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Groupes Cristallographiques
et Polynômes de Chebyshev
en Optimisation Globale

Crystallographic Groups
and Chebyshev Polynomials
in Global Optimization

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Jury

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Abstract

This thesis studies the problem of optimizing a trigonometric polynomial with crystallographic symmetry. Optimization of trigonometric polynomials has been subject to many recent works, but a theory for exploiting symmetries has hardly been developed or generalized. We consider the multiplicative action of a crystallographic group, also known as a Weyl group, on the exponents. This action admits a definition of generalized Chebyshev polynomials. If a trigonometric polynomial is invariant under the action, then it can be written as a sum of such Chebyshev polynomials in fundamental invariants.

By rewriting an invariant trigonometric polynomial as a classical polynomial, the region of optimization is transformed into the orbit space of the multiplicative Weyl group action. This orbit space is the image of fundamental invariants and we show that, for the Weyl groups of types A_{n-1}, B_n, C_n, D_n and G_2, it is a compact basic semi–algebraic set. Furthermore, we give a closed formula for the describing polynomial inequalities through a positive semi–definite Hermite matrix polynomial.

Concerning the optimization problem, our rewriting approach transforms the trigonometric optimization problem into a classical polynomial optimization problem on a basic semi–algebraic set. To solve such problems, one can apply Lasserre's hierarchy of moment relaxations and sums of squares reinforcements. We adapt and implement this hierarchy in the basis of generalized Chebyshev polynomials with a new notion of degree. The optimal value of the original trigonometric optimization problem is then approximated through solutions of semi–definite programs, which are solved numerically.

In classical polynomial optimization and other applications, symmetry adaptation has been studied and implemented, but crystallographic symmetries have not been exploited in trigonometric optimization before. With our approach, we provide an alternative to known strategies. Where other techniques utilize sums of Hermitian squares or generalizations of Lasserre's hierarchy to the complex setting, we exploit symmetry first and then apply techniques from classical polynomial optimization. This reduces the size of arising semi–definite hierarchies and can also improve the quality of the approximation.

As an application, we study the problem of computing lower bounds for the chromatic number of geometric distance graphs. Given a norm and a set of vertices, this problem asks to find the minimal number of colors needed to paint the vertices, so that no two of those of distance 1 between them have the same color. The spectral bound was generalized from finite to infinite graphs to deal with such problems. This bound involves the optimization of a trigonometric polynomial. We focus on norms which are given by polytopes with central and crystallographic symmetry. Then the problem can be tackled with the techniques developed in this thesis. We give several bounds through analytical and numerical computations.

Keywords: Crystallographic Groups, Chebyshev Polynomials, Optimization, Root Systems, Symmetry

Résumé

Cette thèse étudie le problème de l'optimisation d'un polynôme trigonométrique avec symétrie cristallographique. L'optimisation des polynômes trigonométriques était l'objet de nombreux travaux récents, mais une théorie permettant d'exploiter les symétries n'a pas été développée ou généralisée. Nous considérons l'action d'un groupe cristallographique, également connu sous le nom de groupe de Weyl, sur les exposants. Cette action admet une définition des polynômes de Chebychev généralisés. Si un polynôme trigonométrique est invariant sous l'action, il peut être écrit comme une somme de polynômes de Chebyshev généralisés dans les invariants fondamentaux.

En réécrivant un polynôme trigonométrique invariant comme un polynôme classique, la région d'optimisation est transformée en l'espace d'orbit de l'action du groupe de Weyl multiplicatif. Cet espace d'orbite est l'image des invariants fondamentaux et nous montrons que, pour les groupes de Weyl de types A_{n-1}, B_n, C_n, D_n et G_2, il s'agit d'un ensemble compact basic semi–algébrique. En plus, nous donnons les inégalités polynomiales descriptives à par un matrix polynômial positif de Hermite.

En ce qui concerne l'optimisation, notre approche de réécriture transforme le problème d'optimisation trigonométrique dans un problème d'optimisation polynomiale sur un ensemble basic semi–algébrique. Pour résoudre de tels problèmes, on peut appliquer la hiérarchie des relaxations de moment et de somme de carrés de Lasserre. Nous adaptons et implémentons cette hiérarchie sur la base de polynômes de Chebyshev généralisés avec une nouvelle notion de degré. La valeur optimale du problème d'optimisation trigonométrique original est alors approximée par des solutions de programmes semi-définis, qui sont résolus numériquement.

Dans l'optimisation polynomiale classique et d'autres applications, l'adaptation des symétries a été étudiée et implémenté, mais les symétries cristallographiques n'ont pas été exploitées en optimisation trigonométrique auparavant. Avec notre approche, nous fournissons une alternative aux stratégies connues pour l'optimisation trigonométrique. Alors que d'autres techniques utilisent des sommes de carrés Hermitiens ou en généralisant l'hiérarchie de Lasserre au cadre complexe, nous exploitons d'abord la symétrie et appliquons ensuite des techniques d'optimisation polynomiale classique. Cela réduit la taille des relaxations semi-définies qui en découlent et peut également améliorer la qualité de l'approximation.

En guise d'application, nous étudions le problème de calcul des bornes inférieurs pour le nombre chromatique des graphes géométriques. Etant donné une norme et un ensemble de sommets, ce problème demande de trouver le nombre minimal de couleurs nécessaires pour peindre les sommets, de sorte que deux de ceux de distance 1 entre eux n'aient pas la même couleur. La borne spectrale a été généralisée des graphes finis aux graphes infinis pour traiter de tels problèmes. Cette limite implique l'optimisation d'un polynôme trigonométrique. Nous nous concentrons sur les normes qui sont données par des polytopes avec une symétrie cristallographique. Le problème peut alors être abordé avec les techniques développées dans cette thèse. Nous donnons plusieurs bornes à travers des calculs analytiques et numériques.

Mots clés: Groupes Cristallographiques, Polynômes de Chebyshev, Optimisation, Systèmes de Racines, Symétrie

Zusammenfassung

Diese Arbeit untersucht das Problem der Optimierung eines trigonometrischen Polynoms mit kristallographischer Symmetrie. Die Optimierung trigonometrischer Polynome ist Gegenstand vieler neuerer Arbeiten, aber eine Theorie zur Ausnutzung von Symmetrien wurde bisher kaum entwickelt oder verallgemeinert. Wir betrachten die Wirkung einer kristallographischen Gruppe, auch bekannt als Weyl-Gruppe, auf die Exponenten. Diese Wirkung erlaubt eine Definition von verallgemeinerten Chebyshev Polynomen. Wenn ein trigonometrisches Polynom unter der Wirkung invariant ist, dann kann es als Summe von verallgemeinerten Tschebyscheff Polynomen in fundamentalen Invarianten geschrieben werden.

Indem man ein invariantes trigonometrisches Polynom in ein klassisches Polynom umschreibt, wird der Bereich der Optimierung in den Orbitraum der multiplikativen Weyl–Gruppenwirkung transformiert. Dieser Orbitraum ist das Bild der fundamentalen Invarianten und wir zeigen, dass er für die Weyl Gruppen der Typen A_{n-1}, B_n, C_n, D_n und G_2 eine kompakte basisch semi–algebraische Menge ist. Außerdem geben wir die beschreibenden polynomiellen Ungleichungen explizit durch ein positiv semidefinites Hermite–Matrixpolynom an.

Was das Optimierungsproblem betrifft, so wandelt unser Umschreibungsansatz das trigonometrische Optimierungsproblem in ein klassisches polynomiales Optimierungsproblem auf einer basisch semi–algebraischen Grundmenge. Um solche Probleme zu lösen, kann man die Lasserre Hierarchie von Quadratsummen– und Momenten–Relaxierungen anwenden. Wir adaptieren und implementieren diese Hierarchie in der Basis der verallgemeinerten Chebyshev Polynome mit einem angepassten Gradbegriff. Der optimale Wert des ursprünglichen trigonometrischen Optimierungsproblems wird dann durch Lösungen von semidefiniten Programmen angenähert, die numerisch gelöst werden.

In der klassischen polynomiellen Optimierung und anderen Anwendungen wurde die Symmetrieanpassung untersucht und umgesetzt, aber kristallografische Symmetrien wurden in der trigonometrischen Optimierung bisher nicht genutzt. Unser Ansatz bietet eine Alternative zu bekannten Strategien für trigonometrische Optimierung. Wo andere Techniken Hermite'sche Quadratsummen oder Verallgemeinerungen der Lasserre–Hierarchie auf die komplexe Umgebung anwenden, nutzen wir zuerst die Symmetrie und wenden dann Techniken der klassischen polynomiellen Optimierung an. Dies reduziert die Größe der entstehenden semidefiniten Relaxierungen und kann auch die Qualität der Approximation verbessern.

Als Anwendung untersuchen wir das Problem der Berechnung von unteren Schranken für die chromatische Zahl von geometrischen Abstandsgraphen. Gegeben eine Norm und eine Menge von Knoten, stellt sich das Problem, die minimale Anzahl von Farben zu finden, die benötigt werden, um die Knoten so zu färben, dass keine zwei Knoten mit einem Abstand von 1 zueinander die gleiche Farbe haben. Die spektrale Schranke wurde von endlichen auf unendliche Graphen verallgemeinert, um solche Problemen zu bahandeln. Diese Schranke beinhaltet die Optimierung eines trigonometrischen Polynoms. Wir konzentrieren uns auf Normen, die durch Polytope mit kristallographischer Symmetrie gegeben sind. Dann kann das Problem mit den in dieser Arbeit entwickelten Techniken angegangen werden. Wir geben mehrere Schranken durch analytische und numerische Berechnungen an.

Stichwörter: Kristallographische Gruppen, Chebyshev Polynome, Optimierung, Wurzelsysteme, Symmetrie

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Contents

Introduction

This thesis studies a global optimization problem in mathematics with crystallographic symmetries. Optimization is the problem of determining the optimal value of an object under given parameters. Mathematically, this means to find the supremum or infimum of a real–valued map, the so–called objective function, under given constraints, defining the so–called feasible region.

Polynomial optimization

A case of optimization is the one, where the objective function resides in the commutative multivariate polynomial ring with real coefficients and the feasible region is a basic closed semi–algebraic set. This polynomial optimization problem is already in the quadratic case known to be NP–hard [PV91]. Under certain algebraic and geometric circumstances however, one can approximate the optimal value, if it exists. The semi–algebraic constraints, given by finitely many polynomial inequalities, can be replaced by necessary conditions for a polynomial to be positive or nonnegative. This leads to two dual hierarchies of semi–definite problems, which are solvable through numerical methods [Las01, Par03]. The approach is known as the Lasserre hierarchy.

Since Artin's solution of Hilbert's 17–th problem in 1927, the study of positivity and nonnegativity certificates has been essential to real algebraic geometry and neighboring fields of pure mathematics. Examples are the Positivstellensätze of Krivine, Stengle, Schmüdgen, Putinar [Kri64, Ste74, Sch91, Put93], and the matrix versions due to Kojima, Hol, Scherer [Koj03, HS05, HS06]. In [Las01], nonnegativity is replaced with membership in a quadratic module, the necessary condition of Putinar's Positivstellensatz. By restricting to sums of squares with bounded degree, one obtains a hierarchy of semi–definite lower bounds, which are dual to problems of moments and converge to the optimal value. Raising the degree improves the quality of the bound but increases the computational effort. Recent advances on the hierarchy are to be found in [HKL21].

The complexity to solve a semi–definite program obtained from a Lasserre relaxation is not to be underestimated. The arising matrices grow quickly in both size and number along with the order of the relaxation. Hence, techniques to reduce the complexity are required. To keep the parameters, which increase computation time, as small as possible, the keyword in the present thesis is symmetry. If symmetry in the data of the problem can be detected, that is, if there is a group action, which leaves the objective function and the constraints invariant, then this can be exploited. Symmetry–adapted bases for example have seen the size of moment methods decrease and have proven to be successful in the study of optimization problems [GP04, Val08]. Next to group symmetry, sparsity is also a structure that can be exploited in polynomial optimization [Las06, LMW21, MW23].

Trigonometric optimization

Many applications deal with the optimization of trigonometric polynomials, where the objective function is a linear combination of complex exponentials, indexed by a lattice. The problem is usually unconstrained, that is, the feasible region is $\mathbb{R}^n$. Assuming that the coefficients are real and sign–symmetric, a trigonometric polynomial assumes only real values and can be optimized. The same holds true for complex conjugate coefficients. Since such functions are periodic, they assume a maximum and minimum. Equivalently, one can consider a Laurent polynomial on the compact torus with the same constraints on the coefficients.

An approach to optimize trigonometric polynomials utilizes sums of Hermitian squares. In the univariate case, the Riesz–Fejér theorem states that a trigonometric polynomial is non–negative, if it has a so–called spectral factorization. This is similar to the notion of sums of squares in the real setting and gives an analog to the above Positivstellensätze. The Riesz–Fejér theorem was generalized to the multivariate setting, which leads to a hierarchy of semi–definite bounds on the optimal value. For more details, we refer to the book [Dum07], where optimization in the univariate case (Chapter 2) and the multivariate case (Chapter 3 and 4) is applied to filter design (Chapter 5, 6 and 8), stability and robustness (Chapter 7). Sparsity can also be exploited in this setting. We complement this by introducing an approach that exploits symmetry on the level of exponents before the machinery of polynomial optimization is mobilized.

Furthermore, Lasserre's hierarchy can be generalized to the complex setting with semi–algebraic constraints, see for example [JM18]. Trigonometric optimization falls in this context when we add the equality constraints for the compact torus. Optimization of other kinds of exponential functions has been studied in the context of AM/GM and SONC/SAGE polynomials, see [DIW19, MSW19, DHNW20, DNT21, MDSV22, DKW22]. Recently, symmetry has also been exploited in [MNR+21].

Contribution

The contribution of this thesis lies in a new approach to the problem of optimizing trigonometric polynomials with crystallographic symmetry. A crystallographic group, also known as a Weyl group, is a finite group generated by reflections on hyperplanes with certain geometric relations. More precisely, such groups are defined via reflections associated to root systems.

A Weyl group has a multiplicative action on the ring of trigonometric polynomials. Exploiting the symmetry, the problem of optimizing an invariant trigonometric polynomial is reformulated to a polynomial optimization problem. To do this, we introduce a polynomial basis via the action of the Weyl group. These polynomials are called generalized Chebyshev polynomials and allow to rewrite any invariant trigonometric polynomial as a classical polynomial in fundamental invariants. The feasible region, that is, the region of periodicity, is transformed into the orbit space of the group action. We describe the said orbit space as a compact basic semi–algebraic set and give a closed formula. This puts us in the context of classical polynomial optimization, where we have Lasserre's hierarchy to our disposal.

Given that our arising polynomial optimization problem is naturally represented in the generalized Chebyshev polynomials, we adapt and implement Lasserre's hierarchy in this basis. With that approach, the time to model the semi–definite relaxations grows, but the number of matrices and their overall size decreases thanks to a different notion of degree, which reduces the numerical effort. We also compare with other techniques from trigonometric optimization, that do not exploit symmetry.

The problem of optimizing trigonometric polynomials with crystallographic symmetry arises in the computation of the spectral bound for geometric distance graphs due to [BDFV14]. We study several instances of this problem and give bounds through analytical and numerical computations.

The reason to restrict to crystallographic symmetries is a result from multiplicative invariant theory, which we recall in Theorem 1.30. It states that the ring of invariants is a polynomial ring if and only if the considered group is a Weyl group. This property allows us to define generalizations of Chebyshev polynomials uniquely.

Symmetry adaptation and exploitation has seen the complexity of algorithms in polynomial optimization and other related areas decrease, see for example [GP04, ALRT13, CH18]. Crystallographic groups can be studied in numerous contexts and optimization is one of several applications. An example are Lie integration techniques and sampling [MKNR12]. Beyond mathematics, crystallographic structures are of relevance in chemistry [Wyb73] and physics [Woi17]. Recently, the Fields medal was awarded to Maryna Viazovska for proving that the densest possible sphere packing in dimension 8 is obtained from the E_8 root system[1]. In trigonometric optimization on the other hand, the exploitation of crystallographic symmetries has to the knowledge of the author not been advanced through a general theory.

Structure and main results of the thesis

We study the problem of finding

$$f^* = \inf_{u\in\mathbb{R}^n} \sum_{\mu\in\Omega} c_\mu \, \exp(-2\pi\mathrm{i}\,\langle \mu, u\rangle),$$

[1]Fields medals 2022: https://www.mathunion.org/imu-awards/fields-medal/fields-medals-2022

where $\Omega \cong \mathbb{Z}^n$ is a lattice in $\mathbb{R}^n$, $\langle\cdot,\cdot\rangle$ an inner product on $\mathbb{R}^n$ and the $c_\mu \in \mathbb{R}$ are coefficients with only finitely many nonzero. We call the objective function a trigonometric polynomial and write $\mathbb{R}[\Omega]$ for the set of all trigonometric polynomials. For the problem to be well–defined, we require the coefficients to be sign–symmetric, that is, $c_\mu = c_{-\mu}$. If $\Lambda = \Omega^*$ is the dual lattice of Ω, then the objective function is invariant under $u \mapsto u+\lambda$ for $\lambda \in \Lambda$. In other words, the objective function is periodic and the infimum is a minimum, assumed in a periodicity domain, as for instance the Voronoï cell of Λ.

Furthermore, we assume that the problem has orthogonal symmetry in the following sense. Let $\mathcal{W} \subseteq \mathrm{O}_n(\mathbb{R})$ be a finite orthogonal matrix group, such that Ω is a $\mathcal{W}$–lattice, that is, $A\mu \in \Omega$ for all $A \in \mathcal{W}$ and $\mu \in \Omega$. Here, orthogonality is with respect to $\langle\cdot,\cdot\rangle$. Orthogonal symmetry for the optimization problem now means that $c_{A\mu} = c_\mu$. In other words, the objective function is invariant under $u \mapsto Au$ for all $A \in \mathcal{W}$. Indeed, we have $\langle A\mu, u\rangle = \langle \mu, A^t u\rangle = \langle \mu, A^{-1}u\rangle$, and, since $\mathcal{W}$ is a group, $A^{-1} \in \mathcal{W}$.

If the group $\mathcal{W}$ is an essential reflection group, then one can show that the product $\mathcal{W} \ltimes \Lambda$ is semi–direct if and only if $\mathcal{W}$ is the Weyl group of a root system and $\Lambda^* = \Omega$ is the weight lattice. In this case we speak of crystallographic symmetries.

An equivalent problem is to find

$$f^* = \inf_{x\in\mathbb{T}^n} \sum_{\alpha\in\mathbb{Z}^n} c_\alpha\, x^\alpha,$$

where $\mathbb{T}^n$ is the compact torus in $(\mathbb{C}^*)^n$ and c_α is obtained from c_μ through $\mathbb{Z}^n \cong \Omega$. Indeed, if $\Omega = \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_n$ and we define the matrix $W := [\omega_1|\ldots|\omega_n]$, then we have an $\mathbb{R}$–algebra isomorphism $\mathbb{R}[x^\pm] \cong \mathbb{R}[\Omega]$ given by

$$x^\alpha \leftrightarrow \exp(-2\pi \mathrm{i}\, \langle W\alpha, u\rangle).$$

In particular, $x \in \mathbb{T}^n$ if and only if $u \in \mathbb{R}^n$. In the language of Laurent polynomials, orthogonal symmetry now translates to $c_{B\alpha} = c_\alpha$, where $B \in \mathrm{GL}_n(\mathbb{Z})$ is obtained from $A \in \mathcal{W}$ by conjugation with W, that is, $B = W^{-1}AW$. In other words, the objective function is invariant under $x^\alpha \mapsto x^{B\alpha}$. The matrix W is not to be confused with the group $\mathcal{W}$.

Chapter 1. The goal of this chapter is to find a polynomial basis, which allows us to write trigonometric polynomials with crystallographic symmetry as a classical polynomial in new variables. A typical example that comes to mind are the univariate Chebyshev polynomials, which satisfy the property $T_\ell(\cos(2\pi\, u)) = \cos(2\pi\, \ell\, u)$ with $\ell \in \mathbb{N}$. The cosine is a crystallographic invariant in the sense that it is a periodic and even function and thus invariant under change of sign $u \mapsto -u$. When we write $2\,\cos(2\pi\,\ell\,u) = e^{2\pi \mathrm{i}\,\ell\,u} + e^{-2\pi \mathrm{i}\,\ell\,u}$, then it becomes evident that the change of sign is a linear action of the group $\{\pm 1\}$ on the exponents. In fact, this observation suffices to show that the polynomial T_ℓ is unique and well-defined and we say that $\cos(2\pi\, u)$ is a fundamental invariant.

To give a proper generalization, we shall work with root systems. Those are specific generating sets of the Euclidean space, which define hyperplanes. The reflections on these planes generate a finite orthogonal group, which we call Weyl group. Historically, root systems appeared in the classification of the semi–simple complex Lie algebras due to Cartan and Killing in 1880.

The Weyl group $\mathcal{W}$ of a root system has a linear action on the trigonometric polynomials $\mathbb{R}[\Omega]$, given by $\exp(-2\pi \mathrm{i}\,\langle \mu, u\rangle) \mapsto \exp(-2\pi \mathrm{i}\,\langle A\mu, u\rangle)$ for $A \in \mathcal{W}$. Equivalently, the integer matrix group $\mathcal{G}$ of all $B = W^{-1}AW$ has a linear action on the Laurent polynomials $\mathbb{R}[x^\pm]$ by $x^\alpha \mapsto x^{B\alpha}$. Now, a theorem from multiplicative invariant theory, see [Bou68, Chapitre VI, §3, Théorème 1] or [Lor05, Theorem 3.6.1], states

$$\mathbb{R}[\Omega]^{\mathcal{W}} \cong \mathbb{R}[x^\pm]^{\mathcal{G}} = \mathbb{R}[\theta_1, \ldots, \theta_n],$$

where the θ_i are algebraically independent generators of $\mathbb{R}[x^\pm]^{\mathcal{G}}$ as an $\mathbb{R}$–algebra, the so–called fundamental invariants. This theorem is unique for Weyl groups and shall be our workhorse. For $\alpha \in \mathbb{N}^n$, we set $\Theta_\alpha(x) := \frac{1}{|\mathcal{G}|} \sum_{B\in\mathcal{G}} x^{B\alpha}$. Then $\Theta_\alpha \in \mathbb{R}[x^\pm]^{\mathcal{G}}$ and a multivariate polynomial T_α is uniquely defined via $T_\alpha(\theta_1, \ldots, \theta_n) = \Theta_\alpha$. We speak of the generalized Chebyshev polynomials of the first kind, if $\theta_i = \Theta_{e_i}$. Other choices are possible and define different kinds of generalized Chebyshev polynomials. The application of these polynomials has been studied in the context of Fourier analysis [Bee91, MKNR12], cubature [Xu00, LX10, LSX12, Xu15] and sparse interpolation [HS21]. The univariate Chebyshev polynomials fit in this family, as they satisfy the property $T_\ell((x+x^{-1})/2) = (x^\ell + x^{-\ell})/2$ for $\ell \in \mathbb{N}$ with $x^\ell = e^{2\pi\mathrm{i}\,\ell\,u}$.

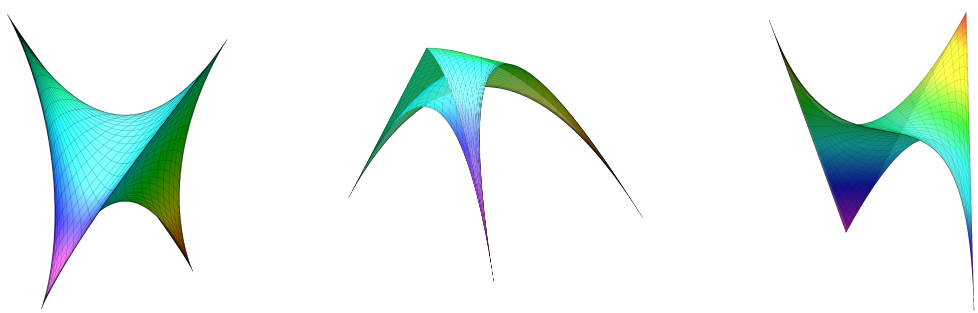
Concerning our original problem of finding f^*, the theorem on the invariant ring allows us to write

$$f^* = \inf_{u\in\mathbb{R}^n} \sum_{\mu\in\Omega} c_\mu \, \exp(-2\pi\mathrm{i}\,\langle\mu,u\rangle) = \inf_{z\in\mathcal{T}} \sum_{\alpha\in\mathbb{N}^n} c_\alpha \, T_\alpha(z),$$

where $\mathcal{T}$ is the image of $\mathbb{T}^n$ under the fundamental invariants θ_i and the T_α are generalized Chebyshev polynomials in $\mathbb{R}[z] = \mathbb{R}[z_1,\ldots,z_n]$. Note that we have reduced the indices α from $\Omega \cong \mathbb{Z}^n$ to $\mathbb{N}^n$ by exploiting symmetry. Since the support of the objective function is finite, this is a factor 2^n.

Chapter 2. We study the problem of characterizing the image of the fundamental invariants $\vartheta : x \mapsto (\theta_1(x),\ldots,\theta_n(x))$ for the multiplicative Weyl group action. Note that the known characterization of orbit spaces for linear actions on representation spaces due to Procesi for the symmetric group [Pro78] and Procesi–Schwarz for compact Lie groups [PS85, (0.10) Main Theorem] does not apply here, because $(\mathbb{C}^*)^n$ is not a representation space. Furthermore, the recipe in [PS85, §4] is only known to provide an implicit formula in terms of invariants and additional computations are required. This extra step can be skipped. In this thesis, we develop an independent theory to treat the multiplicative case.

Main result 1. *For a root system of type* A_{n-1}, C_n, B_n, D_n *or* G_2, *there exist a symmetric matrix polynomial* $P \in \mathbb{R}[z]^{n\times n}$ *and a linear space* $\mathcal{Z} \subseteq \mathbb{C}^n$, *such that, for all* $z \in \mathcal{Z}$, *we have* $P(z) \in \mathbb{R}^{n\times n}$ *and* $\mathcal{T} = \{z \in \mathcal{Z} \,|\, P(z) \succeq 0\}$.



(a) A_3 (b) B_3 (c) C_3

Figure 1: Orbit spaces for root systems of rank 3, given by $P(z) \succeq 0$.

Here, A_{n-1}, B_n, C_n, D_n and G_2 are so–called irreducible root systems. One can show that every other root system can be decomposed into these components or two further special cases $\mathrm{E}_{6,7,8}$ and F_4, which are not treated here. This notation goes back to the classification of the complex semi–simple Lie algebras and is used in representation theory, see [Bou68, Chapitre VI, §4, Théorème 3] for the proof and [Bou68, Planche I–IX] for an overview. We review these cases in Theorem 1.20.

The proof is inspired by Sylvester's version of Sturm's theorem. A novelty and significant difference to [PS85] lies in the presentation of a closed formula for the targeted families of Weyl groups in both the standard monomial basis and the basis of generalized Chebyshev polynomials. The formula only depends on the involved parameters, namely dimension and identification of the symmetry group, but not on generally heavy calculations for invariants. Remarkably, the formula that we present in the chapter is identical for all cases in the Chebyshev basis.

