.2690633 (cit. on p. 77).

[Kis+20] Gergely Kiss et al. "On the discrete Fuglede and Pompeiu problems". In: *Anal. PDE* 13.3 (2020), pp. 765–788. ISSN: 2157-5045. DOI: 10.2140/apde.2020.13.765 (cit. on p. 138).

[Knu94] Donald E. Knuth. "The sandwich theorem". In: *Electron. J. Combin.* 1 (1994), Article 1, approx. 48 pp. (electronic). ISSN: 1077-8926. URL: http://www.combinatorics.org/Volume_1/Abstracts/v1i1a1.html (cit. on p. 45).

[Kob91] Toshiyuki Kobayashi. *Convex domains and Fourier transform on spaces of constant curvature*. https://www.ms.u-tokyo.ac.jp/~toshi/pub/21.html. Lecture notes of the Unesco-Cimpa School on "Invariant differential operators on Lie groups and homogeneous spaces", at WuHan University in P. R. China. 1991 (cit. on p. 138).

[KP02] Mihail N. Kolountzakis and Michael Papadimitrakis. "A class of non-convex polytopes that admit no orthonormal basis of exponentials". In: *Illinois J. Math.* 46.4 (2002), pp. 1227–1232. ISSN: 0019-2082. URL: http://projecteuclid.org/euclid.ijm/1258138476 (cit. on p. 91).

[KP93] Askol'd G. Khovanskii and Alexander V. Pukhlikov. "Integral transforms based on Euler characteristic and their applications". In: *Integral Transform. Spec. Funct.* 1.1 (1993), pp. 19–26. ISSN: 1065-2469. DOI: 10.1080/10652469308819004 (cit. on p. 92).

[KT19] Emily J. King and Xiaoxian Tang. "New upper bounds for equiangular lines by pillar decomposition". In: *SIAM J. Discrete Math.* 33.4 (2019), pp. 2479–2508. ISSN: 0895-4801. DOI: 10.1137/19M1248881 (cit. on pp. 71, 73–79, 81–86).

[Laa+21] David de Laat et al. “k-Point semidefinite programming bounds for equiangular lines”. In: *Math. Program.* (2021). ISSN: 1436-4646. DOI: 10.1007/s10107-021-01638-x (cit. on p. 58).

[Laa16] David de Laat. “Moment methods in extremal geometry”. PhD thesis. Delft University of Technology, 2016. DOI: 10.4233/uuid:fce81f72-8261-484d-b9f4-d3d0c26f0473 (cit. on pp. 10–12, 14).

[Laa19] David de Laat. “Moment methods in energy minimization: New bounds for Riesz minimal energy problems”. In: *Transactions of the American Mathematical Society* (2019). ISSN: 1088-6850. DOI: 10.1090/tran/7976 (cit. on p. 58).

[Las02] Jean B. Lasserre. “An explicit equivalent positive semidefinite program for nonlinear 0-1 programs”. In: *SIAM J. Optim.* 12.3 (2002), pp. 756–769. ISSN: 1052-6234. DOI: 10.1137/S1052623400380079 (cit. on pp. 46, 60).

[Lau03] Monique Laurent. “A comparison of the Sherali-Adams, Lovász-Schrijver, and Lasserre relaxations for 0-1 programming”. In: *Math. Oper. Res.* 28.3 (2003), pp. 470–496. ISSN: 0364-765X. DOI: 10.1287/moor.28.3.470.16391 (cit. on pp. 46, 60).

[Lau09] Monique Laurent. “Sums of squares, moment matrices and optimization over polynomials”. In: *Emerging applications of algebraic geometry*. Vol. 149. IMA Vol. Math. Appl. Springer, New York, 2009, pp. 157–270. DOI: 10.1007/978-0-387-09686-5_7 (cit. on p. 54).

[Law91] Jim Lawrence. “Rational-function-valued valuations on polyhedra”. In: *Discrete and computational geometry (New Brunswick, NJ, 1989/1990)*. Vol. 6. DIMACS Ser. Discrete Math. Theoret. Comput. Sci. Amer. Math. Soc., Providence, RI, 1991, pp. 199–208 (cit. on pp. 93, 94).