Continuing the story of our invariant trigonometric optimization problem, this means that the feasible region is basic semi–algebraic and compact. Under the assumption of the Main result 1, we are now at a point

where we can write
$$f^* = \inf_{u\in\mathbb{R}^n} \sum_{\mu\in\Omega} c_\mu \exp(-2\pi \mathrm{i} \langle \mu, u\rangle) = \inf_{P(z)\succeq 0} \sum_{\alpha\in\mathbb{N}^n} c_\alpha T_\alpha(z).$$

Chapter 3. We address the problem of optimizing a trigonometric polynomial with crystallographic symmetry in practice. Our approach adapts the techniques of Lasserre's hierarchy and utilizes the generalized Chebyshev polynomials, as well as a different notion of degree. The problem is first reformulated to a polynomial optimization problem on the orbit space. A hierarchy of relaxations is formulated in the basis of generalized Chebyshev polynomials and convergence is proven. The approach is extended to bilevel problems with additional linear constraints.

In [Dum07, Chapter 3], it is proposed to solve a hierarchy of sum of Hermitian squares relaxations via semi–definite programming to obtain an approximate solution for f^*. Other techniques are for example generalizations of Lasserre's hierarchy [JM18], but do not exploit symmetry. With our rewriting approach, we are in the context of polynomial optimization and can apply the classical Lasserre hierarchy. Since the objective function and the constraints are represented in the basis of generalized Chebyshev polynomials, we formulate and implement the hierarchy in this way, using a new notion of polynomial degree, that comes naturally with Chebyshev polynomials and root systems.

Furthermore, we apply the positivity certificate due to Hol and Scherer [HS06] for feasible regions given by polynomial matrix inequalities.

This leads to a hierarchy of sums of squares relaxations of reduced complexity compared to other trigonometric optimization techniques. For $d \in \mathbb{N}$ sufficiently large, this hierarchy has standard form

$$\begin{array}{rll} f_{\mathrm{sos}}^d := & \sup & \lambda \\ & \text{s.t.} & \lambda \in \mathbb{R},\, q \in \mathrm{SOS}(\mathcal{F}_d),\, Q \in \mathrm{SOS}(\mathcal{F}_{d-D}^{n\times n}), \\ & & \sum\limits_{\alpha\in\mathbb{N}^n} c_\alpha T_\alpha - \lambda = q + \mathrm{Trace}(P\,Q), \end{array}$$

where $\mathcal{F}_k$ are finite dimensional spaces and D is an additional parameter, specified in Chapter 3. Under an Archimedean assumption, one can then show the following.

Main result 2. *The sequence $(f_{\mathrm{sos}}^d)_{d\in\mathbb{N}}$ is monotonously converging to f^*.*

Numerical evidence is provided to show that f_{sos}^d yields more accurate bounds at lower complexity than the hierarchy in [Dum07]. We then study the dual formulation of f_{sos}^d via moments of generalized Chebyshev polynomials, giving explicit formulae for the entries of the arising SDP matrices. This is implemented in a Maple package GeneralizedChebyshev.

Chapter 4. We study the problem of computing the chromatic number of subgraphs of $\mathbb{R}^n$ for polytope norms. The Hardwiger–Nelson problem (1950) asks for the minimal number of colors needed to paint the space $\mathbb{R}^2$, so that no two points with Euclidean distance 1 have the same color. From a graph–theoretic point, this means to compute the (measurable) chromatic number of the graph $G(\mathbb{R}^2, \|\cdot\|_2)$ with vertices and edges
$$V = \mathbb{R}^2, \quad E = \left\{ \{u, v\} \in \binom{V}{2} \;\middle|\; \|u-v\|_2 = 1 \right\}.$$

Until today, this problem is not solved. According to [Soi09], Isbell was the first to prove that the upper bound for the chromatic number is 7. The current lower bound on the other hand is 5, found by de Grey computationally through a finite subgraph [Gre18]. When it comes to norms, that are defined by space–tiling polytopes instead of $\|\cdot\|_2$, one can prove that the upper bound for the chromatic number of $\mathbb{R}^n$ is 2^n. Equality is conjectured and proven in several cases [BBMP19].

In [BDFV14], the Hoffman and Lovász bounds for chromatic numbers and independence ratios of finite graphs are generalized to the infinite setting via self–adjoint operators on Hilbert spaces. This allows to study the chromatic number χ and the measurable chromatic number χ_m. In particular, we consider the case where the vertices of the graph are $\mathbb{R}^n$ and an edge connects two vertices, if the distance is 1 for a fixed norm on $\mathbb{R}^n$. The spectral bound from [BDFV14] involves the optimization of the Fourier transformation of a centrally–symmetric signed Borel measure on the sphere with radius 1.

In this chapter, we study norms, which are induced by centrally symmetric convex polytopes whose symmetry group is a Weyl group. Then we have a problem of the kind of finding f^* from above and can solve it with the techniques established in the previous chapters. Furthermore, we can optimize on the coefficients of the measure from the spectral bound.

Our strategy is to fix the points on the boundary of the polytope, which are contained in a weight lattice. This defines a discrete subgraph of $\mathbb{R}^n$ and we can compute lower bounds for its chromatic number. The de Bruijn–Erdös theorem implies that the chromatic number of $\mathbb{R}^n$ is obtainable through discrete subgraphs. Hence, our approach allows us to investigate whether the conjectured bound 2^n for tiling polytopes can be obtained through a systematic approach.

In some cases, the restriction to discrete subgraphs allows to prove theoretical results. In others, we obtain approximations by numerically solving the following optimization problem. For $r, d \in \mathbb{N}$, we define a hierarchy

$$\begin{array}{rll} F(r,d) := & \sup & -\mathrm{Trace}(A_0\, X) \\ & \text{s.t.} & X \in \mathrm{Sym}^N_{\succeq 0}, \ \sum\limits_{\alpha \in S_r(\mathbb{N})} \mathrm{Trace}(A_\alpha\, X) = 1, \\ & & \mathrm{Trace}(A_\alpha\, X) \geq 0 \quad \text{for} \quad \alpha \in S_r(\mathbb{N}), \\ & & \mathrm{Trace}(A_\beta\, X) = 0 \quad \text{for} \quad \beta \notin S_r(\mathbb{N}) \cup \{0\}, \end{array}$$

where $S_r(\mathbb{N}) \subseteq \mathbb{N}^n$, $N = \dim(\mathcal{F}_d) + n\, \dim(\mathcal{F}_{d-D})$ and the A_α are specified in Chapter 4 and depend on the Weyl group $\mathcal{W}$.

Main result 3a. *Let Ω be a weight lattice and $\mathcal{P}$ be a centrally symmetric convex polytope with $\mathcal{W}(\mathcal{P}) = \mathcal{P}$, such that $S_r := \Omega \cap \partial(r\,\mathcal{P}) \neq \emptyset$. Then the sequence $(F(r,d))_{d\in\mathbb{N}}$ is monotonously non–decreasing in d and*

$$\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathcal{P}}) \geq \chi(\Omega, S_r) \geq 1 - \frac{1}{F(r,d)}.$$

The sequence converges to an optimal value $F(r) = \lim\limits_{d\to\infty} F(r,d)$ and, for $k \in \mathbb{N}$, we have $F(r) \leq F(k\, r)$.

Main result 3b. *Denote by $\mathbb{B}^1_r$ the sphere of the 1–norm $\|\cdot\|_1$ with radius $r \in \mathbb{N}$ and by e_i the Euclidean standard basis vectors. The spectral bound is analytically proven to be sharp in the following cases.*

1. $\chi(\mathbb{Z}^n, \{\pm e_i \,|\, 1 \leq i \leq n\}) = 2$.
2. $\chi(\mathbb{Z}^n/\langle[1, 1 \ldots, 1]^t\rangle, \{\pm(e_i - e_j) \,|\, 1 \leq i < j \leq n\}) = n$.
3. $\chi(\mathbb{Z}^n, \mathbb{B}^1_2 \cap \mathbb{Z}^n) = 2n$.
4. *For $\mathcal{P} \subseteq \mathbb{R}^n$ the n–cube:* $\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathcal{P}}) = 2^n$.

The following spectral bounds are found numerically.

5. *For $\mathcal{P} \subseteq \mathbb{R}^2$ the hexagon:* $\chi_m(\mathbb{R}^2, \|\cdot\|_{\mathcal{P}}) \geq \chi(\Omega(\mathrm{A}_2), S_2) \geq 1 - 1/F(2,8) \approx 3.571$.
6. *For $\mathcal{P} \subseteq \mathbb{R}^3$ the rhombic dodecahedron:* $\chi_m(\mathbb{R}^3, \|\cdot\|_{\mathcal{P}}) \geq \chi(\Omega(\mathrm{A}_3), S_2) \geq 1 - 1/F(2,8) \approx 6.108$.
7. *For $\mathcal{P} \subseteq \mathbb{R}^4$ the icositetrachoron:* $\chi_m(\mathbb{R}^4, \|\cdot\|_{\mathcal{P}}) \geq \chi(\Omega(\mathrm{D}_4), S_2) \geq 1 - 1/F(2,6) \approx 10.024$.
8. $\chi(\mathbb{Z}^3, \mathbb{B}^1_4 \cap \mathbb{Z}^3) \geq 1 - 1/F(4,9) \approx 6.281$.
9. $\chi(\mathbb{Z}^3, \mathbb{B}^1_8 \cap \mathbb{Z}^3) \geq 1 - 1/F(8,9) \approx 6.305$.
10. $\chi(\mathbb{Z}^4, \mathbb{B}^1_4 \cap \mathbb{Z}^4) \geq 1 - 1/F(4,7) \approx 10.860$.

The first set of bounds is not obtained through numerical relaxation techniques, but analytically through a reformulation of the objective trigonometric function in the basis of generalized Chebyshev polynomials, enabling an easy proof. In the other cases, lower bounds for the spectral bound, and thus for the chromatic number, are obtained through sums of squares relaxations until the point where no further improvement was observable.

Articles

The presented results are based on two articles, "Polynomial description for the $\mathbb{T}$–orbit spaces of multiplicative actions" with Evelyne Hubert and Cordian Riener [HMR22] and "Optimization of trigonometric polynomials with crystallographic symmetry and applications" with Evelyne Hubert, Philippe Moustrou and Cordian Riener [HMMR22]. The third article that has been produced during the doctoral studies, "Computing free non-commutative Gröbner bases over Z with Singular:Letterplace" with Viktor Levandovskyy and Karim Abou Zeid [LMZ23], does not fit in the scope of this thesis and is thus not a part of it.

- E. Hubert, T. Metzlaff, C. Riener. Polynomial description for the $\mathbb{T}$–Orbit Spaces of Multiplicative Actions. *Preprint submitted https://hal.archives-ouvertes.fr/hal-03590007v2*, 2022
- E. Hubert, T. Metzlaff, P. Moustrou, C. Riener. Optimization of trigonometric polynomials with crystallographic symmetry and applications. *Preprint in preparation https://hal.archives-ouvertes.fr/hal-03768067v1*, 2022
- V. Levandovskyy, T. Metzlaff, K. Abou Zeid. Computing free non-commutative Gröbner bases over Z with Singular:Letterplace. *Journal of Symbolic Computations*, 115:201–222, 2023

Notation

$\mathbb{N}, \mathbb{Z}, \mathbb{Q}, \mathbb{R}, \mathbb{C}$	nonnegative integers, integers, rational, real, complex numbers
$\{\ldots\}, \lvert\cdot\rvert$	set, cardinality or absolute value
$V, \dim(V), 0$	vector space (in Chapter 1), dimension, neutral element of addition
$\mathrm{GL}(V), \mathrm{O}(V)$	general linear group, orthogonal group
$\langle\cdot,\cdot\rangle, \lVert\cdot\rVert$	inner product, norm
R, B	root system, base
$\mathrm{A}_{n-1}, \mathrm{C}_n, \mathrm{B}_n, \mathrm{D}_n, \mathrm{E}_{6,7,8}, \mathrm{F}_4, \mathrm{G}_2$	irreducible root systems
$\rho, \rho^\vee, \rho_i, \rho_0$	roots, coroots, simple roots, highest root
s_ρ	reflection associated to a root
$\mathcal{W}, I_n$	Weyl group, neutral group element
$\mathfrak{S}_n, \mathfrak{D}_n$	symmetric group of order $n!$, dihedral group of order $2n$
$\mathrm{Rank}, \mathrm{Det}, \mathrm{Trace}$	rank, determinant, trace
$\mathcal{G}$	finite group of integer matrices
Ω, Λ	dual weight and coroot lattice
μ, ω_i	weights, fundamental weights
W	change of basis from standard Euclidean to fundamental weights
$\mathbb{R}[\Omega]$	group algebra or trigonometric polynomials
$\mathbb{R}[x^\pm], \mathbb{R}[x^\pm]^\mathcal{G}$	multivariate Laurent polynomial ring, ring of invariants
θ_i	fundamental invariants
$\Theta_\alpha, \Upsilon_\alpha$	invariant and anti–invariant orbit polynomials
Ξ_α	character polynomials
$\mathbb{R}[z]$	multivariate polynomial ring
$T_\alpha, \widehat{T}_\alpha$	generalized Chebyshev polynomials of the first kind, real part
U_α	generalized Chebyshev polynomials of the second kind
$\deg(\cdot), \deg_W(\cdot)$	degree, weighted degree
$\mathcal{F}_d$	filtration
$(\mathbb{C}^*)^n, \mathbb{T}^n$	algebraic torus, compact torus
$\star, \cdot$	nonlinear action, multiplicative action
$\mathbb{T}^n/\mathcal{G}$	orbits
ϑ	canonical projection
$\mathcal{T}$	$\mathbb{T}$–orbit space
$\exp, \cos, \sin$	exponential, cosine, sine
$\mathfrak{c}_\mu, \mathfrak{s}_\mu$	generalized cosine, generalized sine
$\nabla, \widetilde{\nabla}$	gradient, gradient of Euler derivations
$\mathscr{L}, \mathbb{H}^\mathscr{L}, \mathcal{H}^\mathscr{L}$	linear functional, Hankel operator, Hankel matrix in Chebyshev basis
$\otimes$	Kronecker product of matrices
G, V, E	graph, vertices (in Chapter 4), edges
$\mathfrak{g}, \mathfrak{h}$	Lie algebra, Cartan subalgebra
$[\cdot,\cdot], \chi_\mathfrak{g}$	Lie bracket, Killing form

If a group acts linearly on a finite dimensional vector space by matrix vector multiplication, both the matrix and the vector are denoted by $[\ldots]$ parentheses. The transpose is $[\ldots]^t$. A symbol for this action is omitted, just as for scalar multiplication. This notation is not to be confused with closed intervals $[\cdot,\cdot] \subseteq \mathbb{R}$ or Lie brackets $[\cdot,\cdot] \in \mathfrak{g}$.

If a space with no matrix group action is considered, the elements are denoted by $(\ldots)$ parentheses. This notation is not to be confused with open intervals $(\cdot,\cdot) \subseteq \mathbb{R}$ or binomial coefficients $\binom{\cdot}{\cdot} \in \mathbb{N}$.

Chapter 1

Multiplicative invariant theory for crystallographic groups

A crystallographic reduced root system defines a finite reflection group, which is known as a crystallographic group or Weyl group. A root system can be decomposed in irreducible components and this leaves us with a finite number of families, which we shall mainly study. The weights of the root system form a lattice, which is invariant under the Weyl group. We define a multiplicative action on the associated group ring. Then the invariants of the action form a polynomial ring. This is a unique property for Weyl groups among all reflection groups and allows us to define multivariate generalizations of Chebyshev polynomials. We introduce the necessary notations and prove minor properties.

1 Crystallographic symmetries

The symmetries studied in this thesis are the crystallographic ones, given by special kinds of reflection groups over real vector spaces. A crystallographic group is the Weyl group of a crystallographic reduced root system. We introduce these notions by revisiting Bourbaki's chapter VI on root systems [Bou68] and chapter VIII on weights of Lie algebras [Bou75]. Historically, root systems were used by Wilhelm Killing and Élie Cartan to classify the complex simple Lie algebras, see Appendix A.

1.1 Root systems and Weyl groups

Let V be an n–dimensional $\mathbb{R}$–vector space with an inner product $\langle \cdot, \cdot \rangle$, that identifies V with its dual. Denote by $\mathrm{GL}(V)$ the group of autormorphisms on V and by $\mathrm{O}(V)$ the orthogonal group.

Definition 1.1. *Let* R *be a finite nonempty subset of* V*. We say that* R *is a* ***root system*** *in* V*, if the following conditions are satisfied.*

1. R *spans* V *and does not contain* 0*.*
2. *If* $\rho, \tilde{\rho} \in \mathrm{R}$*, then* $s_\rho(\tilde{\rho}) \in \mathrm{R}$*, where* s_ρ *is the reflection on* V *defined by* $s_\rho(u) = u - 2\frac{\langle u, \rho \rangle}{\langle \rho, \rho \rangle}\rho$*.*
3. *If* $\rho, \tilde{\rho} \in \mathrm{R}$*, then* $2\frac{\langle \tilde{\rho}, \rho \rangle}{\langle \rho, \rho \rangle} \in \mathbb{Z}$*.*
4. *For* $\rho \in \mathrm{R}$ *and* $c \in \mathbb{R}$*, we have* $c\rho \in \mathrm{R}$ *if and only if* $c = \pm 1$*.*

The elements of R *are called* ***roots****. The* ***rank*** *of* R *is the dimension of* V*.*

In many texts, a root system is defined by only using the first three of the above conditions and if the fourth condition holds, one speaks of a **reduced** root system. Less common is also to define a root system without the third **crystallographic** property, see for example [Kan01]. In this thesis, we assume all root systems to be reduced and crystallographic.

The element

$$\rho^\vee := \frac{2\,\rho}{\langle \rho, \rho \rangle}$$

that appears in the definition of the reflection s_ρ is called the **coroot** of $\rho \in \mathrm{R}$. The set of all coroots is denoted by $\mathrm{R}^\vee$ and this set is again a root system called the **dual root system** with the same reflections as R. We have $(\rho^\vee)^\vee = \rho$ for all $\rho \in \mathrm{R}$.

Definition 1.2. *The* ***Weyl group*** $\mathcal{W} = \mathcal{W}(\mathrm{R})$ *of a root system is the group generated by the reflections* s_ρ *for* $\rho \in \mathrm{R}$*.*

The group $\mathcal{W}$ is a subgroup of the orthogonal group on V with respect to the inner product $\langle \cdot, \cdot \rangle$. In particular, V is a $\mathcal{W}$–module, that is, a representation of $\mathcal{W}$. For $u \in V$, we denote the orbit of u under $\mathcal{W}$ by $\mathcal{W}u$.

1.2 Irreducible root systems

We shall mainly work with the so–called irreducible root systems.

Proposition 1.3. [Bou68, Chapitre VI, §1, Proposition 5] *Let* $k \in \mathbb{N}$ *and* $V_1, \ldots, V_k$ *be finite dimensional* $\mathbb{R}$*–vector subspaces, such that* $V = V_1 \oplus \ldots \oplus V_k$*. Assume that* R *is a root system in* V*. The following statements are equivalent.*

1. *For all* $1 \leq i \leq k$*,* V_i *is a representation of* $\mathcal{W}$*.*

2. *For all* $1 \leq i \leq k$*,* $\mathrm{R}_i := \mathrm{R} \cap V_i$ *is a root system in* V_i *and* $\mathrm{R} = \mathrm{R}_1 \oplus \ldots \oplus \mathrm{R}_k$*.*

A root system is called **irreducible**, if it is not the direct sum of two root systems. By Maschke's Theorem for irreducible representations and the previous statement, we obtain a characterization.

Corollary 1.4. [of Proposition 1.3] *Let* R *be a root system in* V*. Then* R *is irreducible if and only if* V *is an irreducible representation of* $\mathcal{W}$*.*

Remark 1.5. *If* R *is not irreducible, then* $\mathcal{W}$ *is the product of the Weyl groups corresponding to the irreducible components, see the discussion before* [Bou68, Chapitre VI, §1, Proposition 5].

Proposition 1.6. [Bou68, Chapitre VI, §1, Proposition 6 et 7] *Let* R *be a root system. Then* R *can be uniquely decomposed in a direct sum of irreducible root systems* R_i*. Let* V_i *be the* $\mathbb{R}$*–vector subspace generated by* R_i*. Then the* V_i *are pairwise orthogonal with respect to* $\langle \cdot, \cdot \rangle$*.*

The finitely many cases of irreducible root systems are recalled later in a classification with Dynkin graphs.

1.3 Positive roots, chambers and weights

A **chamber** C of R is a connected open subset of V, which is restricted by the invariant hyperplanes of the reflections s_ρ. The **walls** L of a chamber are those hyperplanes, which support a facet.

Proposition 1.7. [Bou68, Chapitre VI, §1, Théorème 2 and 3] *Let* R *be a root system in* V *with Weyl group* $\mathcal{W}$*. The following statements hold.*

1. *The action of* $\mathcal{W}$ *on the set of chambers is simply–transitive.*
2. *A chamber is a simplicial cone and its closure is a fundamental domain for* $\mathcal{W}$*.*
3. *For every wall* L *of a chamber* C*, there exists a unique* $\rho \in \mathrm{R}$*, such that*
$$L = \{u \in V \mid \langle u, \rho \rangle = 0\}$$
and ρ *lies on the same side of* L *as* C*. The set of all such* ρ *is a basis* B *of* V *and we have*
$$C = \{u \in V \mid \forall\, \rho \in \mathrm{B} :\, \langle u, \rho \rangle > 0\}.$$
Every element of R *can be written as a unique linear combination of* B *with coefficients all non–negative or non–positive.*

In particular, the number of chambers is the order of $\mathcal{W}$. We observe that there is a correspondence between linearly independent subsets of R, which define "positive" roots, and the chambers.

Definition 1.8. *Let* R *be a root system in* V*.*

1. *A subset* $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$ *of* R *is called a* ***base****, if the following conditions hold.*
   (a) B *is a basis of the vector space* V*.*
   (b) *Every root* $\rho \in \mathrm{R}$ *can be written as* $\rho = \alpha_1 \rho_1 + \ldots + \alpha_n \rho_n$ *or* $\rho = -\alpha_1 \rho_1 - \ldots - \alpha_n \rho_n$ *for some* $\alpha \in \mathbb{N}^n$*.*

   The elements of B *are called* ***simple roots****.*
2. *The* ***fundamental Weyl chamber*** *in* V *relative to a base* $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$ *is*
$$\Lambda\!\!\Lambda := \{u \in V \mid \forall\, 1 \leq i \leq n :\, \langle u, \rho_i \rangle > 0\}.$$

3. *If* B *is a base, the roots of the form* $\rho = \alpha_1 \rho_1 + \ldots + \alpha_n \rho_n$ *for* $\alpha \in \mathbb{N}^n$ *are called the* ***positive roots*** *and the set of all positive roots is denoted by* R^+.

4. *The* ***Cartan matrix*** *of* R *is the* $(n \times n)$*–matrix with integer entries*

$$\mathrm{Cartan}(\mathrm{R})_{ij} := \frac{\langle \rho_i, \rho_j \rangle}{\langle \rho_j, \rho_j \rangle}.$$

From now on, we fix a base B of R. The closure $\overline{\Lambda}$ of the fundamental Weyl chamber is a fundamental domain of $\mathcal{W}$ [Bou68, Chapitre V, §3, Théorème 2]. Furthermore, we define a partial ordering on V by

$$u \succeq v \quad \Leftrightarrow \quad u - v \text{ is a sum of positive roots.} \tag{1.1}$$

Proposition 1.9. [Bou68, Chapitre VI, §1, Proposition 18 and 25] *Let* B *be a base.*

1. *For* $u \in V$*, we have* $u \in \overline{\Lambda}$*, if and only if, for all* $A \in \mathcal{W}$*,* $u \succeq Au$.

2. *If* R *is irreducible, then there exists a unique maximal positive root* $\rho_0 \in \mathrm{R}^+$ *with respect to* $\succeq$.

We call ρ_0 the **highest root** of R with respect to B.

Definition 1.10. *Let* $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$ *be a base of* R.

1. *An element* μ *of* V *is called a* ***weight*** *of* R*, if, for all* $1 \leq i \leq n$*,*

$$\langle \mu, \rho_i^\vee \rangle \in \mathbb{Z}.$$

   The set of weights forms a lattice Ω*, called the* ***weight lattice****.*

2. *The* ***fundamental weights*** *are the elements* $\{\omega_1, \ldots, \omega_n\}$ *such that* $\langle \omega_i, \rho_j^\vee \rangle = \delta_{i,j}, 1 \leq i, j \leq n$.

3. *A weight* μ *is called* ***radical****, if it is contained in the lattice of roots, that is,* $\mu \in \mathbb{Z}\rho_1 \oplus \ldots \oplus \mathbb{Z}\rho_n$.

4. *A weight* μ *is called* ***strongly dominant****, if* $\langle \mu, \rho_i \rangle > 0$ *for all* $\rho_i \in \mathrm{B}$*. A weight* μ *is called* ***dominant****, if* $\langle \mu, \rho_i \rangle \geq 0$ *for all* $\rho_i \in \mathrm{B}$*. The set of dominant weights is denoted by* Ω^+.

We finish this section with a collection of useful facts.

Lemma 1.11. *The following statements hold.*

1. Ω *is left invariant under the Weyl group, that is, for all* $\mu \in \Omega$*,* $\mathcal{W}\mu \subseteq \Omega$.

2. *The strongly dominant weights are contained in* Λ *and the dominant weights are contained in* $\overline{\Lambda}$.

3. *The fundamental weights lie on the walls of* Λ.

4. *For every* $\mu \in \Omega$*, there exists a unique dominant weight* μ'*, such that* $\mu \in \mathcal{W}\mu'$.

5. *We have*

$$\frac{1}{2} \sum_{\rho \in \mathrm{R}^+} \rho = \sum_{i=1}^{n} \omega_i.$$

   In particular, this is a strongly dominant weight [Bou68, Chapitre VI, §1, Proposition 29].

1.4 Affine Weyl groups

Let R be a root system of rank n in V with Weyl group $\mathcal{W}$, base B and weight lattice Ω. As in Definition 1.1, R is crystallographic and reduced. The coroots $R^\vee$ span a lattice Λ in V, which is an Abelian group of translations. Λ is the dual lattice of the weights, that is, $\Omega^* = \{u \in V \,|\, \forall\, \mu \in \Omega : \langle \mu, u\rangle \in \mathbb{Z}\} = \Lambda$.

With respect to the inner product, we define a norm on V via $\|u\| := \sqrt{\langle u, u\rangle}$.

The **affine Weyl group** $\mathcal{W} \ltimes \Lambda$ of R is the semi–direct product of $\mathcal{W}$ by Λ. The property "semi–direct" is lost when the root system is not crystallographic, see [Bou68, Chapitre VI, §2, Proposition 9].

With respect to the inner product, we define a norm on V via $\|u\| := \sqrt{\langle u, u\rangle}$. Then the **Voronoï cell** of Λ is

$$\mathrm{Vor}(\Lambda) := \{u \in V \,|\, \forall \lambda \in \Lambda : \|u\| \leq \|u - \lambda\|\}$$

and tiles V by Λ–translation, that is,

$$V = \bigcup_{\lambda \in \Lambda} (\mathrm{Vor}(\Lambda) + \lambda). \tag{1.2}$$

The intersection of two distinct cells $\mathrm{Vor}(\Lambda) + \lambda$ and $\mathrm{Vor}(\Lambda) + \tilde{\lambda}$ is empty or contained in a hyperplane [CS99, Chapter 2, §1.2]. Here, "+" denotes the Minkowski sum.

Remark 1.12. *When it comes to the affine Weyl group, Bourbaki replaces the term "chamber" by "alcoves". In particular, $\mathcal{W} \ltimes \Lambda$ acts simply transitively on the set of alcoves and the closure of any alcove is a fundamental domain for $\mathcal{W} \ltimes \Lambda$.*

If R *is irreducible, then any alcove of $\mathcal{W} \ltimes \Lambda$ is an open simplex. Otherwise, any alcove is the product of alcoves corresponding to the irreducible components, see the discussion after* [Bou68, Chapitre VI, §2, Proposition 2].

Proposition 1.13. [Bou68, Chapitre VI, §2, Proposition 4] and [CS99, Chapter 21, §3, Theorem 5] *There is a unique alcove of $\mathcal{W} \ltimes \Lambda$ in $\Lambda\!\!\Lambda$, which contains 0 in its closure. Denote this closure by $\triangle$. Then* $\mathrm{Vor}(\Lambda) = \mathcal{W}\,\triangle$ *is the Voronoï cell of Λ.*

In the case of irreducible root systems, the closure $\triangle$ in the previous statement has a particular representation.

Proposition 1.14. [Bou68, Chapitre VI, §2, Proposition 5] *If* R *is irreducible, then the closed alcove*

$$\triangle = \{u \in \mathbb{R}^n \,|\, \forall\, 1 \leq i \leq n : \langle u, \rho_i\rangle \geq 0 \text{ and } \langle u, \rho_0\rangle \leq 1\}$$

is a fundamental domain for $\mathcal{W} \ltimes \Lambda$.

Lemma 1.15. *Assume that*

$$\rho_0 = \sum_{i=1}^{n} \alpha_i\, \rho_i^\vee$$

is the highest root for some $\alpha \in \mathbb{R}^n$. Then, for $1 \leq i \leq n$, $\alpha_i > 0$ and

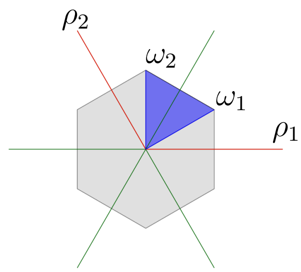
$$\triangle = \mathrm{ConvHull}\left(0, \frac{\omega_1}{\alpha_1}, \ldots, \frac{\omega_n}{\alpha_n}\right).$$

Proof. For $1 \leq i, j \leq n$, we have $\langle \omega_i/\alpha_i, \rho_j^\vee\rangle = \delta_{i,j}/\alpha_i \geq 0$. Thus, ω_i/α_i is contained in a wall of $\Lambda\!\!\Lambda$ and

$$\langle \omega_i/\alpha_i, \rho_0\rangle = \sum_{j=1}^{n} \frac{\alpha_j}{\alpha_i} \langle \omega_i, \rho_j^\vee\rangle = \sum_{j=1}^{n} \frac{\alpha_j}{\alpha_i}\, \delta_{i,j} = \frac{\alpha_i}{\alpha_i} = 1$$

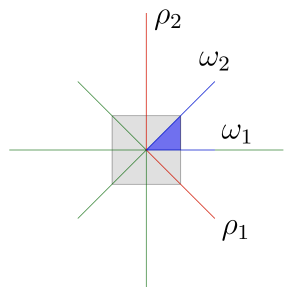
implies that ω_i/α_i is on the hyperplane $\langle \cdot, \rho_0\rangle = 1$. □

Example 1.16. *In the 2–dimensional case, we can consider the following irreducible root systems.*



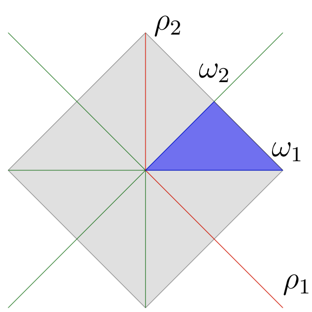
$\mathcal{W}(\mathrm{A}_2) \cong \mathfrak{S}_3$
$\omega_1 = [2, -1, -1]^t/3$
$\omega_2 = [1, 1, -2]^t/3$
$\rho_1 = [1, -1, 0]^t = \rho_1^\vee$
$\rho_2 = [0, 1, -1]^t = \rho_2^\vee$
$\rho_0 = \rho_1^\vee + \rho_2^\vee$

Figure 1.1: The root system A_2 in $\mathbb{R}^3/\langle[1, 1, 1]^t\rangle$.



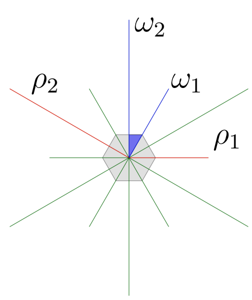
$\mathcal{W}(\mathrm{C}_2) \cong \mathfrak{S}_2 \ltimes \{\pm 1\}^2$
$\omega_1 = [1, 0]^t$
$\omega_2 = [1, 1]^t$
$\rho_1 = [1, -1]^t = \rho_1^\vee$
$\rho_2 = [0, 2]^t = 2\,\rho_2^\vee$
$\rho_0 = 2\,\rho_1^\vee + 2\,\rho_2^\vee$

Figure 1.2: The root system C_2 in $\mathbb{R}^2$.



$\mathcal{W}(\mathrm{B}_2) \cong \mathfrak{S}_2 \ltimes \{\pm 1\}^2$
$\omega_1 = [1, 0]^t$
$\omega_2 = [1, 1]^t/2$
$\rho_1 = [1, -1]^t = \rho_1^\vee$
$\rho_2 = [0, 1]^t = \rho_2^\vee/2$
$\rho_0 = \rho_1^\vee + \rho_2^\vee$

Figure 1.3: The root system B_2 in $\mathbb{R}^2$.



$\mathcal{W}(\mathrm{G}_2) \cong \mathfrak{S}_3 \ltimes \{\pm 1\}$
$\omega_1 = [0, -1, 1,]^t$
$\omega_2 = [-1, -1, 2]^t$
$\rho_1 = [1, -1, 0]^t = \rho_1^\vee$
$\rho_2 = [-2, 1, 1]^t = 3\,\rho_1^\vee$
$\rho_0 = 3\,\rho_1^\vee + 6\,\rho_2^\vee$

Figure 1.4: The root system G_2 in $\mathbb{R}^3/\langle[1, 1, 1]^t\rangle$.

Here, the roots are depicted in green, the base in red and the fundamental weights in blue. The Voronoï cell *of the coroot lattice Λ is the gray shaded region, we have two squares (C_2 and B_2) and two hexagons (A_2 and G_2). The fundamental domain of the affine Weyl group is the blue shaded simplex.*

1.5 Classification by Dynkin graphs

The irreducible root systems can be classified with so–called Dynkin graphs. Let R be a root system of rank n in V with Weyl group $\mathcal{W}$ and base $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$.

The crystallographic property in the definition of a root system reduces the possible lengths and angles of roots to finitely many cases, because

$$\mathbb{N} \ni 2\frac{\langle \tilde{\rho}, \rho\rangle}{\langle \rho, \rho\rangle}\, 2\frac{\langle \rho, \tilde{\rho}\rangle}{\langle \tilde{\rho}, \tilde{\rho}\rangle} = 4\left(\frac{\langle \tilde{\rho}, \rho\rangle}{\|\rho\|\ \|\tilde{\rho}\|}\right)^2 = 4\cos(\phi)^2 \le 4,$$

where ϕ denotes the angle between ρ and $\tilde{\rho}$. The finitely many cases are recalled in Theorem 1.20.

Proposition 1.17. [Bou68, Chapitre VI, §1, Proposition 11 and 12] *Let R be an irreducible root system in V and $\rho, \tilde{\rho} \in \mathrm{R}$. The following statements hold.*

1. *If $\|\rho\| = \|\tilde{\rho}\|$, then $\rho \in \mathcal{W}\tilde{\rho}$.*
2. *The set $\{\|\rho\| \mid \rho \in \mathrm{R}\}$ has cardinality 1 or 2.*

In this sense, one can distinguish between "short" and "long" roots. The highest root ρ_0 is always a long root [Bou68, Chapitre VI, §1, Proposition 25].

Definition 1.18. *The **Dynkin graph** of R is the directed graph with vertices B. For $k \in \mathbb{N}$ and $1 \le i, j \le n$, a k–fold edge connects ρ_i and ρ_j if the product of reflections $s_{\rho_i}\, s_{\rho_j} \in \mathcal{W}$ has order $k+2$. If two roots have distinct lengths, an arrow points to the longer root.*

Denote by $s_i := s_{\rho_i}$ the reflection associated to $\rho_i \in \mathrm{B}$.

Lemma 1.19. *For a root system R, the following statements hold.*

1. *The reflections s_i have order 2. Hence, a simple root is not connected to itself in the Dynkin graph.*
2. *If $i \ne j$ and s_i, s_j commute, then no edge connects ρ_i and ρ_j.*
3. *The Dynkin graph is connected if and only if R is irreducible.*

Theorem 1.20. [Bou68, Chapitre VI, §4, Théorème 3] *Let R be an irreducible root system. Then its Dynkin graph is of type A_{n-1}, B_n, C_n $(n \ge 2)$, D_n $(n \ge 4)$, E_n $(n \in \{6,7,8\})$, F_4 or G_2.*

The undirected version of the Dynkin graph with edges given by the generators s_i of $\mathcal{W}$ is called **Coxeter graph**. For the four infinite families and G_2, on which we shall mainly focus throughout this thesis, these graphs are listed below. Coxeter graphs are furthermore used to classify finite Coxeter systems, see [Bou68, Chapitre VI, §4, Théorème 4].

A_{n-1}

The group $\mathfrak{S}_n$ acts on $\mathbb{R}^n$ by permutation of coordinates and leaves the subspace $V = \mathbb{R}^n/\langle [1, \ldots, 1]^t\rangle = \{u \in \mathbb{R}^n \mid u_1 + \ldots + u_n = 0\}$ invariant. The root system A_{n-1} given in [Bou68, Planche I] is a root system of rank $n-1$ in V with simple roots and fundamental weights

$$\rho_i = e_i - e_{i+1} \quad \text{and} \quad \omega_i = \sum_{j=1}^{i} e_j - \frac{i}{n}\sum_{j=1}^{n} e_j = \frac{1}{n}[\underbrace{n-i, \ldots, n-i}_{i \text{ times}}, \underbrace{-i, \ldots, -i}_{n-i \text{ times}}]^t \tag{1.3}$$

for $1 \le i \le n-1$. Here, the e_i denote the Euclidean standard basis vectors. The Weyl group of A_{n-1} is $\mathcal{W} \cong \mathfrak{S}_n$ and the graph

$$s_1 \text{ --- } s_2 \text{ --- } \dots \text{ --- } s_{n-2} \text{ --- } s_{n-1} \tag{1.4}$$

is the associated Coxeter graph, where the $s_i := s_{\rho_i}$ are the reflections from Definition 1.1, which generate $\mathcal{W}$. The reflection s_i permutes the coordinates i and $i+1$. Thus, $-\omega_{n-i} \in \mathcal{W}\,\omega_i$ and the orbit $\mathcal{W}\,\omega_i$ has cardinality $\binom{n}{i}$ for $1 \le i \le n-1$.

C_n

The groups $\mathfrak{S}_n$ and $\{\pm 1\}^n$ act on $\mathbb{R}^n$ by permutation of coordinates and multiplication of coordinates by ± 1. The root system C_n given in [Bou68, Planche III] is a root system in $\mathbb{R}^n$ with simple roots and fundamental weights

$$\rho_i = e_i - e_{i+1}, \quad \rho_n = 2\,e_n \quad \text{and} \quad \omega_i = e_1 + \ldots + e_i. \tag{1.5}$$

for $1 \le i \le n$. The Weyl group of C_n is $\mathcal{W} \cong \mathfrak{S}_n \ltimes \{\pm 1\}^n$ and the graph

$$s_1 \text{ --- } s_2 \text{ --- } \dots \text{ --- } s_{n-1} = s_n \tag{1.6}$$

is the associated Coxeter graph. We have $-I_n \in \mathcal{W}$ and thus, $-\omega_i \in \mathcal{W}\,\omega_i$. Furthermore, the orbit $\mathcal{W}\,\omega_i$ has cardinality $2^i\binom{n}{i}$ for $1 \le i \le n$.

B_n

The root system B_n given in [Bou68, Planche II] is a root system in $\mathbb{R}^n$. Its Weyl group is isomorphic to that of C_n. The simple roots and fundamental weights are

$$\rho_i = e_i - e_{i+1}, \quad \rho_n = e_n \quad \text{and} \quad \omega_i = e_1 + \ldots + e_i, \quad \omega_n = (e_1 + \ldots + e_n)/2. \tag{1.7}$$

for $1 \le i \le n$. The Weyl group of B_n is $\cong \mathcal{W} \cong \mathfrak{S}_n \ltimes \{\pm 1\}^n$ and the graph

$$s_1 \text{ --- } s_2 \text{ --- } \dots \text{ --- } s_{n-1} = s_n \tag{1.8}$$

is the associated Coxeter graph. We have $-I_n \in \mathcal{W}$ and thus, $-\omega_i \in \mathcal{W}\,\omega_i$. Furthermore, the orbit $\mathcal{W}\,\omega_i$ has cardinality $2^i\binom{n}{i}$ for $1 \le i \le n$.

D_n

The groups $\mathfrak{S}_n$ and $\{\pm 1\}^n_+ := \{\epsilon \in \{\pm 1\}^n \,|\, \epsilon_1 \ldots \epsilon_n = 1\}$ act on $\mathbb{R}^n$ by permutation of coordinates and multiplication of coordinates by ± 1, where only an even amount of sign changes is admissible. The root system D_n given in [Bou68, Planche IV] is a root system in $\mathbb{R}^n$ with simple roots and fundamental weights

$$\begin{aligned} &\rho_i = e_i - e_{i+1}, \quad \rho_n = e_{n-1} + e_n \quad \text{and} \\ &\omega_i = e_1 + \ldots + e_i, \quad \omega_{n-1} = (e_1 + \ldots + e_{n-1} - e_n)/2, \quad \omega_n = (e_1 + \ldots + e_n)/2. \end{aligned} \tag{1.9}$$

The Weyl group of D_n is $\mathcal{W} \cong \mathfrak{S}_n \ltimes \{\pm 1\}^n_+$ and the graph

$$s_1 \text{ --- } s_2 \text{ --- } \dots \text{ --- } s_{n-2} \begin{cases} \text{ --- } s_{n-1} \\ \text{ --- } s_n \end{cases} \tag{1.10}$$

is the associated Coxeter graph. For all $1 \le i \le n$, we have $-\omega_i \in \mathcal{W}\,\omega_i$, except when n is odd, where $-\omega_{n-1} \in \mathcal{W}\,\omega_n$. Furthermore, the orbit $\mathcal{W}\,\omega_i$ has cardinality $2^i\binom{n}{i}$ for $1 \le i \le n-2$ and $|\mathcal{W}\,\omega_{n-1}| = |\mathcal{W}\,\omega_n| = 2^{n-1}$.

G_2

The group $\mathfrak{S}_3 \ltimes \{\pm 1\}$ acts on $\mathbb{R}^3$ by permutation of coordinates and scalar multiplication with ± 1. The subspace $V = \mathbb{R}^3/\langle [1,1,1]^t \rangle = \{u \in \mathbb{R}^n \,|\, u_1 + u_2 + u_3 = 0\}$ is left invariant. The root system G_2 given in [Bou68, Planche IX] is a root system of rank 2 in V with simple roots and fundamental weights

$$\rho_1 = [1,-1,0]^t, \quad \rho_2 = [-2,1,1]^t \quad \text{and} \quad \omega_1 = [1,-1,0]^t, \quad \omega_2 = [-2,1,1]^t. \tag{1.11}$$

The Weyl group of G_2 is $\mathcal{W} \cong \mathfrak{S}_3 \ltimes \{\pm 1\}$ and the graph

$$s_1 \equiv s_2 \tag{1.12}$$

is the associated Coxeter graph. We have $-I_3 \in \mathcal{W}$ and thus, $-\omega_1 \in \mathcal{W}\,\omega_1$ as well as $-\omega_2 \in \mathcal{W}\,\omega_2$. Furthermore, $|\mathcal{W}\,\omega_1| = |\mathcal{W}\,\omega_2| = 6$.

2 Multiplicative invariants

Multiplicative invariant theory studies group actions on lattices and the invariant elements in the associated group algebra. In this thesis, the group is the Weyl group of a root system and the lattice is the weight lattice. We recall essential facts and introduce a notation for multiplicative actions. A more general and detailed introduction is given in the book of Lorenz [Lor05]. The case of root lattices was studied in the PhD thesis of Hamm, see [Ham14].

Let V be an n–dimensional $\mathbb{R}$–vector space with an inner product $\langle \cdot, \cdot \rangle$ and $\Omega \subseteq V$ be a free $\mathbb{Z}$–module of rank n. The **group algebra** of Ω over $\mathbb{R}$ is the $\mathbb{R}$–vector space $\mathbb{R}[\Omega]$ of formal power sums

$$\sum_{\mu \in \Omega} c_\mu \, \mathfrak{e}^\mu,$$

where all but finitely many $c_\alpha \in \mathbb{R}$ are zero. The basis of $\mathbb{R}[\Omega]$ is thus indexed by Ω. Multiplication on $\mathbb{R}[\Omega]$ is defined through

$$\mathfrak{e}^{\mu_1}\, \mathfrak{e}^{\mu_2} = \mathfrak{e}^{\mu_1 + \mu_2}$$

with $\mu_1, \mu_2 \in \Omega$, where we use the notation from [Bou68, Chapitre VI, §3].

Assume that Ω is the weight lattice of a root system in V. Then the Weyl group $\mathcal{W}$ has a linear action on $\mathbb{R}[\Omega]$, given by monomial maps

$$\begin{array}{ccc} \mathcal{W} \times \mathbb{R}[\Omega] & \to & \mathbb{R}[\Omega], \\ (A, \mathfrak{e}^\mu) & \mapsto & \mathfrak{e}^{A\mu}. \end{array}$$

An element $f \in \mathbb{R}[\Omega]$ is called $\mathcal{W}$–**invariant**, if, for all $A \in \mathcal{W}$, A acts trivially on f. The ring of all $\mathcal{W}$–invariants is denoted by $\mathbb{R}[\Omega]^{\mathcal{W}}$. The above action is sometimes referred to as a **multiplicative** one, as the monomials $\mathfrak{e}^\mu$ form a multiplicative group.

2.1 Integer representations

Part of multiplicative invariant theory is to study the algebraic structure of the ring of invariants $\mathbb{R}[\Omega]^{\mathcal{W}}$ and to describe the orbit space through polynomial equations. Doing the latter is discussed in Chapter 2 for Weyl groups and weight lattices. We start by introducing a notation that helps us with computations over $\mathbb{R}[\Omega]$ and simultaneously combines algebraic geometry with multiplicative invariant theory.

For a fixed basis $\{\omega_1, \ldots, \omega_n\}$ of Ω, we have a $\mathbb{Z}$–module isomorphism

$$\begin{array}{rccl} W: & \mathbb{Z}^n & \to & \Omega = \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_n, \\ & [\alpha_1, \ldots, \alpha_n]^t & \mapsto & \alpha_1\,\omega_1 + \ldots + \alpha_n\,\omega_n. \end{array} \tag{1.13}$$

If $V = \mathbb{R}^n$, then $W \in \mathbb{R}^{n\times n}$ is the matrix with columns $\omega_1, \ldots, \omega_n$, see Figure 1.5. Since Ω is left invariant by $\mathcal{W}$, there exists a representation of $\mathcal{W}$ over $\mathbb{Z}$. Indeed, such a representation is given by

$$\begin{array}{rccl} \varrho: & \mathcal{W} & \rightarrow & \mathrm{GL}_n(\mathbb{Z}), \\ & A & \mapsto & W^{-1} A W. \end{array} \tag{1.14}$$

We write $\mathcal{G} := \varrho(\mathcal{W})$. From a computational point of view, it is more convenient to work over $\mathbb{Z}^n$ than over $\mathbb{R}^n$. Hence, we prefer to work with $\mathcal{G}$ instead of $\mathcal{W}$ and introduce the theory in the way it is implemented for the applications in Chapter 3 and Chapter 4.

Example 1.21. *Consider the group $\mathcal{W} = \langle A_1, A_2 \rangle$ with*

$$A_1 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \quad \textit{and} \quad A_2 = \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{bmatrix}.$$

$\mathcal{W} \cong \mathfrak{S}_3 \cong \mathfrak{D}_3$ is of order 6 and leaves the hexagonal lattice $\Omega := \mathbb{Z}\,\omega_1 \oplus \mathbb{Z}\,\omega_2 := \mathbb{Z}\left[\begin{smallmatrix} \sqrt{2}/2 \\ \sqrt{6}/6 \end{smallmatrix}\right] \oplus \mathbb{Z}\left[\begin{smallmatrix} 0 \\ \sqrt{6}/3 \end{smallmatrix}\right]$ invariant, see Figure 1.5. Here $\mathfrak{S}_3$ denotes the symmetric group and $\mathfrak{D}_3$ the dihedral group. Under the change of basis $W = [\omega_1, \omega_2] \in \mathbb{R}^{2\times 2}$, the generators of the integer representation $\mathcal{G}$ are

$$\begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix} \quad \textit{and} \quad \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}.$$

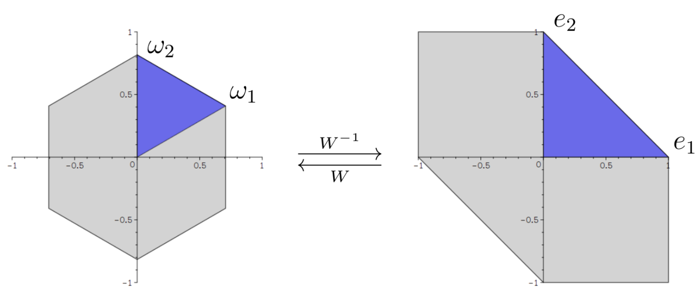


Figure 1.5: The matrix W is the change of basis from $\{e_1, \ldots, e_n\}$ to $\{\omega_1, \ldots, \omega_n\}$.

2.2 Invariant and anti–invariant Laurent polynomials

Let $n \in \mathbb{N}$ and denote by $(\mathbb{C}^*)^n := (\mathbb{C} \setminus \{0\})^n$ the algebraic n–torus. For $x = (x_1, \ldots, x_n) \in (\mathbb{C}^*)^n$ and a column vector $\alpha = [\alpha_1, \ldots, \alpha_n]^t \in \mathbb{Z}^n$, define $x^\alpha := x_1^{\alpha_1} \ldots x_n^{\alpha_n} \in \mathbb{C}^*$. A finite integer matrix group $\mathcal{G} \subseteq \mathrm{GL}_n(\mathbb{Z})$ has a nonlinear action

$$\begin{array}{rccl} \star: & \mathcal{G} \times (\mathbb{C}^*)^n & \rightarrow & (\mathbb{C}^*)^n, \\ & (B,\, x) & \mapsto & B \star x := (x_1, \ldots, x_n)^{B^{-1}} = (x^{B_{\cdot 1}^{-1}}, \ldots, x^{B_{\cdot n}^{-1}}), \end{array} \tag{1.15}$$

where $B_{\cdot i}^{-1} \in \mathbb{Z}^n$ denotes the i–th column vector of $B^{-1} \in \mathcal{G}$.
The coordinate ring of $(\mathbb{C}^*)^n$ with coefficients in $\mathbb{R}$ is $\mathbb{R}[x^\pm] := \mathbb{R}[x_1, x_1^{-1}, \ldots, x_n, x_n^{-1}]$, the ring of multivariate Laurent polynomials. The monomials of $\mathbb{R}[x^\pm]$ are the terms $x^\alpha = x_1^{\alpha_1} \ldots x_n^{\alpha_n}$ for $\alpha \in \mathbb{Z}^n$. $\star$ induces a linear action, given by monomial maps

$$\begin{array}{rccl} \cdot: & \mathcal{G} \times \mathbb{R}[x^\pm] & \rightarrow & \mathbb{R}[x^\pm], \\ & (B,\, x^\alpha) & \mapsto & B \cdot x^\alpha := x^{B\alpha} \end{array} \tag{1.16}$$

on $\mathbb{R}[x^\pm]$. Hence, for $f = \sum_\alpha f_\alpha\, x^\alpha \in \mathbb{R}[x^\pm]$ and $B \in \mathcal{G}$, we write

$$B \cdot f := f(x^B) = \sum_\alpha f_\alpha\, x^{B\alpha}.$$

If $B \cdot f = f$ for all $B \in \mathcal{G}$, then f is called $\mathcal{G}$–**invariant**. The set of all $\mathcal{G}$–invariant Laurent polynomials is denoted by $\mathbb{R}[x^\pm]^\mathcal{G}$.

Remark 1.22. *If $\mathcal{G}$ is the integer representation of a group $\mathcal{W}$ as in Equation (1.14) and Ω a $\mathcal{W}$–lattice, then $\mathbb{R}[x^\pm]^\mathcal{G} \cong \mathbb{R}[\Omega]^\mathcal{W}$ as algebras.*

Proposition 1.23. [Lor05, Corollary 3.3.2] *$\mathbb{R}[x^\pm]^\mathcal{G}$ is a finitely generated $\mathbb{R}$–algebra.*

Definition 1.24. *Assume that $\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\theta_1, \ldots, \theta_m]$ for some $m \in \mathbb{N}$ and $\theta_1, \ldots, \theta_m \in \mathbb{R}[x^\pm]^\mathcal{G}$, not necessarily algebraically independent.*

1. *The generators $\theta_1, \ldots, \theta_m$ are called* ***fundamental invariants*** *of $\mathcal{G}$.*
2. *For $\alpha \in \mathbb{Z}^n$, we call*

$$\Theta_\alpha(x) := \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} x^{B\alpha} \in \mathbb{R}[x^\pm]^\mathcal{G}$$

   the ***invariant orbit polynomial*** *associated to α.*

A basis for $\mathbb{R}[x^\pm]^\mathcal{G}$ as a $\mathbb{R}$–vector space is given by $\{\Theta_\alpha \,|\, \alpha \in \mathbb{N}^n\}$ [Lor05, Equation (3.4)]. The following statement admits a recurrence formula to compute orbit polynomials.

Proposition 1.25. *Let $\alpha, \beta \in \mathbb{N}^n$. We have $\Theta_0 = 1$ and*

$$|\mathcal{G}|\, \Theta_\alpha\, \Theta_\beta = \sum_{B \in \mathcal{G}} \Theta_{\alpha + B\beta}.$$

If $B \cdot f = \mathrm{Det}(B)\, f$ for all $B \in \mathcal{G}$, then f is called $\mathcal{G}$–**anti–invariant**.