[Leb20] Jiri Lebl. *Tasty Bits of Several Complex Variables*. Version 3.4. Lulu.com, 2020. ISBN: 978-0-359-64225-0. URL: https://www.jirka.org/scv/scv.pdf (cit. on p. 139).

[Lin11] Eva Linke. “Rational Ehrhart quasi-polynomials”. In: *J. Combin. Theory Ser. A* 118.7 (2011), pp. 1966–1978. ISSN: 0097-3165. DOI: 10.1016/j.jcta.2011.03.007 (cit. on pp. 104, 119).

[LL19a] Nir Lev and Bochen Liu. “Multi-tiling and equidecomposability of polytopes by lattice translates”. In: *Bulletin of the London Mathematical Society* 51.6 (2019), pp. 1079–1098. DOI: 10.1112/blms.12297 (cit. on pp. 91, 132, 133).

[LL19b] Nir Lev and Bochen Liu. “Spectrality of Polytopes and Equidecomposability by Translations”. In: *International Mathematics Research Notices* (2019). ISSN: 1073-7928. DOI: 10.1093/imrn/rnz191 (cit. on p. 91).

[LM19] Nir Lev and Máté Matolcsi. “The Fuglede conjecture for convex domains is true in all dimensions”. In: *arXiv preprint arXiv:1904.12262* (2019) (cit. on p. 91).

[LOV14] David de Laat, Fernando M. de Oliveira Filho, and Frank Vallentin. “Upper bounds for packings of spheres of several radii”. In: *Forum Math. Sigma* 2 (2014), e23, 42. ISSN: 2050-5094. DOI: 10.1017/fms.2014.24 (cit. on pp. 54, 55).

[Lov79] László Lovász. “On the Shannon capacity of a graph”. In: *IEEE Trans. Inform. Theory* 25.1 (1979), pp. 1–7. ISSN: 0018-9448. DOI: 10.1109/TIT.1979.1055985 (cit. on p. 45).

[LPS17] Bart Litjens, Sven Polak, and Alexander Schrijver. "Semidefinite bounds for nonbinary codes based on quadruples". In: *Des. Codes Cryptogr.* 84.1-2 (2017), pp. 87–100. ISSN: 0925-1022. DOI: 10.1007/s10623-016-0216-5 (cit. on p. 59).

[LRS77] David G. Larman, C. Ambrose Rogers, and Johan J. Seidel. "On two-distance sets in Euclidean space". In: *Bull. London Math. Soc.* 9.3 (1977), pp. 261–267. ISSN: 0024-6093. DOI: 10.1112/blms/9.3.261 (cit. on p. 73).

[LS66] Jacobus H. van Lint and Johan J. Seidel. "Equilateral point sets in elliptic geometry". In: *Indag. Math.* 28 (1966), pp. 335–348 (cit. on pp. 59, 72, 74).

[LS73] P.W.H. Lemmens and Johan J. Seidel. "Equiangular lines". In: *J. Algebra* 24 (1973), pp. 494–512. ISSN: 0021-8693. DOI: 10.1016/0021-8693(73)90123-3 (cit. on pp. 72, 74, 75).

[LV12] Monique Laurent and Frank Vallentin. *Semidefinite optimization.* http://www.mi.uni-koeln.de/opt/wp-content/uploads/2015/06/laurent_vallentin_sdo_2012_05.pdf. Lecture notes. 2012 (cit. on pp. 43, 44, 46, 47).

[LV15] David de Laat and Frank Vallentin. "A semidefinite programming hierarchy for packing problems in discrete geometry". In: *Math. Program.* 151.2, Ser. B (2015), pp. 529–553. ISSN: 0025-5610. DOI: 10.1007/s10107-014-0843-4 (cit. on pp. 42, 58, 62, 78).

[LY19] Yen-chi R. Lin and Wei-Hsuan Yu. "Equiangular lines and the Lemmens-Seidel conjecture". In: *Discrete Mathematics* (2019), p. 111667. ISSN: 0012-365X. DOI: 10.1016/j.disc.2019.111667 (cit. on pp. 75, 78, 81, 82).