Definition 1.26. *For $\alpha \in \mathbb{N}^n$ we call*

$$\Upsilon_\alpha(x) := \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} \mathrm{Det}(B)\, x^{B\alpha} \in \mathbb{R}[x^\pm]$$

the ***anti–invariant orbit polynomial*** *associated to α.*

Proposition 1.27. *Let $\alpha, \beta \in \mathbb{N}^n$. We have $\Upsilon_0 = 1$ and*

$$|\mathcal{G}|\, \Upsilon_\alpha\, \Theta_\beta = \sum_{B \in \mathcal{G}} \Upsilon_{\alpha + B\beta}.$$

2.3 Weyl's character formula and fundamental invariants

For the Weyl group of a rank n root system, let $\mathcal{G} \subseteq \mathrm{GL}_n(\mathbb{Z})$ be the integer representation given by Equation (1.14). The following theorem, which is known as the character formula of Hermann Weyl (1885–1955), states that the $\mathcal{G}$–anti–invariant Laurent polynomials form a free $\mathbb{R}[x^\pm]^\mathcal{G}$–module of rank 1.

Theorem 1.28. [Bou75, Chapitre VIII, §9, Théorème 1] *Let $\alpha \in \mathbb{N}^n$ and set $\delta := [1, \ldots, 1]^t \in \mathbb{N}^n$. Then there exists a unique $\Xi_\alpha \in \mathbb{R}[x^\pm]^\mathcal{G}$, such that*

$$\Xi_\alpha(x)\, \Upsilon_\delta(x) = \Upsilon_{\alpha+\delta}(x).$$

In the context of a semi–simple complex Lie algebra $\mathfrak{g}$, $W\alpha \in \Omega$ is a highest weight and Weyl's character formula allows to compute the character of the irreducible representation of $\mathfrak{g}$ associated to $W\alpha$, see Appendix A and the example following [Bou75, Chapitre VIII, §9, Théorème 1].

Definition 1.29. *Let $\alpha \in \mathbb{N}^n$ and set $\delta := [1, \ldots, 1]^t \in \mathbb{N}^n$. We call $\Xi_\alpha \in \mathbb{R}[x^\pm]^\mathcal{G}$ the* ***character polynomial*** *associated to α and Υ_δ the* ***Weyl denominator****.*

As mentioned above, the ring of invariants is a finitely generated algebra. Given $f \in \mathbb{R}[x^\pm]^\mathcal{G}$, we can write it as a polynomial in the fundamental invariants $\theta_1, \ldots, \theta_m$. However, those may have algebraic dependencies, that is, there exists $0 \neq g \in \mathbb{R}[z_1, \ldots, z_m]$, such that $g(\theta_1, \ldots, \theta_m) = 0$. Such a g is called a **syzygy** and the set of all syzygies forms an ideal, called the syzygy ideal. In the case of Weyl groups, this ideal is trivial.

Theorem 1.30. [Bou68, Chapitre VI, §3, Théorème 1] *Let R be a root system. Assume that $\mathcal{W}$ is the Weyl group with integer representation $\mathcal{G}$ given by Equation (1.14). Then*

1. *$\Theta_{e_1}, \ldots, \Theta_{e_n}$ are algebraically independent over $\mathbb{R}$,*
2. *$\Xi_{e_1}, \ldots, \Xi_{e_n}$ are algebraically independent over $\mathbb{R}$ and*
3. *$\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\Theta_{e_1}, \ldots, \Theta_{e_n}] = \mathbb{R}[\Xi_{e_1}, \ldots, \Xi_{e_n}]$ is a polynomial algebra.*

It is precisely this important result in combination with the following remark, which makes Weyl groups relevant for the topic of this thesis, namely the optimization of trigonometric polynomials.

Remark 1.31. [Far86] *The converse*

$$\mathbb{R}[x^\pm]^\mathcal{G} \text{ is a polynomial algebra} \quad \Rightarrow \quad \mathcal{W} \text{ is a Weyl group}$$

of Theorem 1.30 holds true.

3 Generalized Chebyshev polynomials

The polynomials introduced in this section are named after Pafnuty Lvovich Chebyshev (1821–1894). In the Roman alphabet, other spellings are also common and depend on the language, such as Tchebychev (French) or Tschebyschow (German).

The **Chebyshev polynomial of the first kind** associated to $\ell \in \mathbb{N}$ is the unique univariate polynomial T_ℓ satisfying

$$T_\ell(\cos(2\pi\, u)) = \cos(2\pi\, \ell\, u)$$

with $u \in \mathbb{R}$. We understand this definition in the context of the previous section, that is, in the context of multiplicative group actions. We write $2\cos(2\pi\, u) = x + x^{-1}$, where $x := \exp(-2\pi\, \mathrm{i}\, u)$. Then the Weyl group $\{\pm 1\}$ of the A_1 root system acts multiplicatively on $\mathbb{R}[x^\pm]$ and the ring of invariants is

$$\mathbb{R}[x^\pm]^{\{\pm 1\}} = \mathbb{R}\left[\frac{x + x^{-1}}{2}\right].$$

Thus,

$$T_\ell\left(\frac{x + x^{-1}}{2}\right) = \frac{x^\ell + x^{-\ell}}{2}.$$

Analogously, the **Chebyshev polynomial of the second kind** associated to $\ell \in \mathbb{N}$ is the unique univariate polynomial U_ℓ satisfying

$$U_\ell(\cos(2\pi\, u)) = \frac{\sin(2\pi\,(\ell+1)\, u)}{\sin(2\pi\, u)} \quad \text{or} \quad U_\ell\left(\frac{x + x^{-1}}{2}\right) = \frac{x^{\ell+1} - x^{-\ell-1}}{x - x^{-1}}.$$

3.1 Generalization with Weyl groups

Let R be a root system with Weyl group $\mathcal{W}$. Denote the integer representation of $\mathcal{W}$ by $\mathcal{G}$ as in Equation (1.14). For $1 \leq i \leq n$, denote the orbit polynomial associated to e_i by $\theta_i := \Theta_{e_i}$. According to Theorem 1.30, the ring of invariants is the polynomial algebra $\mathbb{R}[x^{\pm}]^{\mathcal{G}} = \mathbb{R}[\theta_1, \ldots, \theta_n]$. The polynomial ring in n indeterminates is $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_n]$.

Definition 1.32. *The **generalized Chebyshev polynomials of the first kind** associated to $\alpha \in \mathbb{N}^n$ is the unique $T_\alpha \in \mathbb{R}[z]$ satisfying $T_\alpha(\theta_1, \ldots, \theta_n) = \Theta_\alpha$.*

For $\alpha \in \mathbb{Z}^n$, we write α' for the unique element of $\mathbb{N}^n$ with $\alpha' \in \mathcal{G}\alpha$. Then we immediately obtain a recurrence formula for this family of polynomials.

Corollary 1.33. [of Proposition 1.25] *Let $\alpha, \beta \in \mathbb{N}^n$. We have $T_0 = 1$, $T_{e_i} = z_i$ and*

$$|\mathcal{G}|\, T_\alpha\, T_\beta = \sum_{B \in \mathcal{G}} T_{(\alpha + B\beta)'}.$$

Throughout the literature, this definition is one of the most common. When it comes to the other kinds, generalizations differ. The most frequent one for the second kind is the following, see for example [LX10, MP11, MKNR12, CHHM16, HS21].

Definition 1.34. *The **generalized Chebyshev polynomials of the second kind** associated to $\alpha \in \mathbb{N}^n$ is the unique $U_\alpha \in \mathbb{R}[z]$ satisfying $U_\alpha(\theta_1, \ldots, \theta_n) = \Xi_\alpha$.*

Corollary 1.35. [of Proposition 1.27 and Theorem 1.28] *Let $\alpha, \beta \in \mathbb{N}^n$. We have $U_0 = 1$ and*

$$|\mathcal{G}|\, U_\alpha\, T_\beta = \sum_{B \in \mathcal{G}} U_{(\alpha + B\beta)'}.$$

Recall that the choice of a base for a root system defines a partial ordering. On $\mathbb{Z}^n$, we can therefore define

$$\beta \preceq \alpha \Leftrightarrow W(\alpha - \beta) \text{is a sum of positive roots.}$$

A useful consequence of the theorem of the highest weights Theorem A.11 is the following property for generalized Chebyshev polynomials of the first and second kind.

Proposition 1.36. [HS21, Proposition 2.23] *Let $\alpha \in \mathbb{N}^n$. For $\beta \in \mathbb{N}^n$ with $\beta \preceq \alpha$, there exists $t_\beta, u_\beta \in \mathbb{R}$, such that $t_\alpha \neq 0 \neq u_\alpha$ and*

$$T_\alpha(z) = \sum_{\beta \preceq \alpha} t_\beta\, z^\beta, \quad U_\alpha(z) = \sum_{\beta \preceq \alpha} u_\beta\, z^\beta.$$

Example 1.37. *The generalized Chebyshev polynomials of the first kind associated to* A_2 *are*

$$T_{02} = 3\, z_2^2 - 2\, z_1,\, T_{11} = 3/2\, z_1\, z_2 - 1/2,\, T_{20} = 3\, z_1^2 - 2\, z_2,\, T_{03} = 9\, z_2^3 - 9\, z_1\, z_2 + 1,$$
$$T_{12} = 9/2\, z_1\, z_2^2 - 3\, z_1^2 - 1/2\, z_2,\, T_{21} = -3\, z_2^2 - 1/2\, z_1 + 9/2\, z_1^2\, z_2,\, T_{30} = 9\, z_1^3 - 9\, z_1\, z_2 + 1,\, \ldots$$

The generalized Chebyshev polynomials of the first kind associated to B_2 *are*

$$T_{02} = 4\, z_2^2 - 2\, z_1 - 1,\, T_{11} = 2\, z_1\, z_2 - z_2,\, T_{20} = 4\, z_1^2 - 8\, z_2^2 + 4\, z_1 + 1,\, T_{03} = 16\, z_2^3 - 12\, z_1\, z_2 - 3\, z_2,$$
$$T_{12} = 8\, z_1\, z_2^2 - 4\, z_1^2 - 3\, z_1,\, T_{21} = 8\, z_1^2\, z_2 - 16\, z_2^3 + 6\, z_1\, z_2 + 3\, z_2,\, T_{30} = 16\, z_1^3 - 48\, z_1\, z_2^2 + 24\, z_1^2 + 9\, z_1,\, \ldots$$

The generalized Chebyshev polynomials of the second kind associated to A_2 *are*

$$U_{01} = 3\, z_2,\, U_{10} = 3\, z_1,\, U_{02} = 9\, z_2^2 - 3\, z_1,\, U_{11} = 9\, z_1\, z_2 - 1,\, U_{20} = 9\, z_1^2 - 3\, z_2,$$
$$U_{03} = 27\, z_2^3 - 18\, z_1\, z_2 + 1,\, U_{12} = 27\, z_1\, z_2^2 - 9\, z_1^2 - 3\, z_2$$
$$U_{21} = 27\, z_1^2\, z_2 - 9\, z_2^2 - 3\, z_1,\, U_{30} = 27\, z_1^3 - 18\, z_1\, z_2 + 1,\, \ldots$$

The generalized Chebyshev polynomials of the second kind associated to B_2 *are*

$$U_{01} = 4\,z_2,\, U_{10} = 4\,z_1 + 1,\, U_{02} = 16\,z_2^2 - 4\,z_1 - 2,\, U_{11} = 16\,z_2\,z_1,\, U_{20} = 16\,z_1^2 - 16\,z_2^2 + 12\,z_1 + 2,$$
$$U_{03} = 64\,z_2^3 - 32\,z_1\,z_2 - 12\,z_2,\, U_{12} = 64\,z_1\,z_2^2 - 16\,z_1^2 - 12\,z_1 - 1$$
$$U_{21} = 64\,z_1^2\,z_2 - 64\,z_2^3 + 32\,z_1\,z_2 + 8\,z_2,\, U_{30} = 64\,z_1^3 - 128\,z_1\,z_2^2 + 80\,z_1^2 - 16\,z_2^2 + 28\,z_1 + 2,\, \ldots$$

Each of the two introduced families of generalized Chebyshev polynomials forms a basis of $\mathbb{R}[z]$. We mainly work with the generalized Chebyshev polynomials of the first kind. Hence, we omit the notions "generalized" and "of the first kind" unless needed.

3.2 Weighted degrees

The classical notion of degree can be misleading for Chebyshev polynomials.

Example 1.38. *Consider the root system* B_3*. With the recurrence formula, one finds*

$$T_{010}^2 = (2\,T_{200} + 4\,T_{102} + T_{020} + 4\,T_{010} + T_{000})/12$$

and obtains recursively

$$T_{020} = -64\,z_1\,z_3^2 + 12\,z_1^2 + 24\,z_1\,z_2 + 12\,z_2^2 + 8\,z_1 + 8\,z_2 + 1.$$

We observe that $T_{102} = t_{102}\,z^{[1,0,2]^t} + \ldots$ *appears as a term, although we started with* $T_{010}^2 = z_2^2$*, which has degree* $|2\,[0,1,0]^t| = 2$*.*

The problem lies in Proposition 1.36, where $\beta \preceq \alpha$ does not necessarily correspond to $|\beta| \leq |\alpha|$. Hence, the degree of the product $T_\alpha\,T_\beta$ is not necessarily that of $T_{\alpha+\beta}$. We give a more suitable notion of degree.

Assume that R is an irreducible root system with highest root ρ_0 with respect to a fixed base. We denote its coroot by $\rho_0^\vee := (\rho_0)^\vee = 2\,\rho_0/\langle \rho_0, \rho_0\rangle$. This is an element of the coroot lattice Λ, which is the dual of Ω. The change of basis from $\mathbb{Z}^n$ to the weight lattice Ω shall be given by the matrix of fundamental weights $W = [\omega_1| \ldots |\omega_n]$.

Definition 1.39. *Let* $0 \neq f(z) = \sum_\alpha c_\alpha\,T_\alpha(z) \in \mathbb{R}[z]$ *be an arbitrary polynomial with coefficients* $c_\alpha \in \mathbb{R}$ *in the Chebyshev basis. The* ***weighted degree*** *of* f *is*

$$\deg_W(f) := \max\{\langle W\alpha,\, \rho_0^\vee\rangle \,|\, c_\alpha \neq 0\} \in \mathbb{N}.$$

In Example 1.38 we have $\deg(T_{010}) = \deg(z_2) = 1$, but $\deg_W(T_{010}) = \langle W[0,1,0]^t,\, \rho_0^\vee\rangle = \langle \omega_2,\, \rho_0^\vee\rangle = \langle [1,1,0]^t,\, [1,1,0]^t\rangle = 2$.

We show that this is a reasonable definition.

Proposition 1.40. *For* $d \in \mathbb{N}$*, define the finite dimensional* $\mathbb{R}$*–vector subspace*

$$\mathcal{F}_d := \bigoplus_{\ell=0}^{d} \langle \{T_\alpha \,|\, \alpha \in \mathbb{N}^n,\, \deg_W(T_\alpha) = \ell\}\rangle_{\mathbb{R}}$$

of $\mathbb{R}[z]$*. Then* $(\mathcal{F}_d)_{d\in\mathbb{N}}$ *is a filtration of* $\mathbb{R}[z]$ *as an* $\mathbb{R}$*–algebra, that is,*

1. $\mathbb{R}[z] = \bigcup\limits_{d\in\mathbb{N}} \mathcal{F}_d$ *and*

2. *if* $d_1, d_2 \in \mathbb{N}$*, then* $\mathcal{F}_{d_1}\,\mathcal{F}_{d_2} \subseteq \mathcal{F}_{d_1+d_2}$*.*

Proof. *1.* Let $p = \sum_\alpha c_\alpha \, T_\alpha \in \mathbb{R}[z]$. Choose $d \in \mathbb{N}$, such that $d \geq \langle W\alpha, \rho_0^\vee \rangle$ for all $c_\alpha \neq 0$. Then $p \in \mathcal{F}_d$.
2. Let $T_\alpha \in \mathcal{F}_{d_1}$ and $T_\beta \in \mathcal{F}_{d_2}$. Then $|\mathcal{G}| \, T_\alpha \, T_\beta = \sum_B T_{\alpha+B\beta}$. For all $B \in \mathcal{G}$, there exists $A \in \mathcal{G}$, such that $A(\alpha + B\beta) \in \mathbb{N}^n$. By Proposition 1.9, $W(\alpha - A\alpha)$ and $W(\beta - AB\beta)$ are sums of positive roots. Hence, there exists $\gamma \in \mathbb{N}^n$, such that

$$\langle W A(\alpha + B\beta), \rho_0^\vee \rangle = \langle W(\alpha + \beta), \rho_0^\vee \rangle - \sum_{i=1}^{n} \gamma_i \langle \rho_i, \rho_0^\vee \rangle.$$

By [Bou68, Chapitre VI, §1.8, Proposition 25], $\rho_0^\vee \in \overline{\Lambda}$ and thus $\langle \rho_i, \rho_0^\vee \rangle \geq 0$. We obtain

$$\langle W A(\alpha + AB\beta, \rho_0^\vee \rangle \leq \langle W(\alpha + \beta), \rho_0^\vee \rangle \leq d_1 + d_2.$$

Therefore, $T_\alpha \, T_\beta \in \mathcal{F}_{d_1+d_2}$. □

Hence, for an arbitrary $0 \neq f \in \mathbb{R}[z]$, we can write the weighted degree of f as

$$\deg_W(f) = \min\{d \in \mathbb{N} \,|\, f \in \mathcal{F}_d\}.$$

Furthermore, in Example 1.38 we have $\deg(T_{020}) = 3 \neq 2 = \deg(T_{010}^2)$, but $\deg_W(T_{020}) = 4 = \deg_W(T_{010}^2)$. Hence, this new notion of degree is more intuitive. This will be of relevance in Chapter 3. For now, we conclude with the following useful property.

Proposition 1.41. *For $\alpha \in \mathbb{N}^n$, there exists a unique $\widehat{\alpha} \in \mathbb{N}^n$ with $-\alpha \in \mathcal{G}\widehat{\alpha}$. In this case, we have $\deg_W(T_\alpha) = \deg_W(T_{\widehat{\alpha}})$.*

Proof. Let B be the base of R, which admits fundamental weights ω_i, change of basis W and Weyl chamber C. Assume that $A \in \mathcal{W}$ is the Weyl group element taking $-C$ to C. Such an element exists, because $\mathcal{W}$ acts simply–transitively on the chambers of R, see Proposition 1.7. In particular, $-C$ is the Weyl chamber for the base $-$B and A takes $-$B to B. Fix $\widehat{\alpha} := -W^{-1} \, A \, W \, \alpha$. Since the inner product is $\mathcal{W}$–invariant, we have

$$\ell = \langle W\alpha, \rho_0^\vee \rangle = \langle A \, W\alpha, A\rho_0^\vee \rangle = \langle -W\widehat{\alpha}, -\rho_0^\vee \rangle = \langle W\widehat{\alpha}, \rho_0^\vee \rangle.$$

Furthermore, $-W\widehat{\alpha} = A \, W\alpha$ is a dominant weight with respect to $-$B. Thus, $W\widehat{\alpha}$ is dominant with respect to B and so we finally have $\widehat{\alpha} \in \mathbb{N}^n$. □

3.3 Examples of recurrences

As a more general application of the recurrence formula, we give two examples, which are needed later on.

Lemma 1.42. *Let* R *be a root system of type* B_n. *Then*

$$T_{2\,e_n} \,=\, 2^n \, z_n^2 - \sum_{j=1}^{n-1} \binom{n}{j} \, z_j - 1.$$

Proof. We use the recurrence formula and the representation of the B_n root system over $\mathbb{R}^n$ from Equation (1.7). The cardinality of the orbit $\mathcal{G}\, e_n$ is 2^n. Let $\alpha \in \mathcal{G}\, e_n$ and distinguish between the following cases.

1. If $\alpha = e_n$, then $T_{e_n+\alpha} = T_{2\,e_n}$ is the term on the left–hand side of the statement, for which we search an explicit formula.

2. If $\alpha = -e_n$, then $T_{e_n+\alpha} = T_0 = 1$.

3. Denote by W the matrix with columns $\omega_1, \dots, \omega_n$. For any other $\alpha \in \mathcal{G}\, e_n$, there exists $1 \leq j \leq n-1$, such that $\mu := W\alpha \in \mathcal{W}\omega_n \subseteq \mathbb{R}^n$ contains exactly j positive coordinates. Therefore, $\mu + \omega_n$ has exactly j nonzero entries and is contained in the orbit of ω_j under $\mathcal{W}$. The number of μ, for which this is the case, is $\binom{n}{j}$.

We conclude

$$2^n\, z_n^2 = |\mathcal{G}|\, T_{e_n}\, T_{e_n} = \sum_{\alpha \in \mathcal{G}\, e_n} T_{\alpha + e_n} = T_{2\, e_n} + \sum_{j=1}^{n-1} \binom{n}{j} T_{e_j} + 1 = T_{2\, e_n} + \sum_{j=1}^{n-1} \binom{n}{j} z_j + 1$$

and obtain the formula for $T_{2\, e_n}$. □

Lemma 1.43. *Let* R *be a root system of type* D_n. *The following statements hold.*

1. If n is even, then

$$\begin{aligned} T_{e_{n-1}+e_n} &= \frac{2^{n-1}}{n}\, z_{n-1}\, z_n - \frac{1}{n} \sum_{j=1}^{(n-2)/2} \binom{n}{2j-1} z_{2j-1}, \\ T_{2\, e_{n-1}} &= 2^{n-1}\, z_{n-1}^2 - \sum_{j=1}^{(n-2)/2} \binom{n}{2j} z_{2j} - 1 \quad \textit{and} \\ T_{2\, e_n} &= 2^{n-1}\, z_n^2 - \sum_{j=1}^{(n-2)/2} \binom{n}{2j} z_{2j} - 1. \end{aligned}$$

2. If n is odd, then

$$\begin{aligned} T_{e_{n-1}+e_n} &= \frac{2^{n-1}}{n}\, z_{n-1}\, z_n - \frac{1}{n} \sum_{j=1}^{(n-3)/2} \binom{n}{2j} z_{2j} - \frac{1}{n}, \\ T_{2\, e_{n-1}} &= 2^{n-1}\, z_{n-1}^2 - \sum_{j=0}^{(n-3)/2} \binom{n}{2j+1} z_{2j+1} \quad \textit{and} \\ T_{2\, e_n} &= 2^{n-1}\, z_n^2 - \sum_{j=0}^{(n-3)/2} \binom{n}{2j+1} z_{2j+1}. \end{aligned}$$

Proof. Again, we use the recurrence formula and the representation of the D_n root system from Equation (1.9). We have $|\mathcal{G}\, e_{n-1}| = |\mathcal{G}\, e_n| = 2^{n-1}$ and the statement can be obtained from the following combinatorial steps.

1. Assume that n is even. We first prove the equation for $T_{2\, e_n}$ in detail. Let $\alpha \in \mathcal{G}e_n$ and denote by W the matrix with columns $\omega_1, \dots, \omega_n$. Then $\mu := W\alpha \in \mathcal{W}\omega_n$ has $2j$ positive coordinates for some $0 \leq j \leq n/2$. There are precisely $\binom{n}{2j}$ such elements in $\mathcal{W}\,\omega_n$ and an odd amount of positive coordinates is not possible. We distinguish three cases. If $j = 0$, then $\omega_{n-1} + \mu = 0$, and if $j = n/2$, then $\omega_n + \mu = 2\,\omega_n$. Otherwise, $\omega_n + \mu$ has $2j$ nonzero coordinates and must therefore be contained in $\mathcal{W}\,\omega_{2j}$. All in all, we obtain

$$2^{n-1}\, z_n^2 = \sum_{\alpha \in \mathcal{G}\, e_n} T_{e_n + \alpha} = T_{2\, e_n} + \sum_{j=1}^{(n-2)/2} \binom{n}{2j} z_{2j} + 1.$$

Next, let $\alpha \in \mathcal{G}e_{n-1}$. Then $\mu := W\alpha \in \mathcal{W}\omega_{n-1}$ has $2j-1$ positive coordinates for some $1 \le j \le n/2$. We have

$$\omega_{n-1}+\mu \begin{cases} = 0, & \text{if} \quad j=1,\ \mu_n = \dfrac{1}{2} \\ = 2\omega_{n-1}, & \text{if} \quad j=\dfrac{n}{2},\ \mu_n = -\dfrac{1}{2} \\ \in \mathcal{W}\,\omega_{2j}, & \text{otherwise} \end{cases} \quad \text{and} \quad \omega_n+\mu \begin{cases} \in \mathcal{W}\,(\omega_n+\omega_{n-1}), & \text{if} \quad j=\dfrac{n}{2} \\ \in \mathcal{W}\,\omega_{2j-1}, & \text{otherwise} \end{cases}.$$

After counting the number of possibilities in each case, we obtain the two equations

$$2^{n-1}\,z_{n-1}^2 = 1 + T_{2\omega_{n-1}} + \sum_{j=1}^{(n-2)/2} \binom{n}{2j} z_{2j} \quad \text{and} \quad 2^{n-1}\,z_{n-1}\,z_n = n\,T_{e_n+e_{n-1}} + \sum_{j=1}^{(n-2)/2} \binom{n}{2j-1} z_{2j-1}.$$

2. Now assume that n is odd. The arguments are similar to the even case. For $1 \le j \le (n+1)/2$, consider $\mu \in \mathcal{W}\omega_n$ with $2j-1$ positive coordinates. If $j=(n+1)/2$, then $\omega_n+\mu = 2\omega_n$. Otherwise, $\omega_n+\mu$ has $2j-1$ nonzero coordinates. Then $T_{2\,e_n}$ is obtained from

$$2^{n-1}\,z_n^2 = T_{2\,e_n} + \sum_{j=1}^{(n-1)/2} \binom{n}{2j-1} z_{2j-1}.$$

Finally, for $0 \le j \le (n-1)/2$, consider $\mu \in \mathcal{W}\,\omega_{n-1}$ with $2j$ positive coordinates. Then

$$\omega_{n-1}+\mu \begin{cases} = 2\omega_{n-1}, & \text{if} \quad j=\dfrac{n-1}{2},\ \mu_n = -\dfrac{1}{2} \\ \in \mathcal{W}\,\omega_{2j+1}, & \text{otherwise} \end{cases} \quad \text{and} \quad \omega_n+\mu \begin{cases} = 0, & \text{if} \quad j=0 \\ \in \mathcal{W}\,(\omega_n+\omega_{n-1}), & \text{if} \quad j=\dfrac{n-1}{2} \\ \in \mathcal{W}\,\omega_{2j}, & \text{otherwise} \end{cases}.$$

After counting the number of possibilities in each case, we obtain the two equations

$$2^{n-1}\,z_{n-1}^2 = T_{2\,e_{n-1}} + \sum_{j=0}^{(n-3)/2} \binom{n}{2j+1} z_{2j+1} \quad \text{and} \quad 2^{n-1}\,z_{n-1}\,z_n = 1 + n\,T_{e_n+e_{n-1}} + \sum_{j=1}^{(n-3)/2} \binom{n}{2j} z_{2j}.$$

This completes the proof. □

Chapter 2

$\mathbb{T}$–orbit spaces of multiplicative actions

The Weyl group of a crystallographic root system has a nonlinear action on the algebraic torus. This induces a linear action on the ring of Laurent polynomials. Given a set of fundamental invariants, we study the image of the compact torus, which is left invariant under the Weyl group. This set is called the $\mathbb{T}$–orbit space. In this chapter, we characterize the image as a basic semi–algebraic set and give its explicit polynomial description for the Weyl groups associated to irreducible root systems of type A, B, C, D and G. The formula is first given as a Hermite quadratic form in the standard monomial basis via solutions of symmetric polynomial systems. We then obtain a formula in the basis of generalized Chebyshev polynomials and give several examples.