[Mac63] Ian G. Macdonald. "The volume of a lattice polyhedron". In: *Proc. Cambridge Philos. Soc.* 59 (1963), pp. 719–726 (cit. on p. 102).

[Mac71] Ian G. Macdonald. "Polynomials associated with finite cell-complexes". In: *J. London Math. Soc. (2)* 4 (1971), pp. 181–192. ISSN: 0024-6107. DOI: 10.1112/jlms/s2-4.1.181 (cit. on p. 102).

[Mat02] Jiří Matoušek. *Lectures on discrete geometry.* Vol. 212. Graduate Texts in Mathematics. Springer-Verlag, New York, 2002, pp. xvi+481. ISBN: 0-387-95373-6. DOI: 10.1007/978-1-4613-0039-7 (cit. on p. 1).

[Mat10] Jiří Matoušek. *Thirty-three miniatures.* Vol. 53. Student Mathematical Library. Mathematical and algorithmic applications of linear algebra. American Mathematical Society, Providence, RI, 2010, pp. x+182. ISBN: 978-0-8218-4977-4. DOI: 10.1090/stml/053 (cit. on p. 59).

[McM79] Peter McMullen. "Lattice invariant valuations on rational polytopes". In: *Arch. Math. (Basel)* 31.5 (1978/79), pp. 509–516. ISSN: 0003-889X. DOI: 10.1007/BF01226481 (cit. on pp. 103, 119).

[McM93] Peter McMullen. "Valuations and dissections". In: *Handbook of convex geometry, Vol. A, B.* North-Holland, Amsterdam, 1993, pp. 933–988 (cit. on p. 92).

[MR19] Fabrício C. Machado and Sinai Robins. "Coefficients of the solid angle and Ehrhart quasi-polynomials". In: *arXiv preprint* (2019). arXiv:1912.08017 (cit. on p. 34).

[MS83] Peter McMullen and Rolf Schneider. "Valuations on convex bodies". In: *Convexity and its applications.* Birkhäuser, Basel, 1983, pp. 170–247 (cit. on p. 92).

[Mus08] Oleg R. Musin. "The kissing number in four dimensions". In: *Ann. of Math. (2)* 168.1 (2008), pp. 1–32. ISSN: 0003-486X. DOI: 10.4007/annals.2008.168.1 (cit. on p. 58).

[Mus14] Oleg R. Musin. "Multivariate positive definite functions on spheres". In: *Discrete geometry and algebraic combinatorics.* Vol. 625. Contemp. Math. Amer. Math. Soc., Providence, RI, 2014, pp. 177–190. DOI: 10.1090/conm/625/12498 (cit. on pp. 19, 22, 23, 67).

[Nak10] Maho Nakata. "A numerical evaluation of highly accurate multiple-precision arithmetic version of semidefinite programming solver: SDPA-GMP,-QD and-DD." In: *Computer-Aided Control System Design (CACSD), 2010 IEEE International Symposium on.* IEEE. 2010, pp. 29–34 (cit. on p. 77).

[Neu89] Arnold Neumaier. "Graph representations, two-distance sets, and equiangular lines". In: *Linear Algebra Appl.* 114/115 (1989), pp. 141–156. ISSN: 0024-3795. DOI: 10.1016/0024-3795(89)90456-4 (cit. on p. 75).

[NV12] Gabriele Nebe and Boris Venkov. "On tight spherical designs". In: *Algebra i Analiz* 24.3 (2012), pp. 163–171. ISSN: 0234-0852. DOI: 10.1090/S1061-0022-2013-01249-0 (cit. on p. 73).

[Olg19] Juan C. Vera Olga Kuryatnikova. "Generalizations of Schoenberg's theorem on positive definite kernels". In: *arXiv preprint arXiv:1904.02538* (2019) (cit. on p. 58).