The results are based on joint work with Evelyne Hubert (Inria) and Cordian Riener (Tromsø) [HMR22].

Public availability:
https://hal.archives-ouvertes.fr/hal-03590007v2

1 Orbit spaces

The goal of this chapter is to characterize the image of the compact torus under the fundamental invariants from Theorem 1.30. This will help us in optimizing invariant trigonometric polynomials later in Chapter 3. Recall the identity

$$\mathbb{R}[x^{\pm}]^{\mathcal{G}} = \mathbb{R}[\theta_1, \ldots, \theta_n],$$

where $\mathcal{G}$ will be the integer representation of a Weyl group and the θ_i algebraically independent orbit or character polynomials.

The image of fundamental invariants is usually called an orbit space, because it separates orbits, that is, it contains exactly one representative per orbit. Historically, characterizations were for example given for the action of the symmetric group on the classical multivariate polynomial ring in [Pro78]. Later, a characterization for any compact Lie group with a real linear representation was proven in [PS85, Main Theorem]. Polynomial descriptions for orbit spaces are used in several domains such as equivariant dynamical systems [Gat00], symmetry exploitation in optimization [GP04, ALRT13, HMMR22], complex analysis [Sja93] and quantum systems [Dub98, GKP13].

We shall now establish the concept of orbit spaces for our kind of group action and subsequently show that, for certain Weyl groups, the image of fundamental invariants is semi–algebraic. We do this by giving an explicit and closed formula, which is new and obtained independently from [PS85, §4].

1.1 $\mathbb{T}$–orbit spaces of nonlinear actions

Let $\mathcal{G} \subseteq \mathrm{GL}_n(\mathbb{Z})$ be a finite group. Recall from Equation (1.15) that $\mathcal{G}$ has a nonlinear action

$$\begin{array}{rccl} \star: & \mathcal{G} \times (\mathbb{C}^*)^n & \to & (\mathbb{C}^*)^n, \\ & (B,\, x) & \mapsto & B \star x := (x_1, \ldots, x_n)^{B^{-1}} = (x^{B^{-1}_{\cdot 1}}, \ldots, x^{B^{-1}_{\cdot n}}), \end{array}$$

on the algebraic torus, which induces the multiplicative action

$$\begin{array}{rccl} \cdot: & \mathcal{G} \times \mathbb{R}[x^{\pm}] & \to & \mathbb{R}[x^{\pm}], \\ & (B,\, x^{\alpha}) & \mapsto & B \cdot x^{\alpha} := x^{B\alpha} \end{array}$$

on the ring of Laurent polynomials $\mathbb{R}[x^{\pm}]$, see Equation (1.16).

Define $\mathbb{T} := \{x \in \mathbb{C} \,|\, x\,\overline{x} = 1\} \subseteq \mathbb{C}^*$, where $\overline{x}$ is the complex conjugate. Note that complex conjugation on $\mathbb{T}$ is equivalent to inversion. We write $\mathbb{T}^n$ for the **compact** n**–torus**.

Remark 2.1. *$\mathbb{T}^n$ is left invariant by the action $\star$, that is, $\mathcal{G} \star \mathbb{T}^n = \mathbb{T}^n$. Furthermore, if $f \in \mathbb{R}[x^{\pm}]$ satisfies $(-I_n) \cdot f = f$, then f is real–valued on $\mathbb{T}^n$.*

Given fundamental invariants, we can define a canonical mapping of orbits. Let us first consider the univariate case.

Lemma 2.2. *The map*

$$\begin{array}{ccc} \mathbb{C}^* & \to & \mathbb{C}, \\ x & \mapsto & (x + x^{-1}) \end{array}$$

is surjective and the preimage of $[-2, 2]$ is $\mathbb{T}$.

Proof. For $r \in \mathbb{C}$, consider the univariate polynomial $p := x^2 - r\,x + 1 \in \mathbb{C}[x]$. Then 0 is not a root of p and $p(x) = 0$ if and only if $r = x + x^{-1}$, that is, r is in the image of the map. Hence, we have proven the property surjective.

If $r \in [-2, 2]$, then $p \in \mathbb{R}[x]$ has discriminant $(r/2)^2 - 1 \leq 0$ and its two roots are $x, \overline{x} = x, x^{-1} = r/2 \pm \mathrm{i}\sqrt{1 - (r/2)^2} \in \mathbb{T}$. On the other hand, for $x \in \mathbb{T}$, we have $x + x^{-1} = x + \overline{x} = 2\,\Re(x) \in [-2, 2]$. □

In the previous lemma, $x + x^{-1}$ is the fundamental invariant for the multiplicative action of $\{\pm 1\}$ on the univariate Laurent polynomial ring. As we have just proven, the image of $\mathbb{C}^*$ is $\mathbb{C}$ in this case. Of relevance is the restriction to $\mathbb{T}$, which yields a proper subset of $\mathbb{R}$.

Definition 2.3. *Assume that $\theta_1, \ldots, \theta_m \in \mathbb{R}[x^\pm]$ are such that $\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\theta_1, \ldots, \theta_m]$. We define the map*

$$\begin{array}{rccl} \vartheta : & (\mathbb{C}^*)^n & \to & \mathbb{C}^m, \\ & x & \mapsto & (\theta_1(x), \ldots, \theta_m(x)). \end{array}$$

The interpretation of Lemma 2.2 is now the following. The image of the compact torus $\mathbb{T}^n$ under ϑ can be properly embedded in the reals. Before we formalize this claim, let us verify that ϑ yields an orbit space.

Theorem 2.4. *The map*

$$\begin{array}{ccc} \mathbb{T}^n/\mathcal{G} & \to & \vartheta(\mathbb{T}^n), \\ \mathcal{G} \star x & \mapsto & \vartheta(x) \end{array}$$

is well–defined and bijective.

Proof. We follow the proof of [CLO15, Chapter 7, §4, Theorem 10] for linear actions. For $x, y \in \mathbb{T}^n$ with $\mathcal{G} \star x = \mathcal{G} \star y$, we have $\theta_i(x) = \theta_i(y)$ for all $1 \leq i \leq n$ by definition. Therefore, the map is well–defined and surjective.

For injectiveness, assume that $x, y \in \mathbb{T}^n$ with $\mathcal{G} \star x \cap \mathcal{G} \star y = \emptyset$. Define the set $X := \mathcal{G} \star x \cup \mathcal{G} \star y \setminus \{y\} \subseteq \mathbb{T}^n$. Since $\mathcal{G}$ is finite, X is finite and there exists $\tilde{f} \in \mathbb{C}[x_1, \ldots, x_n]$ with $\tilde{f}(X) = \{0\}$, $\tilde{f}(y) \neq 0$. For example,

$$\tilde{f} = \prod_{x' \in X} \prod_{i=1}^{n} (x_i - x'_i)$$

has the desired property. Take $\mathbb{C}[x^\pm]$ as a ring extension of $\mathbb{C}[x_1, \ldots, x_n]$ and define

$$f := \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} B \cdot \tilde{f} \in \mathbb{C}[x^\pm]^\mathcal{G}.$$

Then $f(x) = 0$ and $f(y) = |\mathrm{Stab}_\mathcal{G}(y)|/|\mathcal{G}|\, \tilde{f}(y) \neq 0$ by definition, where $\mathrm{Stab}_\mathcal{G}(y)$ denotes the stabilizer subgroup of y in $\mathcal{G}$. Since $\theta_1, \ldots, \theta_m$ are fundamental invariants, we have $\mathbb{C}[x^\pm]^\mathcal{G} = \mathbb{C}[\theta_1, \ldots, \theta_m]$. With $f(x) \neq f(y)$, we obtain $\theta_i(x) \neq \theta_i(y)$ for some $1 \leq i \leq m$ and thus $\vartheta(x) \neq \vartheta(y)$. ☐

We conclude that there is a one–to–one correspondence between the orbits $\mathbb{T}^n/\mathcal{G}$ and the image of $\mathbb{T}^n$.

Definition 2.5. *We call $\mathcal{T} := \vartheta(\mathbb{T}^n)$ the $\mathbb{T}$–**orbit space** of $\mathcal{G}$.*

Our goal is to describe this set as a basic semi–algebraic one and to give an explicit formula.

1.2 Fundamental invariants and the real $\mathbb{T}$–orbit space

Let R be a crystallographic irreducible root system in an n–dimensional $\mathbb{R}$–vector space V. Denote by $\mathcal{W}$ its Weyl group and $\Omega = \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_n$ the weight lattice. For $W : \mathbb{R}^n \to V$ the isomorphism, which takes e_i to ω_i, let $\mathcal{G}$ be the integer representation of $\mathcal{W}$ as in Equation (1.14). Note that $-I_n \in \mathcal{W}$ if and only if $-I_n \in \mathcal{G}$.

Furthermore, for $1 \leq i \leq n$, we denote by $\theta_i := \Theta_{e_i} = \frac{1}{|\mathcal{G}|} \sum\limits_{B \in \mathcal{G}} x^{B\, e_i}$ the orbit sum corresponding to the i–th fundamental weight. By Theorem 1.30, we have $\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\theta_1, \ldots, \theta_n]$ and this property is only true when $\mathcal{W}$ is a Weyl group. The $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$ is the image of $\mathbb{T}^n$ under the map $x \mapsto \vartheta(x) = (\theta_1(x), \ldots, \theta_n(x))$.

Proposition 2.6. *The following statements hold.*

1. *For $z = (z_1, \ldots, z_n) \in \mathcal{T}$ and $1 \leq i \leq n$, we have $|z_i| \leq 1$.*
2. *If $-I_n \in \mathcal{G}$, then $\mathcal{T} \subseteq [-1, 1]^n \subseteq \mathbb{R}^n$.*
3. *If $-I_n \notin \mathcal{G}$, then there exists $\sigma \in \mathfrak{S}_n$ of order 2, such that, for all $1 \leq i \leq n$, $\theta_i(x^{-I_n}) = \theta_{\sigma(i)}(x)$.*

Proof. *1.* and *2.* Let $z = \vartheta(x)$ for some $x \in \mathbb{T}^n$. Then $|z_i| = |\theta_i(x)| \leq \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} |x^{B e_i}| = 1$. Furthermore, if $-I_n \in \mathcal{G}$ we have $\overline{\theta_i(x)} = \theta_i(x^{-I_n}) = \theta_i(x) \in \mathbb{R}$ for all $x \in \mathbb{T}^n$. Hence, by the first statement, $\mathcal{T}$ is contained in the cube $[-1, 1]^n$.
3. Let $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$ be a base admitting fundamental weights $\omega_1, \ldots, \omega_n$. We prove that there exists a permutation $\sigma \in \mathfrak{S}_n$, such that, for all $1 \leq i \leq n$, $-\omega_{\sigma(i)} \in \mathcal{W}\, \omega_i$.
By Proposition 1.7, there exist $A \in \mathcal{W}$ and $\sigma \in \mathfrak{S}_n$ with $A\, \rho_i^\vee = -\rho_{\sigma(i)}^\vee$. We have

$$\langle -\omega_{\sigma(i)}, -\rho_{\sigma(j)}^\vee \rangle = \delta_{ij} = \langle \omega_i, \rho_j^\vee \rangle = \langle A\, \omega_i, A\, \rho_j^\vee \rangle = \langle A\, \omega_i, -\rho_{\sigma(j)}^\vee \rangle,$$

because σ is a permutation and the inner product is $\mathcal{W}$–invariant. Since $-\mathrm{B}^\vee$ is a basis of V, $A\, \omega_i = -\omega_{\sigma(i)}$. Especially, $-\omega_{\sigma(i)} \in \mathcal{W}\, \omega_i \cap \mathcal{W}\, \omega_{\sigma^2(i)}$ and so $\mathcal{W}\, \omega_i = \mathcal{W}\, \omega_{\sigma^2(i)}$. As the closure of $\Lambda\!\!\Lambda$ is a fundamental domain for $\mathcal{W}$ and both ω_i and $\omega_{\sigma^2(i)}$ lie on the walls of $\Lambda\!\!\Lambda$, we must have $\sigma^2 = 1$. ☐

The $\mathbb{T}$–orbit space of $\mathcal{G}$ is contained in the variety of the syzygies for the fundamental invariants. In the case of Weyl groups, those are algebraically independent and thus the $\mathbb{T}$–orbit space is in $\mathbb{C}^n$. To describe it as a basic semi–algebraic set in $\mathbb{R}^n$, we can now make the following adjustment.

Remark 2.7. *Let $1 \leq i \leq n$. When $i = \sigma(i)$, we leave the i–th coordinate of ϑ as it is. When $i < \sigma(i)$, we replace the i–th and $\sigma(i)$–th coordinate of ϑ by $\theta_{i,\mathbb{R}} := (\theta_i + \theta_{\sigma(i)})/2$ and $\theta_{\sigma(i),\mathbb{R}} := (\theta_i - \theta_{\sigma(i)})/(2\mathrm{i})$. The resulting map*

$$\begin{array}{rccl} \vartheta_{\mathbb{R}}: & \mathbb{T}^n & \to & \mathbb{R}^n, \\ & x & \mapsto & (\theta_{1,\mathbb{R}}(x), \ldots, \theta_{n,\mathbb{R}}(x)) \end{array} \tag{2.1}$$

*has image $\mathcal{T}_{\mathbb{R}} \subseteq [-1, 1]^n$, which we call the **real** $\mathbb{T}$–**orbit space** of $\mathcal{G}$.*

Proposition 2.8. *Let $\alpha \in \mathbb{N}^n$ with $-\alpha \in \mathcal{G}\widehat{\alpha}$. Then $\deg_W(T_\alpha) = \deg_W(T_{\widehat{\alpha}})$ and there exist unique $\widehat{T}_\alpha, \widehat{T}_{\widehat{\alpha}} \in \mathbb{R}[z]$, such that*

$$T_\alpha(\vartheta(x)) = \widehat{T}_\alpha(\vartheta_{\mathbb{R}}(x)) + \mathrm{i}\, \widehat{T}_{\widehat{\alpha}}(\vartheta_{\mathbb{R}}(x)) \quad \text{and} \quad T_{\widehat{\alpha}}(\vartheta(x)) = \widehat{T}_\alpha(\vartheta_{\mathbb{R}}(x)) - \mathrm{i}\, \widehat{T}_{\widehat{\alpha}}(\vartheta_{\mathbb{R}}(x)).$$

Proof. If $-I_n \in \mathcal{G}$, then there is nothing to show. By Proposition 2.6, T_α and $T_{\widehat{\alpha}}$ have the same weighted degree and $|\mathcal{G}\alpha| = |\mathcal{G}\widehat{\alpha}|$. Thus,

$$(T_\alpha + T_{\widehat{\alpha}})(\theta_1(x), \ldots, \theta_n(x)) = \frac{1}{|\mathcal{G}\alpha|} \sum_{\tilde{\alpha} \in \mathcal{G}\alpha} x^{\tilde{\alpha}} + x^{-\tilde{\alpha}}$$

is invariant under the multiplicative action of both $\mathcal{G}$ and $\{\pm 1\}$. We have

$$(\mathbb{R}[x^{\pm}]^{\mathcal{G}})^{\{\pm 1\}} \cong \langle \{\theta_i + \theta_{\sigma(i)} \mid 1 \leq i \leq \sigma(i) \leq n\} \rangle_{\mathbb{R}}$$

as $\mathbb{R}$–algebras and so $(T_\alpha + T_{\widehat{\alpha}})(\vartheta(x))/2$ can be written as a polynomial $\widehat{T}_\alpha$ in $\vartheta_{\mathbb{R}}(x)$. Similarly,

$$(T_\alpha - T_{\widehat{\alpha}})(\theta_1(x), \ldots, \theta_n(x)) = \frac{1}{|\mathcal{G}\alpha|} \sum_{\tilde{\alpha} \in \mathcal{G}\alpha} x^{\tilde{\alpha}} - x^{-\tilde{\alpha}}$$

is invariant under $\mathcal{G}$, but anti–invariant under $\{\pm 1\}$. The elements of $\mathbb{R}[x^\pm]^\mathcal{G}$, which are anti–invariant under $\{\pm 1\}$, are as an $\mathbb{R}$–algebra isomorphic to

$$\langle \{\theta_i - \theta_{\sigma(i)} \mid 1 \leq \sigma(i) < i \leq n\} \rangle_\mathbb{R}.$$

Hence, $(T_\alpha + T_{\widehat{\alpha}})(\vartheta(x))/(2\mathrm{i})$ can be written as a polynomial $\widehat{T}_{\widehat{\alpha}}$ in $\vartheta_\mathbb{R}$.

Since $\widehat{T}_\alpha$ and $\widehat{T}_{\widehat{\alpha}}$ are globally defined as the real and imaginary part of T_α, they are unique. □

Example 2.9. *Consider the root system* A_2 *with* $\mathcal{W} \cong \mathfrak{S}_3$*. Then* $-\omega_1 \in \mathcal{W}\omega_2$*, or equivalently* $\widehat{\left[\begin{smallmatrix}1\\0\end{smallmatrix}\right]} = \left[\begin{smallmatrix}0\\1\end{smallmatrix}\right] \in \mathbb{Z}^2$*, and* $\rho_0 = \omega_1 + \omega_2$*, see Equation (1.3) and Example 1.21. The generalized Chebyshev polynomials with weighted degree* 2 *are*

$$T_{20} = 3\,z_1^2 - 2\,z_2, \quad T_{11} = 3/2\,z_1\,z_2 - 1/2, \quad T_{02} = 3\,z_2^2 - 2\,z_1 \in \mathbb{R}[z].$$

After substitution $z_1 \mapsto z_1 + \mathrm{i}\,z_2, z_2 \mapsto z_1 - \mathrm{i}\,z_2$*, we have*

$$\begin{array}{rcl} T_{20} & = & (3\,z_1^2 - 3\,z_2^2 - 2\,z_1) + (6\,z_1\,z_2 + 2\,z_2)\,\mathrm{i}, \\ T_{11} & = & (3/2\,z_1^2 + 3/2\,z_2^2 - 1/2) + 0\,\mathrm{i}, \\ T_{02} & = & (3\,z_1^2 - 3\,z_2^2 - 2\,z_1) - (6\,z_1\,z_2 + 2\,z_2)\,\mathrm{i}, \end{array}$$

and the new polynomials from Proposition 2.8 are

$$\widehat{T}_{20} = 3\,z_1^2 - 3\,z_2^2 - 2\,z_1, \quad \widehat{T}_{11} = 3/2\,z_1^2 + 3/2\,z_2^2 - 1/2, \quad \widehat{T}_{02} = 6\,z_1\,z_2 + 2\,z_2.$$

At higher degrees, the generalized Chebyshev polynomials of the first kind associated to A_2 *admit the new polynomials*

$$\widehat{T}_{03} = 27\,z_1^2\,z_2 - 9\,z_2^3, \quad \widehat{T}_{12} = 6\,z_1\,z_2 - 1/2\,z_2 + 9/2\,z_1^2\,z_2 + 9/2\,z_2^3,$$
$$\widehat{T}_{21} = -3\,z_1^2 + 3\,z_2^2 - 1/2\,z_1 + 9/2\,z_1^3 + 9/2\,z_1\,z_2^2, \quad \widehat{T}_{30} = 9\,z_1^3 - 27\,z_1\,z_2^2 - 9\,z_1^2 - 9\,z_2^2 + 1,$$
$$\widehat{T}_{04} = 108\,z_1^3\,z_2 - 108\,z_1\,z_2^3 - 36\,z_1^2\,z_2 - 36\,z_2^3 - 12\,z_1\,z_2 + 4\,z_2,$$
$$\widehat{T}_{13} = 27/2\,z_2^3 - 5/2\,z_2 + 27\,z_1\,z_2^3 + 27/2\,z_1^2\,z_2 + 27\,z_1^3\,z_2 - 3\,z_1\,z_2,$$
$$\widehat{T}_{22} = -18\,z_1^3 - 1/2 + 54\,z_1\,z_2^2 + 6\,z_1^2 + 6\,z_2^2 + 27/2\,z_1^4 + 27\,z_1^2\,z_2^2 + 27/2\,z_2^4,$$
$$\widehat{T}_{31} = -27/2\,z_1^3 - 27/2\,z_1\,z_2^2 + 5/2\,z_1 - 3/2\,z_1^2 + 3/2\,z_2^2 + 27/2\,z_1^4 - 27/2\,z_2^4,$$
$$\widehat{T}_{40} = 27\,z_1^4 - 162\,z_1^2\,z_2^2 + 27\,z_2^4 - 36\,z_1^3 - 36\,z_1\,z_2^2 + 6\,z_1^2 - 6\,z_2^2 + 4\,z_1.$$

2 Symmetric polynomial systems

In order to give a polynomial description for the $\mathbb{T}$–orbit space of a Weyl group, our first step is to study solutions of symmetric systems. We do this, because the symmetric group $\mathfrak{S}_n$ can be represented as a subgroup of all Weyl groups of A_{n-1}, B_n, C_n, D_n and G_2. The contents of this section are mostly consequences of the material in [CLO05, Chapter 2] and needed later for the results in Sections 3 to 8.

2.1 Solutions in the compact torus

For $1 \leq i \leq n$, denote the i–th elementary symmetric function in n indeterminates by σ_i. We shall be confronted with the following two types of polynomial systems in unknown $y_1, \ldots, y_n$.

$$\begin{array}{llcllll} \text{(I)} & \sigma_i(y_1, \ldots, y_n) & = & (-1)^i\,c_i & \text{for} & 1 \leq i \leq n & \text{with} \quad c_1, \ldots, c_n \in \mathbb{C} \\ \text{(II)} & \sigma_i\left(\frac{y_1 + y_1^{-1}}{2}, \ldots, \frac{y_n + y_n^{-1}}{2}\right) & = & (-1)^i\,c_i & \text{for} & 1 \leq i \leq n & \text{with} \quad c_1, \ldots, c_n \in \mathbb{R} \end{array}$$

The goal is to determine, whether all solutions $y = (y_1, \ldots, y_n) \in \mathbb{C}^n$ of system (I), respectively system (II), are contained in $\mathbb{T}^n$.

Lemma 2.10.

1. *System* (I) *always has a solution* $y \in \mathbb{C}^n$. *It is is unique up to permutation of coordinates.*
2. *System* (II) *always has a solution in* $y \in (\mathbb{C}^*)^n$. *It is is unique up to permutation and inversion of coordinates.*

Proof. 1. By Vieta's formula, a solution of system (I) is the vector of roots of a polynomial with coefficients given by the right hand side of system (I). Since $\mathbb{C}$ is algebraically closed, the statement follows.

2. By Lemma 2.2, we can write the roots $r_1, \ldots, r_n$ of the polynomial with coefficients given by the right hand side of system (II) as $r_i = (y_i + y_i^{-1})/2$ for some $y \in (\mathbb{C}^*)^n$. Then y is a unique solution of (II) up to permutation and inversion. □

From now on, we speak of *the* solution of system (I), respectively (II).

Proposition 2.11. *For* $c_1, \ldots, c_n \in \mathbb{R}$*, the solution of system* (II) *is contained in* $\mathbb{T}^n$ *if and only if all the roots of the univariate polynomial*

$$x^n + c_1\, x^{n-1} + \ldots + c_{n-1}\, x + c_n$$

are contained in $[-1, 1]$.

Proof. Let $p := x^n + c_1\, x^{n-1} + \ldots + c_n$ be the univariate polynomial with roots $r_1, \ldots, r_n \in \mathbb{C}$. If $y \in (\mathbb{C}^*)^n$ is the solution of system (II), then for all $1 \leq i \leq n$, $y_i + y_i^{-1}$ is a root of p by Vieta's formula. Applying Lemma 2.10 yields $y \in \mathbb{T}^n$ if and only if $r_1, \ldots, r_n \in [-1, 1]$. □

Similarly, we can characterize solutions of system (I). The **Chebyshev polynomial of the first kind** associated to $\ell \in \mathbb{N}$ is the unique univariate polynomial T_ℓ with $T_\ell((x + x^{-1})/2) = (x^\ell + x^{-\ell})/2$. For $0 \neq p \in \mathbb{R}[x]$ or $\mathbb{C}[x]$, denote by $\operatorname{Coeff}(x^\ell, p)$ the coefficient of the monomial x^ℓ in p for $0 \leq \ell \leq \deg(p)$.

Proposition 2.12. *For* $c_1, \ldots, c_{n-1} \in \mathbb{C}$ *with* $\overline{c_i} = (-1)^n\, c_{n-i}$ *and* $c_0 := (-1)^n\, c_n := 1$*, the solution of system* (I) *is contained in* $\mathbb{T}^n$ *if and only if all the roots of the univariate polynomial*

$$T_n(x) + d_1\, T_{n-1}(x) + \ldots + d_{n-1}\, T_1(x) + \frac{d_n}{2}\, T_0(x) \quad \textit{with} \quad d_\ell = \sum_{i=0}^{\ell} \overline{c_i}\, c_{\ell-i} \in \mathbb{R}$$

are contained in $[-1, 1]$.

Proof. By Vieta's formula, the solution of system (I) is contained in $\mathbb{T}^n$ if and only if all the roots of the univariate polynomial $p := x^n + c_1\, x^{n-1} + \ldots + c_n$ are contained in $\mathbb{T}$.