[Oli16] Fernando Mário de Oliveira Filho. *Semidefinite programming upper-bounds for packing problems.* https://www.ime.usp.br/~spschool2016/wp-content/uploads/2016/07/Oliveira.pdf. Lecture notes. 2016 (cit. on p. 50).

[OV15] F.M. de Oliveira Filho and F. Vallentin. "Mathematical optimization for packing problems". In: *SIAG/OPT Views and News* 23.2 (2015), pp. 5–14 (cit. on pp. 41, 54).

[OV18] Fernando Mário de Oliveira Filho and Frank Vallentin. "Computing upper bounds for the packing density of congruent copies of a convex body". In: *New trends in intuitive geometry.* Vol. 27. Bolyai Soc. Math. Stud. János Bolyai Math. Soc., Budapest, 2018, pp. 155–188 (cit. on p. 41).

[OY16] Takayuki Okuda and Wei-Hsuan Yu. "A new relative bound for equiangular lines and nonexistence of tight spherical designs of harmonic index 4". In: *European Journal of Combinatorics* 53 (2016), pp. 96–103. DOI: 10.1016/j.ejc.2015.11.003 (cit. on pp. 71, 74).

[PK92] A. V. Pukhlikov and A. G. Khovanskiĭ. "The Riemann-Roch theorem for integrals and sums of quasipolynomials on virtual polytopes". In: *Algebra i Analiz* 4.4 (1992), pp. 188–216. ISSN: 0234-0852 (cit. on pp. 93, 94).

[PM62] Daniel P. Petersen and David Middleton. "Sampling and reconstruction of wave-number-limited functions in N-dimensional Euclidean spaces". In: *Information and Control* 5 (1962), pp. 279–323. ISSN: 0019-9958. DOI: 10.1016/S0019-9958(62)90633-2 (cit. on p. 89).

[Pom29a] D Pompeiu. "Sur une propriété des fonctions continues dépendent de plusieurs variables". In: *Bull. Sci. Math* 2.53 (1929), pp. 328–332 (cit. on p. 137).

[Pom29b] D Pompeiu. "Sur une propriété intégrale des fonctions de deux variables réelles". In: *Bull. Sci. Acad. Roy. Belgique* 5.15 (1929), pp. 265–269 (cit. on p. 137).

[Pom93] James E. Pommersheim. "Toric varieties, lattice points and Dedekind sums". In: *Math. Ann.* 295.1 (1993), pp. 1–24. ISSN: 0025-5831. DOI: 10.1007/BF01444874 (cit. on pp. 106, 124).

[PT04] James E. Pommersheim and Hugh Thomas. “Cycles representing the Todd class of a toric variety”. In: *J. Amer. Math. Soc.* 17.4 (2004), pp. 983–994. ISSN: 0894-0347. DOI: 10.1090/S0894-0347-04-00460-6 (cit. on p. 103).

[Rad64] Hans Rademacher. “Some remarks on certain generalized Dedekind sums”. In: *Acta Arith.* 9 (1964), pp. 97–105. ISSN: 0065-1036. DOI: 10.4064/aa-9-1-97-105 (cit. on pp. 106, 109).

[Ran69] Burton Randol. “On the Fourier transform of the indicator function of a planar set”. In: *Trans. Amer. Math. Soc.* 139 (1969), pp. 271–278. ISSN: 0002-9947. DOI: 10.2307/1995319 (cit. on p. 90).

[Ran97] Burton Randol. “On the number of integral lattice-points in dilations of algebraic polyhedra”. In: *Internat. Math. Res. Notices* 6 (1997), pp. 259–270. ISSN: 1073-7928. DOI: 10.1155/S1073792897000196 (cit. on p. 88).

[Rob21] Sinai Robins. *A friendly invitation to Fourier analysis on polytopes.* 33° Colóquio Brasileiro de Matemática. IMPA, 2021, pp. xi+252. ISBN: 978-65-89124-35-1 (cit. on p. 2).

[Roy17a] Tiago Royer. “Reconstruction of rational polytopes from the real-parameter Ehrhart function of its translates”. In: *arXiv preprint arXiv:1712.01973* (2017) (cit. on p. 104).