The roots of p are nonzero, because $p(0) = c_n = (-1)^n \neq 0$. We fix another univariate polynomial $\tilde{p} := x^n + \overline{c_1}\, x^{n-1} + \ldots + \overline{c_n}$. Since $\tilde{p}(x) = (-x)^n\, p(x^{-1})$, the roots of $p\tilde{p}$ are the union of the roots of p and their inverses. Especially, all the roots of $p\tilde{p}$ are contained in $\mathbb{T}$ if and only if the roots of p are. The coefficients of $p\tilde{p}$ satisfy

$$\operatorname{Coeff}(x^\ell, p\tilde{p}) = \sum_{i=0}^{\ell} c_{n-i}\, \overline{c_{n-\ell+i}} = \sum_{i=0}^{\ell} \overline{c_i}\, c_{\ell-i} = \begin{cases} \sum_{i=0}^{\ell} \operatorname{Coeff}(x^{n-i}, \tilde{p}) \operatorname{Coeff}(x^{n-\ell+i}, p) = \operatorname{Coeff}(x^{2n-\ell}, p\tilde{p}) \\ \sum_{i=0}^{\lfloor(\ell-1)/2\rfloor} \underbrace{(\overline{c_i}\, c_{\ell-i} + \overline{c_{\ell-i}}\, c_i)}_{\in \mathbb{R}} + \begin{cases} c_{\ell/2}\, \overline{c_{\ell/2}}, & \ell \text{ even} \\ 0, & \ell \text{ odd} \end{cases} \in \mathbb{R} \end{cases}$$

for $0 \le \ell \le n$. Thus, $\mathrm{Coeff}(x^{\ell}, p\tilde{p}) = \mathrm{Coeff}(x^{2n-\ell}, p\tilde{p}) = d_{\ell} \in \mathbb{R}$ and we can write

$$p\tilde{p} = \sum_{\ell=1}^{n} d_{n-\ell}(x^{n+\ell}+x^{n-\ell})+d_n = 2x^n\left(\sum_{\ell=1}^{n} d_{n-\ell}T_{\ell}\left(\frac{x+x^{-1}}{2}\right)+\frac{d_n}{2}T_0\left(\frac{x+x^{-1}}{2}\right)\right) =: 2x^n g\left(\frac{x+x^{-1}}{2}\right).$$

With Lemma 2.10, we see that $x \in \mathbb{T}$ is a root of $p\tilde{p}$ if and only if $(x+x^{-1})/2 \in [-1,1]$ is a root of g. □

2.2 Characterization via Hermite quadratic forms

Let $p, q \in \mathbb{R}[x]$ be univariate polynomials. The multiplication by q in the $\mathbb{R}$–algebra $\mathbb{R}[x]/\langle p\rangle$ is

$$\begin{array}{rrcl} m_q: & \mathbb{R}[x]/\langle p\rangle & \rightarrow & \mathbb{R}[x]/\langle p\rangle, \\ & f+\langle p\rangle & \mapsto & q\,f+\langle p\rangle. \end{array}$$

For simplicity, we write f for the residue class $f+\langle p\rangle$. If $p = x^n + c_1\,x^{n-1} + \ldots + c_{n-1}\,x + c_n$, then the matrix of m_x in the basis $\{1, x, \ldots, x^{n-1}\}$ of $\mathbb{R}[x]/\langle p\rangle$ is the companion matrix

$$\begin{bmatrix} 0 & & 0 & -c_n \\ 1 & \ddots & & \vdots \\ & \ddots & 0 & -c_2 \\ 0 & & 1 & -c_1 \end{bmatrix} \tag{2.1}$$

of p, because $x\,x^i = x^{i+1}$ for $0 \le i \le n-2$ and $x\,x^{n-1} = x^n \equiv -c_1\,x^{n-1} - \ldots - c_{n-1}\,x - c_n \mod \langle p\rangle$.
On the other hand, the univariate Chebyshev polynomials of the first kind up to degree $n-1$ also form a basis $\{T_0, T_1, \ldots, T_{n-1}\}$ of $\mathbb{R}[x]/\langle p\rangle$. If $p = T_n + d_1\,T_{n-1} + \ldots + d_{n-1}\,T_1 + d_n/2\,T_0 \in \mathbb{R}[x]$ and $n \ge 3$, then the matrix of m_x in this basis is

$$\begin{bmatrix} 0 & 1/2 & & & 0 & -d_n/4 \\ 1 & 0 & \ddots & & & -d_{n-1}/2 \\ & 1/2 & \ddots & \ddots & & \vdots \\ & & \ddots & \ddots & 1/2 & -d_3/2 \\ & & & \ddots & 0 & (1-d_2)/2 \\ 0 & & & & 1/2 & -d_1/2 \end{bmatrix}, \tag{2.2}$$

where the rows and columns are indexed by $T_0, T_1, \ldots, T_{n-1}$. The entries in the columns originate from the recurrence formula $x\,T_0 = T_1$ and $2\,x\,T_j = T_{j+1} + T_{j-1}$ for $1 \le j \le n-1$. Especially,

$$2\,x\,T_{n-1} = T_n + T_{n-2} \equiv -d_1\,T_{n-1} + (1-d_2)\,T_{n-2} - d_3\,T_{n-3} - \ldots - d_{n-1}\,T_1 - d_n/2\,T_0 \mod \langle p\rangle$$

yields the last column.

Example 2.13. *Let $p = x^3 - c\,x^2 + \overline{c}\,x - 1 \in \mathbb{C}[x]$ with $c \in \mathbb{C}$. Following the proof of Proposition 2.12, we* *consider the palindromic polynomial* $p\tilde{p} \in \mathbb{R}[x]$ *with*

$$\begin{aligned}
&\frac{1}{2x^3}\, p(x)\tilde{p}(x) \\
&= \frac{1}{2x^3}\left((x^6+1) - (c+\overline{c})(x^5+x) + (c\,\overline{c}+c+\overline{c})(x^4+x^2) - \frac{c^2+\overline{c}^2+2}{2}\,x^3\right) \\
&= \frac{x^3+x^{-3}}{2} - (c+\overline{c})\,\frac{x^2+x^{-2}}{2} + (c\,\overline{c}+c+\overline{c})\,\frac{x+x^{-1}}{2} - \frac{c^2+\overline{c}^2+2}{2} \\
&= T_3\left(\frac{x+x^{-1}}{2}\right) - (c+\overline{c})\,T_2\left(\frac{x+x^{-1}}{2}\right) + (c\,\overline{c}+c+\overline{c})\,T_1\left(\frac{x+x^{-1}}{2}\right) - \frac{c^2+\overline{c}^2+2}{2}\,T_0\left(\frac{x+x^{-1}}{2}\right) \\
&= g\left(\frac{x+x^{-1}}{2}\right).
\end{aligned}$$

The matrix of the multiplication by x *in* $\mathbb{R}[x]/\langle g\rangle$ *in the basis of Chebyshev polynomials is*

$$\begin{bmatrix} 0 & 1/2 & (c^2+\overline{c}^2+2)/4 \\ 1 & 0 & (1-c\,\overline{c}-c-\overline{c})/2 \\ 0 & 1/2 & (c+\overline{c})/2 \end{bmatrix} \in \mathbb{R}^{3\times 3}$$

and all the roots of p *are contained in* $\mathbb{T}$ *if and only if all the roots of* g *are contained in* $[-1,1]$.

To characterize univariate polynomials with roots in $[-1,1]$, we can now use the next statement, which is essentially Sylvester's version for Sturm's theorem for Hermite quadratic forms.

Theorem 2.14. *Let* $p \in \mathbb{R}[x]$ *be of degree* n *and* $q \in \mathbb{R}[x]$. *Then all the roots of* p *are contained in* $S(q) := \{x \in \mathbb{R} \,|\, q(x) \geq 0\}$ *if and only if the Hermite quadratic form*

$$\begin{array}{rccl} P(p,q): & \mathbb{R}[x]/\langle p\rangle & \to & \mathbb{R}, \\ & f+\langle p\rangle & \mapsto & \mathrm{Trace}(m_{q\,f^2}) \end{array}$$

is positive semi–definite.

Proof. Let $P \in \mathbb{R}^{n\times n}$ be the symmetric matrix associated to $P(p,q)$ for a fixed basis of $\mathbb{R}[x]/\langle p\rangle$. Denote by N_+, respectively N_-, the number of strictly positive, respectively negative, eigenvalues of P, including their multiplicities. By [CLO05, Chapter 2, Theorem 5.2], the rank and the signature of $P(p,q)$ are

$$\begin{array}{rcccl} N_+ + N_- & = & \mathrm{Rank}(P(p,q)) & = & |\{x \in \mathbb{C} \,|\, p(x)=0,\, q(x)\neq 0\}|, \\ N_+ - N_- & = & \mathrm{Sign}(P(p,q)) & = & \underbrace{|\{x \in \mathbb{R} \,|\, p(x)=0,\, q(x)>0\}|}_{=:n_+} - \underbrace{|\{x \in \mathbb{R} \,|\, p(x)=0,\, q(x)<0\}|}_{=:n_-}. \end{array}$$

If all the roots of p are contained in $S(q)$, then $n_- = 0$, and thus

$$N_+ + N_- = \mathrm{Rank}(P(p,q)) = \mathrm{Sign}(P(p,q)) = n_+ = N_+ - N_-.$$

Hence, $N_- = 0$ and all eigenvalues of P are nonnegative, that is, $P(p,q)$ is positive semi–definite.
For the converse, assume that $P(p,q)$ is positive semi–definite. Then $N_- = 0$ and

$$N_+ = \mathrm{Sign}(P(p,q)) = n_+ - n_- \leq \mathrm{Rank}(P(p,q)) = N_+,$$

that is, $n_+ - n_- = \mathrm{Rank}(P(p,q))$. On the other hand, $\mathrm{Rank}(P(p,q)) \geq n_+ + n_-$. Hence, $n_- = 0$ and $\mathrm{Rank}(P(p,q)) = n_+$ implies that all the roots of p are real and contained in $S(q)$. □

Corollary 2.15. *Let $n \geq 3$. For $c_1, \dots, c_n \in \mathbb{C}$ with $\overline{c_i} = (-1)^n c_{n-i}$ for $1 \leq i \leq n-1$ and $c_0 := (-1)^n c_n := 1$, the solution of system* (I) *is contained in $\mathbb{T}^n$ if and only if the matrix $P \in \mathbb{R}^{n\times n}$ with entries*

$$P_{ij} = \mathrm{Trace}(C^{i+j-2} - C^{i+j}), \quad \textit{where}$$

$$C = \begin{bmatrix} 0 & 1/2 & & & 0 & -d_n/4 \\ 1 & 0 & \ddots & & & -d_{n-1}/2 \\ & 1/2 & \ddots & \ddots & & \vdots \\ & & \ddots & \ddots & 1/2 & -d_3/2 \\ & & & \ddots & 0 & (1-d_2)/2 \\ 0 & & & & 1/2 & -d_1/2 \end{bmatrix} \in \mathbb{R}^{n\times n} \quad \textit{and} \quad d_\ell = \sum_{i=0}^{\ell} c_i \,\overline{c_{\ell-i}} \quad \textit{for} \quad 1 \leq \ell \leq n,$$

is positive semi–definite.

Proof. P is the matrix associated to the Hermite quadratic form $P(p,q)$ from Theorem 2.14 with $q = 1 - x^2$ in the basis $\{1, x, x^2, \dots, x^{n-1}\}$. Indeed, by [CLO05, Chapter 2, Proposition 4.2], the entries of the associated matrix are

$$\mathrm{Trace}(m_{q\,x^{i-1}\,x^{j-1}}) = \mathrm{Trace}(m_{x^{i+j-2}-x^{i+j}}) = \mathrm{Trace}(m_x^{i+j-2} - m_x^{i+j})$$

for $1 \leq i, j \leq n$. Since the trace is independent of the basis for $\mathbb{R}[x]/\langle p\rangle$, we can consider the matrix of m_x in the basis of univariate Chebyshev polynomials of the first kind, which according to Equation (2.2) is C. The statement now follows from Proposition 2.12. □

Corollary 2.16. *For $c_1, \dots, c_n \in \mathbb{R}$, the solution of system* (II) *is contained in $\mathbb{T}^n$ if and only if the matrix $P \in \mathbb{R}^{n\times n}$ with entries*

$$P_{ij} = \mathrm{Trace}(C^{i+j-2} - C^{i+j}), \quad \textit{where}$$

$$C = \begin{bmatrix} 0 & \cdots & 0 & -c_n \\ 1 & & 0 & -c_{n-1} \\ & \ddots & & \vdots \\ 0 & & 1 & -c_1 \end{bmatrix} \in \mathbb{R}^{n\times n},$$

is positive semi–definite.

Proof. The proof is analogous to the one of Corollary 2.15 with Equation (2.1) and Proposition 2.11. □

For some smaller examples, the following observation will come in handy.

Remark 2.17. *Let $P \in \mathbb{R}^{n\times n}$ be a symmetric matrix with characteristic polynomial*

$$\mathrm{Det}(x\, I_n - P) = x^n + \sum_{i=1}^{n} (-1)^i\, p_i\, x^{n-i} \in \mathbb{R}[x].$$

It follows from Descartes' rule of signs [BPR06, Theorem 2.33] *that P is positive semi–definite if and only if $p_i \geq 0$ for all $1 \leq i \leq n$.*

3 Hermite characterization of $\mathcal{T}_{\mathbb{R}}$ with Chebyshev polynomials

We give a unifying formula for the real $\mathbb{T}$–orbit space $\mathcal{T}_{\mathbb{R}}$ in the basis of real generalized Chebyshev polynomials of the first kind from Proposition 2.8. The proof relies on the results of Sections 4 to 8 that now come together as one.

When giving a description for $\mathcal{T}$ or equivalently $\mathcal{T}_{\mathbb{R}}$, it suffices to consider the irreducible root systems. Indeed, the Weyl group $\mathcal{W}$ is the outer product of the Weyl groups corresponding to the irreducible components. If $\mathrm{R} = \mathrm{R}^{(1)} \cup \ldots \cup \mathrm{R}^{(k)}$, then $\mathcal{T}_{\mathbb{R}}$ can be written as a Cartesian product of real $\mathbb{T}$–orbit spaces $\mathcal{T}_{\mathbb{R}}^{(1)} \times \ldots \times \mathcal{T}_{\mathbb{R}}^{(k)}$.

In this section, let $n \in \mathbb{N}$ and R be a root system with Dynkin graph of type A_{n-1}, B_n, C_n, D_n or G_{n-1}. Assume that the Weyl group has integer representation $\mathcal{G} \subseteq \mathrm{GL}_{\mathrm{Rank(R)}}(\mathbb{Z})$ given by the fundamental weights Equations (1.3), (1.5), (1.7), (1.9) and (1.11). For $\alpha \in \mathbb{Z}^n$, the orbit polynomial associated to α is denoted by $\Theta_\alpha = \frac{1}{|\mathcal{G}|} \sum\limits_{B \in \mathcal{G}} x^{B\alpha}$.

Lemma 2.18. *In $\mathbb{R}[x^{\pm}]$, define the $2\,n$ distinct monomials $\{y_1^{\pm 1}, \ldots, y_n^{\pm 1}\} := \mathcal{G} \cdot x_1 \cup \mathcal{G} \cdot x_1^{-1}$. Then, for $x \in (\mathbb{C}^*)^{\mathrm{Rank(R)}}$ and $k \in \mathbb{N}$, we have*

$$\frac{1}{n} \sum_{i=1}^{n} y_i(x)^k + y_i(x)^{-k} = \Theta_{k\, e_1}(x) + \Theta_{-k\, e_1}(x).$$

Proof. This follows immediately from Propositions 2.21, 2.24, 2.27, 2.30 and 2.33. □

Denote by $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_{\mathrm{Rank(R)}}]$ the multivariate polynomial ring.

Theorem 2.19. *Define the matrix $P \in \mathbb{R}[z]^{n \times n}$ by*

$$\begin{aligned} 2^{i+j}\, P(z)_{ij} = & -\widehat{T}_{(i+j)\, e_1}(z) + \sum_{\ell=1}^{\lceil (i+j)/2 \rceil - 1} \left(4 \binom{i+j-2}{\ell-1} - \binom{i+j}{\ell} \right) \widehat{T}_{(i+j-2\,\ell)\, e_1}(z) \\ & + \frac{1}{2} \begin{cases} 4\binom{i+j-2}{(i+j)/2-1} - \binom{i+j}{(i+j)/2}, & \text{if} \quad i+j \quad \text{is even} \\ 0, & \text{if} \quad i+j \quad \text{is odd} \end{cases}. \end{aligned}$$

Then the real $\mathbb{T}$–orbit space of $\mathcal{G}$ is $\mathcal{T}_{\mathbb{R}} = \{ z \in \mathbb{R}^{\mathrm{Rank(R)}} \,|\, P(z) \succeq 0 \}$.

Proof. The $\mathbb{T}$–orbit space of $\mathcal{G}$ is $\mathcal{T} = \{ \vartheta(x) \,|\, x \in \mathbb{T}^{\mathrm{Rank(R)}} \} = \{ \tilde{z} \in \mathcal{Z} \,|\, P(\tilde{z}) \succeq 0 \}$, where $P \in \mathbb{R}[z]^{n \times n}$ is the Hermite matrix polynomial with entries $P_{ij} = \mathrm{Trace}(C^{i+j-2} - C^{i+j})$ and $\mathcal{Z}$ the $\mathbb{R}$–vector space with $\dim(\mathcal{Z}) = \mathrm{Rank(R)}$ from Theorems 2.23, 2.26, 2.29, 2.32 and 2.35.

To obtain a formula for the entries of P in the basis of generalized Chebyshev polynomials, we shall now utilize the theory that we have developed in Section 2. For $x \in \mathbb{T}^{\mathrm{Rank(R)}}$ and $\tilde{z} = \vartheta(x) \in \mathcal{T}$, $C(\tilde{z})$ is by construction the matrix of the multiplication map associated to a univariate polynomial p with roots $(y_i(x) + y_i(x)^{-1})/2 \in [-1, 1]$, see Equations (2.1) and (2.2). Hence, those roots are the eigenvalues of $C(\tilde{z})$

and, for $2 \leq k \leq 2\,n$, the trace of the k–th power is

$$\begin{aligned}
\mathrm{Trace}(C(\tilde{z})^k) &= \sum_{i=1}^{n} \left(\frac{y_i(x) + y_i(x)^{-1}}{2} \right)^k = \frac{1}{2^k} \sum_{i=1}^{n} \left(\sum_{\ell=0}^{k} \binom{k}{\ell} y_i(x)^{k-\ell}\, y_i(x)^{-\ell} \right) \\
&= \frac{1}{2^k} \sum_{i=1}^{n} \left(\sum_{\ell=0}^{\lceil k/2 \rceil - 1} \binom{k}{\ell} y_i(x)^{k-2\,\ell} + \sum_{\ell=\lfloor k/2 \rfloor + 1}^{k} \binom{k}{\ell} y_i(x)^{k-2\,\ell} + \begin{cases} \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases} \right) \\
&= \frac{1}{2^k} \sum_{\ell=0}^{\lceil k/2 \rceil - 1} \left(\binom{k}{\ell} \sum_{i=1}^{n} \left(y_i(x)^{k-2\,\ell} + y_i(x)^{2\,\ell - k} \right) \right) + \frac{n}{2^k} \begin{cases} \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases} \\
&= \frac{n}{2^k} \sum_{\ell=0}^{\lceil k/2 \rceil - 1} \left(\binom{k}{\ell} \left(\Theta_{(k-2\,\ell)\,e_1}(x) + \Theta_{(2\,\ell-k)\,e_1}(x) \right) \right) + \frac{n}{2^k} \begin{cases} \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases},
\end{aligned}$$

where the last step follows from Lemma 2.18. Now, we use the definition of the generalized Chebyshev polynomials and Proposition 2.8 to write

$$\Theta_{(k-2\,\ell)\,e_1}(x) + \Theta_{(2\,\ell-k)\,e_1}(x) = T_{(k-2\,\ell)\,e_1}(\vartheta(x)) + T_{(2\,\ell-k)\,e_1}(\vartheta(x)) = 2\,\widehat{T}_{(k-2\,\ell)\,e_1}(\vartheta_{\mathbb{R}}(x)).$$

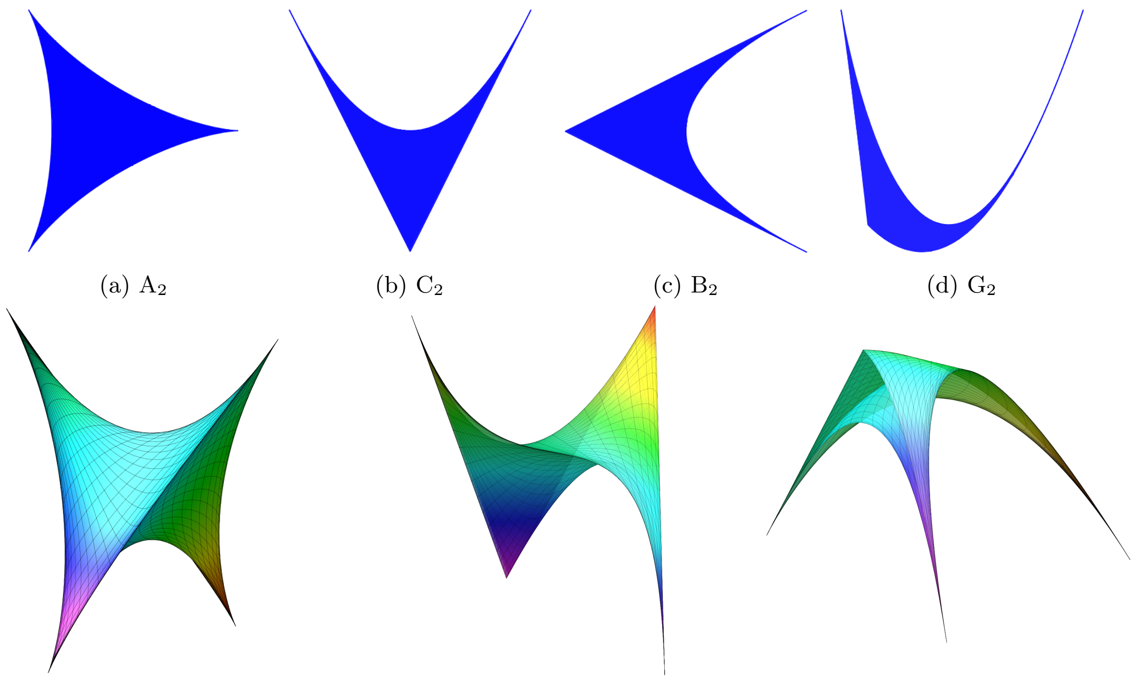
Let $1 \leq i, j \leq n$ and $k = i + j$. Then the entry $P(z)_{ij}$ of the Hermite matrix polynomial in $z := \vartheta_{\mathbb{R}}(x)$ is

$$\begin{aligned}
&\mathrm{Trace}(C(\tilde{z})^{k-2}) - \mathrm{Trace}(C(\tilde{z})^k) \\
&= \frac{2\,n}{2^k} \left(4 \sum_{\ell=0}^{\lceil k/2 \rceil - 2} \left(\binom{k-2}{\ell} \widehat{T}_{(k-2\,(\ell+1))\,e_1}(z) \right) - \sum_{\ell=0}^{\lceil k/2 \rceil - 1} \left(\binom{k}{\ell} \widehat{T}_{(k-2\,\ell)\,e_1}(z) \right) \right) \\
&\quad + \frac{n}{2^k} \begin{cases} 4\binom{k-2}{k/2-1} - \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases} \\
&= \frac{2\,n}{2^k} \left(4 \sum_{\ell=1}^{\lceil k/2 \rceil - 1} \left(\binom{k-2}{\ell-1} \widehat{T}_{(k-2\,\ell)\,e_1}(z) \right) - \sum_{\ell=0}^{\lceil k/2 \rceil - 1} \left(\binom{k}{\ell} \widehat{T}_{(k-2\,\ell)\,e_1}(z) \right) \right) \\
&\quad + \frac{n}{2^k} \begin{cases} 4\binom{k-2}{k/2-1} - \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases} \\
&= \frac{2\,n}{2^k} \left(-\widehat{T}_{k\,e_1}(z) + \sum_{\ell=1}^{\lceil k/2 \rceil - 1} \left(4\binom{k-2}{\ell-1} - \binom{k}{\ell} \right) \widehat{T}_{(k-2\,\ell)\,e_1}(z) \right) + \frac{n}{2^k} \begin{cases} 4\binom{k-2}{k/2-1} - \binom{k}{k/2}, & k \quad \text{even} \\ 0, & k \quad \text{odd} \end{cases}.
\end{aligned}$$

Dividing by $2\,n$ does not change whether P is positive semi–definite in z and so we obtain the formula. □

Remark 2.20. *The matrix polynomial $P \in \mathbb{R}[z]^{n \times n}$ from Theorem 2.19 follows the pattern*

$$\begin{bmatrix}
\frac{\widehat{T}_0 - \widehat{T}_{2\,e_1}}{2} & \frac{\widehat{T}_{e_1} - \widehat{T}_{3\,e_1}}{4} & \frac{\widehat{T}_0 - \widehat{T}_{4\,e_1}}{8} & \frac{2\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - \widehat{T}_{5\,e_1}}{16} & \cdots \\
\frac{\widehat{T}_{e_1} - \widehat{T}_{3\,e_1}}{4} & \frac{\widehat{T}_0 - \widehat{T}_{4\,e_1}}{8} & \frac{2\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - \widehat{T}_{5\,e_1}}{16} & \frac{2\widehat{T}_0 + \widehat{T}_{2\,e_1} - 2\widehat{T}_{4\,e_1} - \widehat{T}_{6\,e_1}}{32} & \cdots \\
\frac{\widehat{T}_0 - \widehat{T}_{4\,e_1}}{8} & \frac{2\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - \widehat{T}_{5\,e_1}}{16} & \frac{2\widehat{T}_0 + \widehat{T}_{2\,e_1} - 2\widehat{T}_{4\,e_1} - \widehat{T}_{6\,e_1}}{32} & \frac{5\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - 3\widehat{T}_{5\,e_1} - \widehat{T}_{7\,e_1}}{64} & \cdots \\
\frac{2\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - \widehat{T}_{5\,e_1}}{16} & \frac{2\widehat{T}_0 + \widehat{T}_{2\,e_1} - 2\widehat{T}_{4\,e_1} - \widehat{T}_{6\,e_1}}{32} & \frac{5\widehat{T}_{e_1} - \widehat{T}_{3\,e_1} - 3\widehat{T}_{5\,e_1} - \widehat{T}_{7\,e_1}}{64} & \frac{5\widehat{T}_0 + 4\widehat{T}_{2\,e_1} - 4\widehat{T}_{4\,e_1} - 4\widehat{T}_{6\,e_1} - \widehat{T}_{8\,e_1}}{128} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}.$$



(a) A_2 (b) C_2 (c) B_2 (d) G_2

(e) A_3 (f) C_3 (g) B_3

Figure 2.1: The real $\mathbb{T}$–orbit space for the irreducible root systems of rank 2 and 3.

1. *P only depends on the $\widehat{T}_\alpha$, where $\alpha \in \mathbb{N}^n$ is a multiple of e_1.*

2. *P has Hankel structure, that is, if $i + j = k + \ell$, then $P_{ij} = P_{k\ell}$.*

3. *Denote by $P^{(n)}$ the matrix P for fixed n. Then the leading submatrices of P have the structure of $P^{(k)}$ for $k \leq n$.*

4. *If R is of type B_n, C_n or G_2, then $\mathcal{T} = \mathcal{T}_\mathbb{R}$ and the $\widehat{T}_{k\,e_i}$ are the usual generalized Chebyshev polynomials of the first kind from Definition 1.32. The same holds for D_n, n even. If n is odd on the other hand, then $T_{k\,e_i}(z) = \widehat{T}_{k\,e_i}(\tilde{z})$ with $\frac{z_{n-1}+z_n}{2} = \tilde{z}_{n-1}$ and $\frac{z_{n-1}-z_n}{2\mathrm{i}} = \tilde{z}_n$. Finally, for A_{n-1}, we have $\frac{T_{k\,e_i}(z)+T_{-k\,e_i}(z)}{2} = \frac{T_{k\,e_i}(z)+T_{k\,e_{n-i}}(z)}{2} = \widehat{T}_{k\,e_i}(\tilde{z})$ with $\frac{z_{n-i}+z_i}{2} = \tilde{z}_i$ and $\frac{z_{n-i}-z_i}{2\mathrm{i}} = \tilde{z}_{n-i}$.*

5. *If R is of type A_2 or G_2, then P is a (3×3)–matrix.*

It now remains to show that a polynomial description of $\mathcal{T}$ via matrices of Hermite quadratic forms as in the proof of Theorem 2.19 exists for the individual cases.