[Roy17b] Tiago Royer. “Semi-reflexive polytopes”. In: *arXiv preprint arXiv:1712.04381* (2017) (cit. on p. 104).

[RS19] Maren H. Ring and Achill Schürmann. “Local formulas for Ehrhart coefficients from lattice tiles”. In: *Beiträge zur Algebra und Geometrie / Contributions to Algebra and Geometry* (2019). ISSN: 2191-0383. DOI: 10.1007/s13366-019-00457-8 (cit. on p. 103).

[RS72] Michael Reed and Barry Simon. *Methods of modern mathematical physics. I. Functional analysis.* Academic Press, New York-London, 1972, pp. xvii+325 (cit. on pp. 14, 30, 31).

[Rud62] Walter Rudin. *Fourier analysis on groups.* Interscience Tracts in Pure and Applied Mathematics, No. 12. Interscience Publishers (a division of John Wiley and Sons), New York-London, 1962, pp. ix+285 (cit. on pp. 5, 29, 31).

[Rud87] Walter Rudin. *Real and complex analysis.* Third. McGraw-Hill Book Co., New York, 1987, pp. xiv+416. ISBN: 0-07-054234-1 (cit. on pp. 11, 28, 38).

[Sch05] Alexander Schrijver. “New code upper bounds from the Terwilliger algebra and semidefinite programming”. In: *IEEE Trans. Inform. Theory* 51.8 (2005), pp. 2859–2866. ISSN: 0018-9448. DOI: 10.1109/TIT.2005.851748 (cit. on pp. 48, 58).

[Sch42] Isaac J. Schoenberg. “Positive definite functions on spheres”. In: *Duke Math. J.* 9 (1942), pp. 96–108. ISSN: 0012-7094 (cit. on pp. 19, 58, 66).

[Sch47] Laurent Schwartz. “Théorie générale des fonctions moyenne-périodiques”. In: *Ann. of Math. (2)* 48 (1947), pp. 857–929. ISSN: 0003-486X. DOI: 10.2307/1969386 (cit. on p. 138).

[Sch79] Alexander Schrijver. “A comparison of the Delsarte and Lovász bounds”. In: *IEEE Trans. Inform. Theory* 25.4 (1979), pp. 425–429. ISSN: 0018-9448. DOI: 10.1109/TIT.1979.1056072 (cit. on p. 45).

[Ser77] Jean-Pierre Serre. *Linear representations of finite groups.* Translated from the second French edition by LL Scott, Graduate Texts in Mathematics, Vol. 42. Springer-Verlag, New York-Heidelberg, 1977, pp. x+170. ISBN: 0-387-90190-6 (cit. on p. 5).

[She67] Geoffrey C. Shephard. "Polytopes with centrally symmetric faces". In: *Canadian J. Math.* 19 (1967), pp. 1206–1213. ISSN: 0008-414X. DOI: 10.4153/CJM-1967-109-3 (cit. on p. 131).

[Skr98] Maxim M. Skriganov. "Ergodic theory on SL(n), Diophantine approximations and anomalies in the lattice point problem". In: *Invent. Math.* 132.1 (1998), pp. 1–72. ISSN: 0020-9910. DOI: 10.1007/s002220050217 (cit. on p. 90).

[Slo18] Neil J.A. Sloane editor. *The On-Line Encyclopedia of Integer Sequences.* Published electronically at https://oeis.org. 2018 (cit. on p. 59).

[Spi65] Michael Spivak. *Calculus on manifolds. A modern approach to classical theorems of advanced calculus.* W. A. Benjamin, Inc., New York-Amsterdam, 1965, pp. xii+144 (cit. on p. 16).

[SS00] Maxim M. Skriganov and Alexander N. Starkov. "On logarithmically small errors in the lattice point problem". In: *Ergodic Theory Dynam. Systems* 20.5 (2000), pp. 1469–1476. ISSN: 0143-3857. DOI: 10.1017/S0143385700000791 (cit. on p. 90).

[SW71] Elias M. Stein and Guido Weiss. *Introduction to Fourier analysis on Euclidean spaces.* Princeton Mathematical Series, No. 32. Princeton University Press, Princeton, N.J., 1971, pp. x+297 (cit. on pp. 17, 19, 27–30, 32–34, 110, 132).

[Sze39] Gabor Szegö. *Orthogonal Polynomials.* American Mathematical Society Colloquium Publications, v. 23. American Mathematical Society, New York, 1939, pp. ix+401 (cit. on p. 19).

[Tay71] Donald E. Taylor. "Some topics in the theory of finite groups". PhD thesis. University of Oxford, 1971 (cit. on p. 72).

[Tem96] Nico M. Temme. *Special functions.* A Wiley-Interscience Publication. An introduction to the classical functions of mathematical physics. John Wiley & Sons, Inc., New York, 1996, pp. xiv+374. ISBN: 0-471-11313-1. DOI: 10.1002/9781118032572 (cit. on p. 140).

[Tra14] Giancarlo Travaglini. *Number theory, Fourier analysis and geometric discrepancy.* Vol. 81. London Mathematical Society Student Texts. Cambridge University Press, Cambridge, 2014, pp. x+240. ISBN: 978-1-107-61985-2. DOI: 10.1017/CBO9781107358379 (cit. on pp. 27, 88).

[Tun10] Levent Tunçel. *Polyhedral and semidefinite programming methods in combinatorial optimization.* Vol. 27. Fields Institute Monographs. American Mathematical Society, Providence, RI; Fields Institute for Research in Mathematical Sciences, Toronto, ON, 2010, pp. x+219. ISBN: 978-0-8218-3352-0. DOI: 10.1090/fim/027 (cit. on p. 43).

[Via17] Maryna S. Viazovska. "The sphere packing problem in dimension 8". In: *Ann. of Math. (2)* 185.3 (2017), pp. 991–1015. ISSN: 0003-486X. DOI: 10.4007/annals.2017.185.3.7 (cit. on p. 56).

[Vil68] Neil Ja. Vilenkin. *Special functions and the theory of group representations.* Translations of Mathematical Monographs, Vol. 22. Translated from the Russian by V. N. Singh. American Mathematical Society, Providence, R. I., 1968, pp. x+613 (cit. on pp. 5, 9, 14, 15, 19).

[Wil76] Stephen A. Williams. "A partial solution of the Pompeiu problem". In: *Math. Ann.* 223.2 (1976), pp. 183–190. ISSN: 0025-5831. DOI: 10.1007/BF01360881 (cit. on pp. 3, 137–140).

[Wit92] Edward Witten. "Two dimensional gauge theories revisited". In: *Journal of Geometry and Physics* 9.4 (1992), pp. 303–368. ISSN: 0393-0440. DOI: https://doi.org/10.1016/0393-0440(92)90034-X (cit. on p. 35).

[Wol03] Thomas H. Wolff. *Lectures on harmonic analysis.* Vol. 29. University Lecture Series. With a foreword by Charles Fefferman and a preface by Izabella Łaba, Edited by Łaba and Carol Shubin. American Mathematical Society, Providence, RI, 2003, pp. x+137. ISBN: 0-8218-3449-5. DOI: 10.1090/ulect/029 (cit. on p. 30).

[Yu17] Wei-Hsuan Yu. "New bounds for equiangular lines and spherical two-distance sets". In: *SIAM J. Discrete Math.* 31.2 (2017), pp. 908–917. ISSN: 0895-4801. DOI: 10.1137/16M109377X (cit. on pp. 71, 74).

[Yu18] Wei-Hsuan Yu. "Saturated configuration and new large construction of equiangular lines". In: *arXiv preprint arXiv:1801.04502* (2018) (cit. on p. 72).

[Zie95] Günter M. Ziegler. *Lectures on polytopes.* Vol. 152. Graduate Texts in Mathematics. Springer-Verlag, New York, 1995, pp. x+370. ISBN: 0-387-94365-X. DOI: 10.1007/978-1-4613-8431-1 (cit. on pp. 87, 131).