4 Type A_{n-1}

In this section, we give a closed formula for the matrix polynomial from Theorem 2.19 in the standard monomial basis for A_{n-1}. The ring of Laurent polynomials is $\mathbb{R}[x^\pm] = \mathbb{R}[x_1, x_1^{-1}, \ldots, x_{n-1}, x_{n-1}^{-1}]$ and the polynomial ring is $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_{n-1}]$.

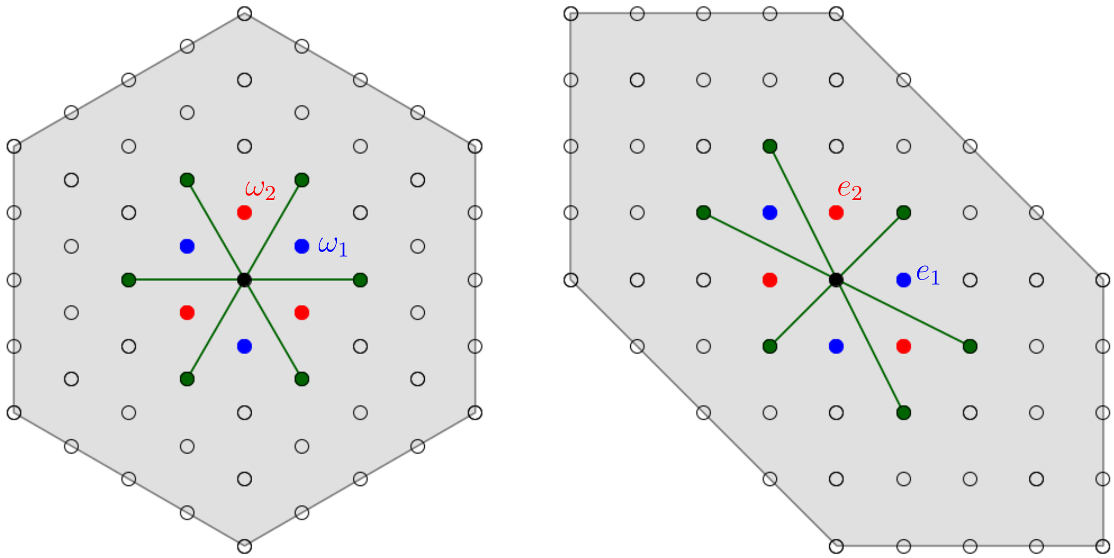


Figure 2.2: The root system A_2 and the weight lattice in the usual orthogonal representation and the integer representation. The orbits of the fundamental weights are the blue and red lattice elements.

4.1 Orbit polynomials

We denote by $\mathcal{G} \in \mathrm{GL}_{n-1}(\mathbb{Z})$ the integer representation of $\mathfrak{S}_n$ with respect to the fundamental weights in Equation (1.3). Then the orbit $\mathcal{G} \cdot x_1 = \{x^\alpha \in \mathbb{R}[x^\pm] \,|\, \exists B \in \mathcal{G} : \alpha = Be_1\}$ consists of the n distinct monomials

$$y_1 = x_1, \quad y_2 = x_2\, x_1^{-1}, \quad \ldots, \quad y_{n-1} = x_{n-1}\, x_{n-2}^{-1}, \quad y_n = x_{n-1}^{-1}. \tag{2.1}$$

For $1 \leq i \leq n$, let σ_i be the i–th elementary symmetric function in n indeterminates and recall that, for $i \leq n-1$, θ_i is the $\mathcal{G}$–invariant orbit polynomial associated to $e_i \in \mathbb{Z}^{n-1}$.

Proposition 2.21. *For $x \in (\mathbb{C}^*)^{n-1}$, we have*

$$\sigma_i(y_1(x), \ldots, y_n(x)) = \binom{n}{i}\, \theta_i(x) \quad \text{and} \quad \sigma_n(y_1(x), \ldots, y_n(x)) = 1.$$

Proof. It follows from Equation (2.1) that $x_i = y_1(x) \ldots y_i(x)$ and $\mathcal{G}$ acts on the $y_i(x)$ by permutation. Hence,

$$\theta_i(x) = \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} x^{B\, e_i} = \frac{|\mathrm{Stab}_{\mathcal{G}}(x_i)|}{|\mathcal{G}|} \sum_{\substack{J \subseteq \{1,\ldots,n\} \\ |J| = i}} \prod_{j \in J} y_j(x) = \frac{1}{|\mathcal{G} \cdot x_i|}\, \sigma_i(y_1(x), \ldots, y_n(x)).$$

With $|\mathcal{G} \cdot x_i| = \binom{n}{i}$ and $1 = y_1(x) \ldots y_n(x)$, we obtain the statement. □

We set $\mathbb{T}_1^n := \{x \in \mathbb{T}^n \mid x_1 \ldots x_n = 1\}$.

Lemma 2.22. *The map*

$$\begin{array}{rccl} \psi : & (\mathbb{C}^*)^{n-1} & \to & (\mathbb{C}^*)^n, \\ & x & \mapsto & (y_1(x), \ldots, y_n(x)), \end{array}$$

is injective and the image contains $\mathbb{T}_1^n$. The preimage of $\mathbb{T}_1^n$ is $\mathbb{T}^{n-1}$.

Proof. This follows immediately from Equation (2.1). □

4.2 Hermite characterization with standard monomials

We now characterize, whether a given point z is contained in the $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$, that is, if the equation $\theta_i(x) = z_i$ has a solution $x \in \mathbb{T}^n$. As we have shown in the previous subsection, this is now equivalent to determining the solutions of a symmetric polynomial system of type (I), which can be done with the techniques from Section 2. Hence, we can state our main result for A_{n-1} in the standard monomial basis. For $n = 2$, we are in the univariate case with $\mathcal{T} = [-1, 1]$.

Theorem 2.23. *Let $n \geq 3$. Define the $(n-1)$–dimensional $\mathbb{R}$–vector space $\mathcal{Z} := \{z \in \mathbb{C}^{n-1} \,|\, \forall\, 1 \leq i \leq n-1 : \overline{z_i} = z_{n-i}\}$ and the matrix $P \in \mathbb{R}[z]^{n\times n}$ by*

$$P(z)_{ij} = \mathrm{Trace}((C(z))^{i+j-2} - (C(z))^{i+j}), \quad \textit{where} \quad C(z) = \begin{bmatrix} 0 & 1/2 & & & 0 & -d_n(z)/4 \\ 1 & 0 & \ddots & & & -d_{n-1}(z)/2 \\ & 1/2 & \ddots & \ddots & & \vdots \\ & & \ddots & \ddots & 1/2 & -d_3(z)/2 \\ & & & \ddots & 0 & (1-d_2(z))/2 \\ 0 & & & & 1/2 & -d_1(z)/2 \end{bmatrix},$$

$$d_\ell(z) = (-1)^\ell \sum_{i=0}^{\ell} \binom{n}{i} \binom{n}{\ell - i} z_i\, z_{n-\ell+i} \Big|_{z_0 = z_n = 1} \quad \textit{for} \quad 1 \leq \ell \leq n.$$

For $z \in \mathcal{Z}$, $P(z) \in \mathbb{R}^{n\times n}$ and $\mathcal{T} = \{z \in \mathcal{Z} \,|\, P(z) \succeq 0\}$.

Proof. For $z \in \mathbb{C}^{n-1}$, define $c_0 := 1$, $c_n := (-1)^n$, $c_i := (-1)^i \binom{n}{i} z_i \in \mathbb{C}$ for $1 \leq i \leq n-1$ as well as $d_\ell := d_\ell(z)$ for $1 \leq \ell \leq n$.

To show "$\subseteq$", assume that $z \in \mathcal{T}$ and fix $x \in \mathbb{T}^{n-1}$, such that $\theta_i(x) = z_i$. By Proposition 2.21, the unique solution of

$$\text{(I)} \quad \sigma_i(y_1, \ldots, y_n) = (-1)^i\, c_i \quad \text{for} \quad 1 \leq i \leq n$$

is $y = \psi(x) \in \mathbb{T}_1^n$, where ψ is the map from Lemma 2.22. Note that $\theta_j(x)$ and $\theta_{n-j}(x)$ are complex conjugates, because $-\omega_j \in \mathcal{W}\,\omega_{n-j}$. Therefore, $z \in \mathcal{Z}$ and $d_\ell = \sum_{i=0}^{\ell} c_i\, \overline{c_{\ell-i}} \in \mathbb{R}$ yields the last column of $C(z)$. Corollary 2.15 gives us $P(z) \succeq 0$.

For "$\supseteq$" on the other hand, assume $z \in \mathcal{Z}$ with $P(z) \succeq 0$. By Corollary 2.15, the solution y of system (I) is contained in $\mathbb{T}_1^n$. Let $x \in \mathbb{T}^{n-1}$ be the unique preimage of y under ψ. Then by Proposition 2.21,

$$z_i = (-1)^i \binom{n}{i}^{-1} c_i = \binom{n}{i}^{-1} \sigma_i(y_1, \ldots, y_n) = \theta_i(x)$$

for $1 \leq i \leq n-1$ and so $z = \vartheta(x) \in \mathcal{T}$. □

Example: A_2

Let $z_1, z_2 \in \mathbb{R}$ and $z = (z_1 + \mathrm{i} z_2, z_1 - \mathrm{i} z_2)$. We give conditions for the membership of z in the $\mathbb{T}$–orbit space. The matrix $C \in \mathbb{R}[z]^{3\times 3}$ from Theorem 2.23 is

$$C(z) = \begin{bmatrix} 0 & 1/2 & (1 + 9\, z_1^2 - 9\, z_2^2)/2 \\ 1 & 0 & (1 - 9\, z_1^2 - 9\, z_2^2 - 6\, z_1)/2 \\ 0 & 1/2 & 3\, z_1 \end{bmatrix}.$$

Define the matrix $P \in \mathbb{R}[z]^{3\times 3}$ with entries $(P(z))_{ij} = \mathrm{Trace}(C(z)^{i+j-2}) - \mathrm{Trace}(C(z)^{i+j})$. Then $z \in \mathcal{T}$ if and only if $P(z)$ is positive semi–definite. Assume that

$$\mathrm{Det}(x\, I_3 - P(z)) = x^3 - p_1(z)\, x^2 + p_2(z)\, x - p_3(z)$$

is the characteristic polynomial of $P(z)$, where

$$\begin{aligned}
p_3(z) &= -\mathrm{Coeff}(x^0, \mathrm{Det}(x\, I_3 - P(z))) \quad \text{(solid)}\\
&= 2187/64\, z_2^4\, (3\, z_1 + 1)^2\, (-3\, z_1^4 - 6\, z_1^2\, z_2^2 - 3\, z_2^4 + 8\, z_1^3 - 24\, z_1\, z_2^2 - 6\, z_1^2 - 6\, z_2^2 + 1)\\
p_2(z) &= \quad \mathrm{Coeff}(x^1, \mathrm{Det}(x\, I_3 - P(z))) \quad \text{(dots)}\\
&= 243/256\, z_2^2\, (-243\, z_1^8 - 972\, z_1^6\, z_2^2 - 1458\, z_1^4\, z_2^4 - 972\, z_1^2\, z_2^6 - 243\, z_2^8 + 324\, z_1^7 - 1620\, z_1^5\, z_2^2\\
&\quad -4212\, z_1^3\, z_2^4 - 2268\, z_1\, z_2^6 - 432\, z_1^6 - 2052\, z_1^4\, z_2^2 - 5400\, z_1^2\, z_2^4 - 324\, z_2^6 + 180\, z_1^5 - 3384\, z_1^3\, z_2^2\\
&\quad -684\, z_1\, z_2^4 + 18\, z_1^4 - 804\, z_1^2\, z_2^2 + 42\, z_2^4 + 76\, z_1^3 + 404\, z_1\, z_2^2 - 8\, z_1^2 - 108\, z_2^2 + 60\, z_1 + 25),\\
p_1(z) &= -\mathrm{Coeff}(x^2, \mathrm{Det}(x\, I_3 - P(z))) \quad \text{(dash)}\\
&= 1/32\, (-729\, z_1^6 + 1458\, z_1^5 + (10935\, z_2^2 - 1215)\, z_1^4 + (-2916\, z_2^2 + 540)\, z_1^3 + 351\, z_2^2 + 63\\
&\quad +(-10935\, z_2^4 + 1458\, z_2^2 - 135)\, z_1^2 + (-4374\, z_2^4 + 972\, z_2^2 + 18)\, z_1 + 729\, z_2^6 - 1215\, z_2^4).
\end{aligned}$$

Then $P(z)$ is positive semi–definite if and only if $p_i(z) \geq 0$ for $1 \leq i \leq 3$. We visualize the problem "$z \in \mathcal{T}$?" by evaluating p_1, p_2, p_3 in $(z_1, z_2) \in \mathbb{R}^2$. In Figure 2.3, a solid red line, blue dots and green dashes indicate the varieties of these three polynomials.

From the plots, we suspect that the real $\mathbb{T}$–orbit space is invariant under the dihedral group $\mathfrak{D}_3$ of order 6 with its canonical action on $\mathbb{R}^2$. The $\mathfrak{D}_3$–invariants are $\mathbb{R}[z]^{\mathfrak{D}_3} = \mathbb{R}[g_1, g_2]$ with $g_1(z) := z_1^2 + z_2^2$ and $g_2(z) := z_1\, (z_1^2 - 3\, z_2^2)$. Then we have

$$p_3(z) = \underbrace{2187/64\, z_2^4\, (3\, z_1 + 1)^2}_{\geq 0}\, \underbrace{(-6\, g_1(z) - 3\, g_1(z)^2 + 8\, g_2(z) + 1)}_{\mathfrak{D}_3\text{–invariant}}.$$

and the variety of the $\mathfrak{D}_3$–invariant part gives the boundary of $\mathcal{T}_\mathbb{R}$.

We now identify the vertices of $\mathcal{T}$, which correspond to the fundamental weights and the origin. With $\vartheta_\mathbb{R} = \left(\frac{\theta_1+\theta_2}{2}, \frac{\theta_1-\theta_2}{2\mathrm{i}}\right)$, those are

$$\mathrm{Vertex}_1 := \vartheta_\mathbb{R}(\exp(-2\pi\mathrm{i}\, \langle \omega_1, \omega_1\rangle), \exp(-2\pi\mathrm{i}\, \langle \omega_2, \omega_1\rangle)) = \vartheta_\mathbb{R}\left(\exp\left(-\frac{4}{3}\pi\mathrm{i}\right), \exp\left(-\frac{2}{3}\pi\mathrm{i}\right)\right) = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right),$$

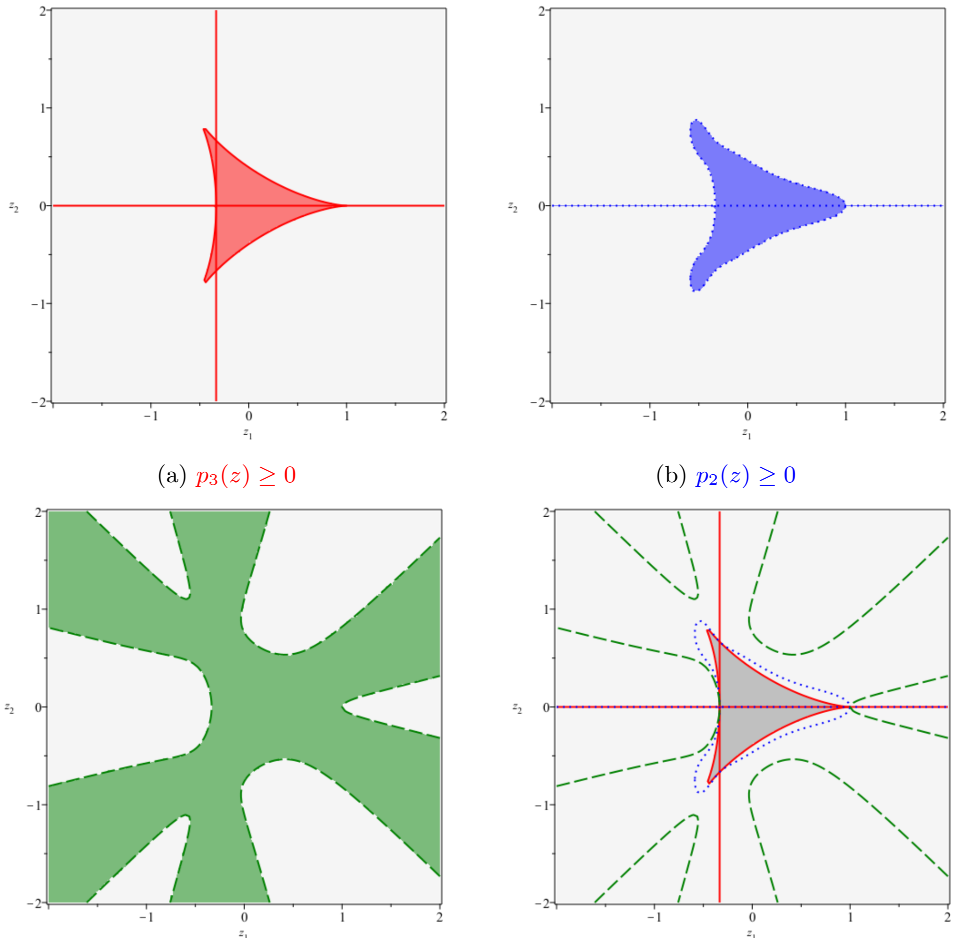
$$\mathrm{Vertex}_2 := \vartheta_\mathbb{R}(\exp(-2\pi\mathrm{i}\, \langle \omega_1, \omega_2\rangle), \exp(-2\pi\mathrm{i}\, \langle \omega_2, \omega_2\rangle)) = \vartheta_\mathbb{R}\left(\exp\left(-\frac{2}{3}\pi\mathrm{i}\right), \exp\left(-\frac{4}{3}\pi\mathrm{i}\right)\right) = \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2}\right),$$

$$\mathrm{Vertex}_3 := \vartheta_\mathbb{R}(\exp(-2\pi\mathrm{i}\, \langle \omega_1, 0\rangle), \exp(-2\pi\mathrm{i}\, \langle \omega_2, 0\rangle)) = \vartheta_\mathbb{R}(1, 1) = (1, 0)\,.$$

For a generic point $(z_1, z_2) \in \mathbb{R}^2$, $P(z)$ has rank 3. We observe an intersection of all three varieties in Vertex_3, in which case the rank of $P(\mathrm{Vertex}_3)$ vanishes. This also occurs at

$$\vartheta_\mathbb{R}(\exp(-2\pi\mathrm{i}\langle \omega_1, (\omega_1+\omega_2)/2\rangle), \exp(-2\pi\mathrm{i}\langle \omega_2, (\omega_1+\omega_2)/2\rangle)) = \vartheta_\mathbb{R}(\exp(-\pi\mathrm{i}), \exp(\pi\mathrm{i})) = \left(-\frac{1}{3}, 0\right).$$

Furthermore, the rank of both $P(\mathrm{Vertex}_1), P(\mathrm{Vertex}_2)$ is 1, we only have an intersection of "$p_3(z) = 0$" with "$p_2(z) = 0$". Two more intersections of "$p_3(z) = 0$" with "$p_1(z) = 0$" lie at $(-1/3, 2/3)$ and $(-1/3, -2/3)$. Every other point on the boundary of $\mathcal{T}$ admits rank 2.



(a) $p_3(z) \geq 0$

(b) $p_2(z) \geq 0$

(c) $p_1(z) \geq 0$

(d) $p_1(z), p_2(z), p_3(z) \geq 0$

Figure 2.3: Varieties and positivity regions for the coefficients of the characteristic polynomial of $P(z)$.

5 Type C_n

In this section, we give a closed formula for the matrix polynomial from Theorem 2.19 in the standard monomial basis for C_n. This is a root system of rank n. Hence, the ring of Laurent polynomials is $\mathbb{R}[x^\pm] = \mathbb{R}[x_1, x_1^{-1}, \ldots, x_n, x_n^{-1}]$ and the polynomial ring is $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_n]$.

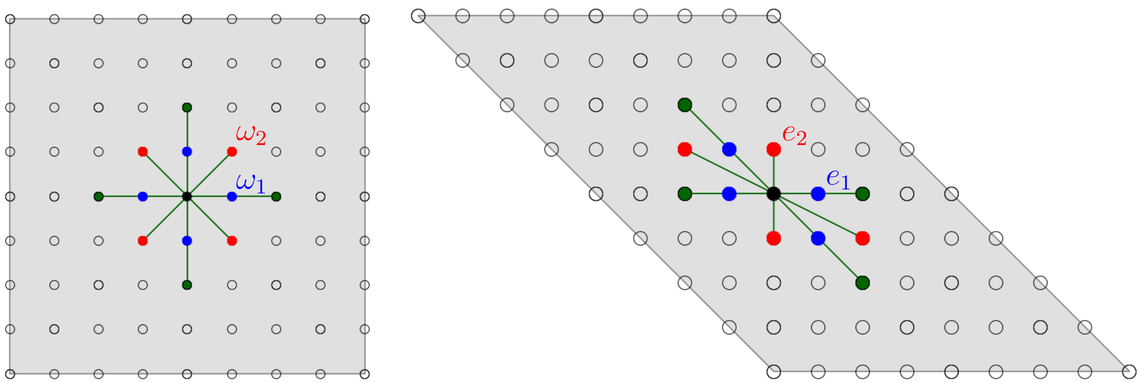


Figure 2.4: The root system C_2 and the weight lattice in the usual orthogonal representation and the integer representation. The orbits of the fundamental weights are the blue and red lattice elements.

5.1 Orbit polynomials

We denote by $\mathcal{G} \in \mathrm{GL}_n(\mathbb{Z})$ the integer representation of $\mathfrak{S}_n \ltimes \{\pm 1\}^n$ with respect to the fundamental weights in Equation (1.5). Then the orbit $\mathcal{G} \cdot x_1 = \{x^\alpha \in \mathbb{R}[x^\pm] \,|\, \exists\, B \in \mathcal{G} : \alpha = B e_1\}$ consists of $2\,n$ distinct monomials, given by

$$y_1 = x_1, \quad y_2 = x_2\, x_1^{-1}, \quad \ldots, \quad y_n = x_n\, x_{n-1}^{-1} \tag{2.1}$$

and their inverses. For $1 \leq i \leq n$, let σ_i be the i–th elementary symmetric function in n indeterminates and recall that θ_i is the $\mathcal{G}$–invariant orbit polynomial associated to $e_i \in \mathbb{Z}^n$.

Proposition 2.24. *For $x \in (\mathbb{C}^*)^n$, we have*

$$\sigma_i \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) = \binom{n}{i} \theta_i(x).$$

Proof. It follows from Equation (2.1) that $x_i = y_1(x) \ldots y_i(x)$ and $\mathcal{G}$ acts on the $y_i^{\pm 1}(x)$ by permutation. Hence,

$$\theta_i(x) = \frac{1}{|\mathcal{G}|} \sum_{B \in \mathcal{G}} x^{B\, e_i} = \frac{|\mathrm{Stab}_{\mathcal{G}}(x_i)|}{|\mathcal{G}|} \sum_{\substack{J \subseteq \{1,\ldots,n\} \\ |J| = i}} \sum_{\delta \in \{\pm 1\}^J} \prod_{j \in J} y_j(x)^{\delta_j} = \frac{1}{|\mathcal{G} \cdot x_i|} \sum_{\substack{J \subseteq \{1,\ldots,n\} \\ |J| = i}} \prod_{j \in J} (y_j(x) + y_j(x)^{-1})$$

With $|\mathcal{G} \cdot x_i| = 2^i \binom{n}{i}$, we obtain the statement. □

Lemma 2.25. *The map*

$$\begin{array}{cccc} \psi: & (\mathbb{C}^*)^n & \to & (\mathbb{C}^*)^n, \\ & x & \mapsto & (y_1(x), \ldots, y_n(x)). \end{array}$$

is bijective and the preimage of $\mathbb{T}^n$ is $\mathbb{T}^n$.

Proof. This follows immediately from Equation (2.1). □

5.2 Hermite characterization with standard monomials

We now characterize, whether a given point z is contained in the $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$, that is, if the equation $\theta_i(x) = z_i$ has a solution $x \in \mathbb{T}^n$. As we have shown in the previous subsection, this is now equivalent to determining the solutions of a symmetric polynomial system of type (II), which can be done with the techniques from Section 2.

Theorem 2.26. *Define the matrix $P \in \mathbb{R}[z]^{n\times n}$ by*

$$P(z)_{ij} = \mathrm{Trace}(C(z)^{i+j-2} - C(z)^{i+j}), \quad \textit{where} \quad C(z) = \begin{bmatrix} 0 & \cdots & 0 & -c_n(z) \\ 1 & & 0 & -c_{n-1}(z) \\ & \ddots & & \vdots \\ 0 & & 1 & -c_1(z) \end{bmatrix},$$

$$c_i(z) = (-1)^i \binom{n}{i} z_i \quad \textit{for} \quad 1 \leq i \leq n.$$

Then $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$.

Proof. Let $z \in \mathbb{R}^n$ and set $c_i := c_i(z) \in \mathbb{R}$ for $1 \leq i \leq n$.

To show "$\subseteq$", assume that $z \in \mathcal{T}$. Then there exists $x \in \mathbb{T}^n$, such that $\theta_i(x) = z_i$ for $1 \leq i \leq n$. By Proposition 2.24, the solution of the symmetric polynomial system

$$\text{(II)} \quad \sigma_i\left(\frac{y_1 + y_1^{-1}}{2}, \ldots, \frac{y_n + y_n^{-1}}{2}\right) = (-1)^i c_i \quad \text{for} \quad 1 \leq i \leq n$$

is $y = \psi(x) \in \mathbb{T}^n$, where ψ is the map from Lemma 2.25. Applying Corollary 2.16 yields $P(z) \succeq 0$.

For "$\supseteq$" on the other hand, assume $P(z) \succeq 0$. By Corollary 2.16, the solution y of the above system (II) is contained in $\mathbb{T}^n$. Let $x \in \mathbb{T}^n$ be the unique preimage of y under ψ. Then $z_i = \theta_i(x)$ and so $z = \vartheta(x)$ is contained in $\mathcal{T}$. □

Example: C_2

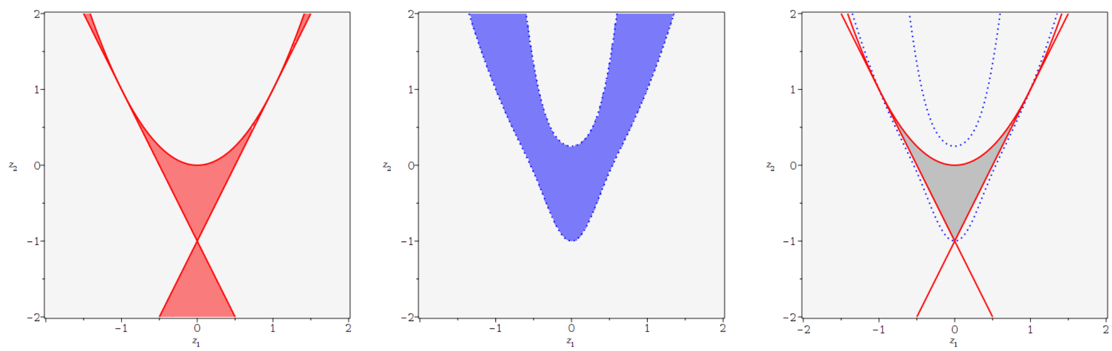
Let $z = (z_1, z_2) \in \mathbb{R}^2$. The matrix $C \in \mathbb{R}[z]^{2\times 2}$ from Theorem 2.26 is

$$C(z) = \begin{bmatrix} 0 & -z_2 \\ 1 & 2\,z_1 \end{bmatrix}.$$

Then z is contained in $\mathcal{T}$ if and only if the resulting Hermite matrix

$$P(z) = \begin{bmatrix} -4\,z_1^2 + 2\,z_2 + 2 & -8\,z_1^3 + 6\,z_1\,z_2 + 2\,z_1 \\ -8\,z_1^3 + 6\,z_1\,z_2 + 2\,z_1 & -16\,z_1^4 + 16\,z_1^2\,z_2 + 4\,z_1^2 - 2\,z_2^2 - 2\,z_2 \end{bmatrix}$$

is positive semi–definite, which is equivalent to its determinant and trace being nonnegative. The varieties of these two polynomials in z_1, z_2 are depicted below.



(a) $\mathrm{Det}(P(z) \geq 0$ (b) $\mathrm{Trace}(P(z) \geq 0$ (c) $\mathrm{Det}(P(z), \mathrm{Trace}(P(z) \geq 0$

Figure 2.5: Vanishing points and positivity regions for determinant and trace of $P(z)$.

$$\begin{array}{rcll} \mathrm{Det}(P(z)) & = & -4\,(z_1^2 - z_2)\,(2\,z_1 + 1 + z_2)\,(2\,z_1 - 1 - z_2) & \text{(solid)} \\ \mathrm{Trace}(P(z)) & = & -16\,z_1^4 + 16\,z_1^2\,z_2 - 2\,z_2^2 + 2 & \text{(dots)} \end{array}$$

We observe three intersections of “$\mathrm{Det}(P(z)) = 0$” (red solid line) and “$\mathrm{Trace}(P(z)) = 0$” (blue dots) in the the vertices

$$\begin{aligned} \mathrm{Vertex}_1 &:= \vartheta(\exp(-2\pi\mathrm{i}\,\langle \omega_1, \omega_1/2\rangle), \exp(-2\pi\mathrm{i}\,\langle \omega_2, \omega_1/2\rangle)) = \vartheta(-1,-1) = (0,-1), \\ \mathrm{Vertex}_2 &:= \vartheta(\exp(-2\pi\mathrm{i}\,\langle \omega_1, \omega_2/2\rangle), \exp(-2\pi\mathrm{i}\,\langle \omega_2, \omega_2/2\rangle)) = \vartheta(-1,1) = (-1,1), \\ \mathrm{Vertex}_3 &:= \vartheta(\exp(-2\pi\mathrm{i}\,\langle \omega_1, 0\rangle), \exp(-2\pi\mathrm{i}\,\langle \omega_2, 0\rangle)) = \vartheta(1,1) = (1,1). \end{aligned}$$

The shape of this domain is dictated by the determinant, but from the positivity condition one can observe that the trace is also required. Alternatively the inequation given by the trace could be replaced by the constraint that the orbit space is contained in the square $[-1,1]^2$.

6 Type B_n

In this section, we give a closed formula for the matrix polynomial from Theorem 2.19 in the standard monomial basis for B_n. This is a root system of rank n. Hence, the ring of Laurent polynomials is $\mathbb{R}[x^\pm] = \mathbb{R}[x_1, x_1^{-1}, \ldots, x_n, x_n^{-1}]$ and the polynomial ring is $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_n]$.

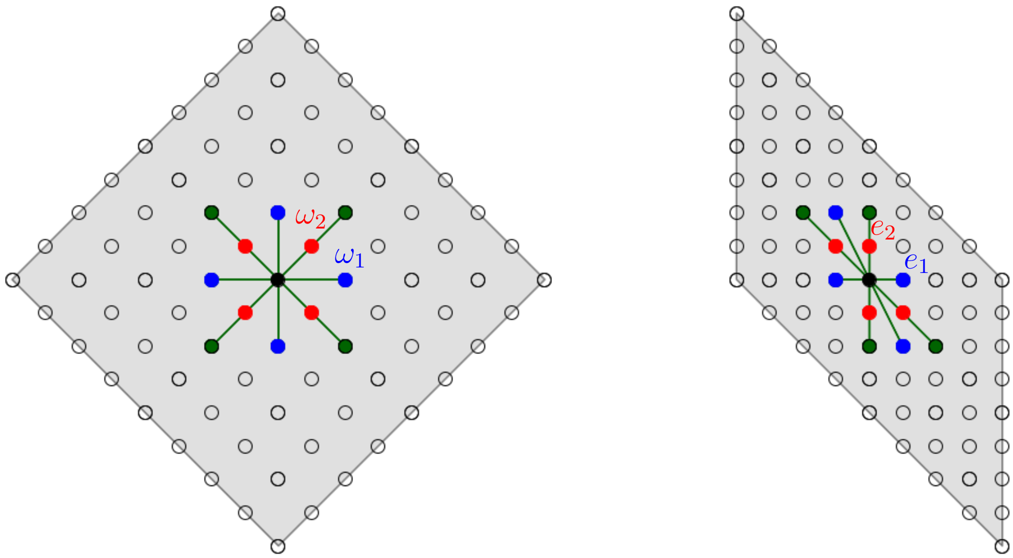


Figure 2.6: The root system B_2 and the weight lattice in the usual orthogonal representation and the integer representation. The orbits of the fundamental weights are the blue and red lattice elements.

6.1 Orbit polynomials

We denote by $\mathcal{G} \in \mathrm{GL}_n(\mathbb{Z})$ the integer representation of $\mathfrak{S}_n \ltimes \{\pm 1\}^n$ with respect to the fundamental weights in Equation (1.7). Then the orbit $\mathcal{G} \cdot x_1 = \{x^\alpha \in \mathbb{R}[x^\pm] \,|\, \exists\, B \in \mathcal{G} : \alpha = B e_1\}$ consists of $2\,n$ distinct monomials, given by

$$y_1 = x_1, \quad y_2 = x_2\, x_1^{-1}, \quad \ldots, \quad y_{n-1} = x_{n-1}\, x_{n-2}^{-1}, \quad y_n = x_n^2\, x_{n-1}^{-1} \tag{2.1}$$

and their inverses. For $1 \leq i \leq n$, let σ_i be the i–th elementary symmetric function in n indeterminates and recall that θ_i is the $\mathcal{G}$–invariant orbit polynomial associated to $e_i \in \mathbb{Z}^n$.

Proposition 2.27. *For $x \in (\mathbb{C}^*)^n$, we have*

$$\begin{aligned} \sigma_i \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) &= \binom{n}{i} \theta_i(x) \\ \text{and} \quad \sigma_n \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) &= \Theta_{2\,e_n}(x). \end{aligned}$$

Proof. It follows from Equation (2.1) that $x_i = y_1(x) \ldots y_i(x)$ and $x_n^2 = y_1(x) \ldots y_n(x)$. Then the proof is analogous to Proposition 2.24. ☐

We have computed the explicit expression for the right hand side of Proposition 2.27 in Lemma 1.42.

Lemma 2.28. *The map*

$$\begin{array}{rccl} \psi : & (\mathbb{C}^*)^n & \to & (\mathbb{C}^*)^n, \\ & x & \mapsto & (y_1(x), \ldots, y_n(x)). \end{array}$$

is surjective and the preimage of $\mathbb{T}^n$ is $\mathbb{T}^n$. Furthermore, every $y \in \mathbb{T}^n$ has exactly two distinct preimages $x, x' \in \mathbb{T}^n$ with

$$\theta_i(x) = \theta_i(x') \quad \text{and} \quad \theta_n(x) = -\theta_n(x').$$

Proof. For all $y \in (\mathbb{C}^*)^n$, there exists $x \in (\mathbb{C}^*)^n$ with $x_1 = y_1, x_2 = y_1\, x_1, \ldots, x_{n-1} = y_{n-1}\, x_{n-2}$ and $x_n^2 = y_n\, x_{n-1}$. Thus, x is a preimage of y under ψ and uniquely determined by y up to a sign in the last coordinate. We have $y \in \mathbb{T}^n$ if and only if $x \in \mathbb{T}^n$.

We have $\mathcal{W}(\mathrm{B}_n) = \mathcal{W}(\mathrm{A}_{n-1}) \ltimes \{\pm 1\}^n$ and $\mathrm{Stab}_{\mathcal{W}(\mathrm{B}_n)}(\omega_n) \cong \mathcal{W}(\mathrm{A}_{n-1})$. Hence, $\mathcal{W}(\mathrm{B}_n)\, \omega_n = \{\pm 1\}^n\, \omega_n$. Now let $\mu \in \mathcal{W}(\mathrm{B}_n)\, \omega_n$. Then there exist $\epsilon_i = \pm 1$ and $\nu \in \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_{n-1}$, such that $\mu = \epsilon_n\, \omega_n + \nu$. Indeed,

$$\mu = \frac{\epsilon_1}{2}\, e_1 + \ldots + \frac{\epsilon_n}{2}\, e_n = \frac{\epsilon_1}{2}\, \omega_1 + \sum_{i=2}^{n-1} \frac{\epsilon_i}{2}\, (\omega_i - \omega_{i-1}) + \frac{\epsilon_n}{2}\, (2\, \omega_n - \omega_{n-1}) = \epsilon_n\, \omega_n + \nu.$$

Let W be the isomorphism that takes e_i to ω_i and let $\alpha, \beta \in \mathbb{Z}^n$, such that $\mu = W\alpha$, $\nu = W\beta$. Then $\beta_n = 0$ and the monomial in θ_n corresponding to μ is $x^\alpha = x_1^{\beta_1} \ldots x_{n-1}^{\beta_{n-1}}\, x_n^{\epsilon_n}$. Thus, x^α is linear in x_n. Since every monomial in θ_n can be written in terms of such β and ϵ_i, θ_n is linear in x_n and with x, x' as above we have $\theta_n(x) = -\theta_n(x')$. □

6.2 Hermite characterization with standard monomials

We now characterize, whether a given point z is contained in the $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$, that is, if the equation $\theta_i(x) = z_i$ has a solution $x \in \mathbb{T}^n$. As we have shown in the previous subsection, this is now equivalent to determining the solutions of a symmetric system of type (II).

Theorem 2.29. *Define the matrix* $P \in \mathbb{R}[z]^{n\times n}$ *by*

$$P(z)_{ij} = \mathrm{Trace}(C(z)^{i+j-2} - C(z)^{i+j}), \quad \textit{where} \quad C(z) = \begin{bmatrix} 0 & \cdots & 0 & -c_n(z) \\ 1 & & 0 & -c_{n-1}(z) \\ & \ddots & & \vdots \\ 0 & & 1 & -c_1(z) \end{bmatrix},$$

$$c_i(z) = (-1)^i \binom{n}{i} z_i \quad \textit{for} \quad 1 \le i \le n-1,$$

$$c_n(z) = (-1)^n \left(2^n\, z_n^2 - \sum_{i=1}^{n-1} \binom{n}{i} z_i - 1 \right).$$

Then $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$.

Proof. Let $z \in \mathbb{R}^n$ and set $c_i := c_i(z) \in \mathbb{R}$ for $1 \le i \le n$.

To show "$\subseteq$", assume that $z \in \mathcal{T}$. Then there exists $x \in \mathbb{T}^n$, such that $\theta_i(x) = z_i$ for $1 \le i \le n$. By Proposition 2.27 and Lemma 1.42, the solution of the symmetric polynomial system

$$\text{(II)} \quad \sigma_i \left(\frac{y_1 + y_1^{-1}}{2}, \ldots, \frac{y_n + y_n^{-1}}{2} \right) = (-1)^i\, c_i \quad \text{for} \quad 1 \le i \le n$$

is $y = \psi(x) \in \mathbb{T}^n$, where ψ is the map from Lemma 2.28. Applying Corollary 2.16 yields $P(z) \succeq 0$.

For "$\supseteq$" on the other hand, assume $P(z) \succeq 0$. By Corollary 2.16, the solution y of system (II) with coefficients c_i is contained in $\mathbb{T}^n$. According to Lemma 2.28, y has exactly two distinct preimages $x, x' \in \mathbb{T}^n$ under ψ with $x_1 = x_1', \ldots, x_{n-1} = x_{n-1}'$ and $x_n = -x_n'$. We have $z_i = \theta_i(x) = \theta_i(x')$ for $1 \le i \le n-1$ and $z_n^2 = \theta_n(x)^2 = \theta_n(x')^2$ with $\theta_n(x) = -\theta_n(x')$. Therefore, $z_n = \theta_n(x)$ or $z_n = \theta_n(x') = -\theta_n(x)$ and thus, z is contained in $\mathcal{T}$. □

Example: B_2

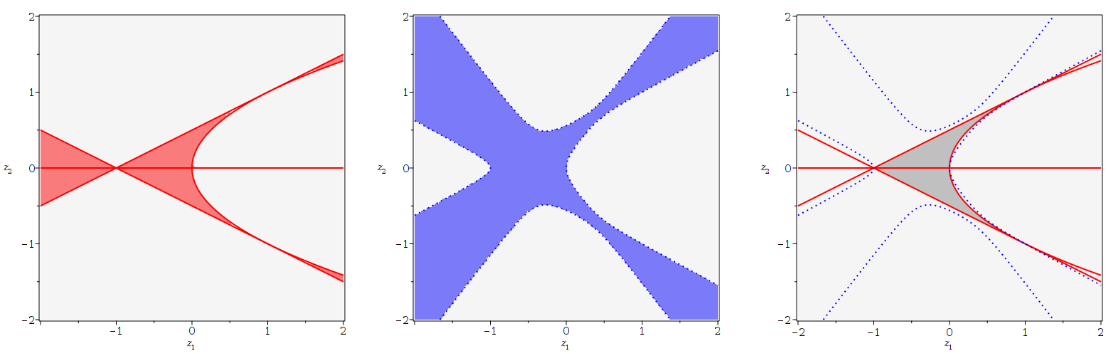
Let $z = (z_1, z_2) \in \mathbb{R}^2$. The matrix $C \in \mathbb{R}[z]^{2\times 2}$ from Theorem 2.29 is

$$C(z) = \begin{bmatrix} 0 & -4\,z_2^2 + 2\,z_1 + 1 \\ 1 & 2\,z_1 \end{bmatrix}.$$

Then z is contained in $\mathcal{T}$ if and only if the resulting Hermite matrix

$$P(z) = 16 \begin{bmatrix} -4\,z_1^2 + 8\,z_2^2 - 4\,z_1 & -8\,z_1^3 + 24\,z_1\,z_2^2 - 12\,z_1^2 - 4\,z_1 \\ -8\,z_1^3 + 24\,z_1\,z_2^2 - 12\,z_1^2 - 4\,z_1 & -16\,z_1^4 + 64\,z_1^2\,z_2^2 - 32\,z_2^4 - 32\,z_1^3 + 32\,z_1\,z_2^2 - 20\,z_1^2 + 8\,z_2^2 - 4\,z_1 \end{bmatrix}$$

is positive semi–definite, which is equivalent to its determinant and trace being nonnegative. The varieties of these two polynomials in z_1, z_2 are depicted below.



(a) $\mathrm{Det}(P(z)) \geq 0$ (b) $\mathrm{Trace}(P(z)) \geq 0$ (c) $\mathrm{Det}(P(z), \mathrm{Trace}(P(z)) \geq 0$

Figure 2.7: Vanishing points and positivity regions for determinant and trace of $P(z)$.

$$\begin{aligned} \mathrm{Det}(P(z)) &= -64\,z_2^2\,(-z_2^2 + z_1)\,(z_1 + 1 + 2\,z_2)\,(z_1 + 1 - 2\,z_2) && \text{(solid)} \\ \mathrm{Trace}(P(z)) &= -16\,z_1^4 + 64\,z_1^2\,z_2^2 - 32\,z_2^4 - 32\,z_1^3 + 32\,z_1\,z_2^2 - 24\,z_1^2 + 16\,z_2^2 - 8\,z_1 && \text{(dots)} \end{aligned}$$

The $\mathbb{T}$–orbit space in the B_2–case is obtained from the C_2–case in Figure 2.5 by permuting z_1, z_2. Apart from that, we also observe that the determinant has an additional irreducible factor. Indeed, the determinant of $P(z)$ is 0 on the line "$z_2 = 0$"and the rank is 0 in $z = (0, 0)$, although this is not a vertex.

7 Type D_n

In this section, we give a closed formula for the matrix polynomial from Theorem 2.19 in the standard monomial basis for D_n. This is a root system of rank n. Hence, the ring of Laurent polynomials is $\mathbb{R}[x^\pm] = \mathbb{R}[x_1, x_1^{-1}, \ldots, x_n, x_n^{-1}]$ and the polynomial ring is $\mathbb{R}[z] = \mathbb{R}[z_1, \ldots, z_n]$.

7.1 Orbit polynomials

We denote by $\mathcal{G} \in \mathrm{GL}_n(\mathbb{Z})$ the integer representation of $\mathfrak{S}_n \ltimes \{\pm 1\}_+^n$ with respect to the fundamental weights in Equation (1.9). Then the orbit $\mathcal{G} \cdot x_1 = \{x^\alpha \in \mathbb{R}[x^\pm] \,|\, \exists\, B \in \mathcal{G} : \alpha = B e_1\}$ consists of $2\,n$ distinct monomials, given by

$$y_1 = x_1, \quad y_2 = x_2\,x_1^{-1}, \quad \ldots, \quad y_{n-2} = x_{n-2}\,x_{n-3}^{-1}, \quad y_{n-1} = x_n\,x_{n-1}\,x_{n-2}^{-1}, \quad y_n = x_n\,x_{n-1}^{-1} \tag{2.1}$$

and their inverses. For $1 \le i \le n$, let σ_i be the i–th elementary symmetric function in n indeterminates and recall that θ_i is the $\mathcal{G}$–invariant orbit polynomial associated to $e_i \in \mathbb{Z}^n$.

Proposition 2.30. *For $x \in (\mathbb{C}^*)^n$, we have*

$$\begin{aligned}
\sigma_i \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) &= \binom{n}{i} \theta_i(x),\\
\sigma_{n-1} \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) &= n\, \Theta_{e_{n-1}+e_n}(x),\\
\sigma_n \left(\frac{y_1(x) + y_1(x)^{-1}}{2}, \ldots, \frac{y_n(x) + y_n(x)^{-1}}{2} \right) &= \frac{\Theta_{2\,e_{n-1}}(x) + \Theta_{2\,e_n}(x)}{2}.
\end{aligned}$$

Proof. For $1 \le i \le n-2$, it follows from Equation (2.1) that $x_i = y_1(x) \ldots y_i(x)$. Then the statement for θ_i is proven analogously to Proposition 2.24. With $x_n\, x_{n-1} = y_1(x) \ldots y_{n-1}(x)$, we obtain the equation for $\Theta_{e_{n-1}+e_n}(x)$ as well.

Finally, we have $x_{n-1}^2 = y_1(x) \ldots y_{n-1}(x)\, y_n(x)^{-1}$ and $x_n^2 = y_1(x) \ldots y_n(x)$ and thus obtain

$$\frac{\Theta_{2\,e_{n-1}}(x) + \Theta_{2\,e_n}(x)}{2} = \frac{1}{2^n} \left(\sum_{\substack{\epsilon \in \{\pm 1\}^n \\ \epsilon_1 \ldots \epsilon_n = -1}} y^\epsilon(x) + \sum_{\substack{\epsilon \in \{\pm 1\}^n \\ \epsilon_1 \ldots \epsilon_n = 1}} y^\epsilon(x) \right) = \frac{1}{2^n} \sum_{\epsilon \in \{\pm 1\}^n} y^\epsilon(x) = \frac{1}{2^n} \prod_{i=1}^{n} y_i(x) + y_i(x)^{-1},$$

where $y^\epsilon(x) := y_1^{\epsilon_1}(x) \ldots y_n^{\epsilon_n}(x)$. This proves the last equation. □

We have computed the explicit expression for the right hand side of Proposition 2.30 in Lemma 1.43.

Proposition 2.31. *The map*

$$\begin{array}{rccc}
\psi: & (\mathbb{C}^*)^n & \to & (\mathbb{C}^*)^n,\\
& x & \mapsto & (y_1(x), \ldots, y_n(x)).
\end{array}$$

is surjective and the preimage of $\mathbb{T}^n$ is $\mathbb{T}^n$. Furthermore, every $y \in \mathbb{T}^n$ has exactly two distinct preimages $x, x' \in \mathbb{T}^n$ with

$$\theta_i(x) = \theta_i(x') \quad \text{for} \quad 1 \le i \le n-2 \quad \text{and} \quad \theta_{n-1}(x) = -\theta_{n-1}(x'), \quad \theta_n(x) = -\theta_n(x').$$

Moreover, for all $x \in \mathbb{T}$, there exists $\tilde{x} \in \mathbb{T}$, such that

$$\theta_i(x) = \theta_i(\tilde{x}) \quad \text{for} \quad 1 \le i \le n-2 \quad \text{and} \quad \theta_{n-1}(x) = \theta_n(\tilde{x}), \quad \theta_n(x) = \theta_{n-1}(\tilde{x}).$$

Proof. For all $y \in (\mathbb{C}^*)^n$, there exists $x \in (\mathbb{C}^*)^n$ with $x_1 = y_1, x_2 = y_1\, x_1, \ldots, x_{n-2} = y_{n-2}\, x_{n-3}$ and $x_{n-1}^2 = y_n^{-1}\, y_{n-1}\, x_{n-2}$, $x_n = y_n\, x_{n-1}$. Hence, x is uniquely determined by y up to a sign in x_{n-1} and x_n. We have $y \in \mathbb{T}^n$ if and only if $x \in \mathbb{T}^n$.

For $1 \le i \le n-2$, we have $\theta_i(x) = \theta_i(x')$, because $y_k(x) = y_k(x')$ for all $1 \le k \le n$.

Similar to Lemma 2.28, we have $\mathcal{W}(\mathrm{D}_n)\, \omega_{n-1} = \{\pm 1\}_+^n\, \omega_{n-1}$ and $\mathcal{W}(\mathrm{D}_n)\, \omega_n = \{\pm 1\}_+^n\, \omega_n$. Now let $\mu \in \mathcal{W}(\mathrm{D}_n)\, \omega_n$. Then there exist $\epsilon_i = \pm 1$ and $\nu \in \mathbb{Z}\, \omega_1 \oplus \ldots \oplus \mathbb{Z}\, \omega_{n-2}$, such that

$$\begin{aligned}
\mu = & \quad \frac{\epsilon_1}{2}\, e_1 + \ldots + \frac{\epsilon_n}{2}\, e_n = \frac{\epsilon_1}{2}\, \omega_1 + \sum_{i=2}^{n-2} \frac{\epsilon_i}{2}\, (\omega_i - \omega_{i-1}) + \frac{\epsilon_{n-1}}{2}\, (\omega_n + \omega_{n-1} - \omega_{n-2}) + \frac{\epsilon_n}{2}\, (\omega_n - \omega_{n-1})\\
= & \quad \frac{\epsilon_{n-1} + \epsilon_n}{2}\, \omega_n + \frac{\epsilon_{n-1} - \epsilon_n}{2}\, \omega_{n-1} + \nu \in \Omega
\end{aligned}$$

and $\epsilon_1 \ldots \epsilon_n = 1$. Let W be the isomorphism that takes e_i to ω_i and let $\alpha, \beta \in \mathbb{Z}^n$, such that $\mu = W\alpha, \nu = W\beta$. Then $\beta_{n-1} = \beta_n = 0$ and the monomial in θ_n corresponding to μ is

$$x^\alpha = x_1^{\beta_1} \ldots x_{n-2}^{\beta_{n-2}}\, x_{n-1}^{(\epsilon_{n-1} - \epsilon_n)/2}\, x_n^{(\epsilon_{n-1} + \epsilon_n)/2}$$

with $(\epsilon_{n-1} \pm \epsilon_n)/2 \in \{-1, 0, 1\}$. Therefore, x^α is linear in x_{n-1} and independent of x_n or vice versa. With x, x' as above we have $x^\alpha = -(x')^\alpha$. Since every monomial in θ_n can be written in terms of such β and ϵ_i, we obtain $\theta_n(x) = -\theta_n(x')$. Analogously for $\mu \in \mathcal{W}(\mathrm{D}_n)\,\omega_{n-1}$, we have $\epsilon_1 \ldots \epsilon_n = -1$ and obtain the statement for θ_{n-1}.

The last statement holds for $\tilde{x} = (x_1, \ldots, x_{n-2}, x_n, x_{n-1})$. □

7.2 Hermite characterization with standard monomials

We now characterize, whether a given point z is contained in the $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$, that is, if the equation $\theta_i(x) = z_i$ has a solution $x \in \mathbb{T}^n$. As we have shown in the previous subsections, this is now equivalent to determining the solutions of a symmetric polynomial system of type (II), which can be done with the techniques from Section 2.

Theorem 2.32. *Define the n–dimensional $\mathbb{R}$–vector space*

$$\mathcal{Z} := \begin{cases} \mathbb{R}^n, & \text{if } n \text{ is even} \\ \{z \in \mathbb{C}^n \,|\, z_1, \ldots, z_{n-2} \in \mathbb{R}, \overline{z_n} = z_{n-1}\}, & \text{if } n \text{ is odd} \end{cases}.$$

and the matrix $P \in \mathbb{R}[z]^{n \times n}$ by

$$P(z)_{ij} = \mathrm{Trace}(C(z)^{i+j-2} - C(z)^{i+j}), \quad \text{where} \quad C(z) = \begin{bmatrix} 0 & \cdots & 0 & -c_n(z) \\ 1 & & 0 & -c_{n-1}(z) \\ & \ddots & & \vdots \\ 0 & & 1 & -c_1(z) \end{bmatrix},$$

$$c_i(z) = (-1)^i \binom{n}{i} z_i \quad \text{for} \quad 1 \leq i \leq n-2,$$

$$c_{n-1}(z) = (-1)^{n-1} \begin{cases} 2^{n-1}\, z_n\, z_{n-1} - \sum\limits_{j=1}^{(n-2)/2} \binom{n}{2j-1} z_{2j-1}, & \text{if } n \text{ is even} \\ 2^{n-1}\, z_n\, z_{n-1} - \sum\limits_{j=1}^{(n-3)/2} \binom{n}{2j} z_{2j} - 1, & \text{if } n \text{ is odd} \end{cases},$$

$$c_n(z) = (-1)^n \begin{cases} 2^{n-2}\,(z_n^2 + z_{n-1}^2) - \sum\limits_{j=1}^{(n-2)/2} \binom{n}{2j} z_{2j} - 1, & \text{if } n \text{ is even} \\ 2^{n-2}\,(z_n^2 + z_{n-1}^2) - \sum\limits_{j=0}^{(n-3)/2} \binom{n}{2j+1} z_{2j+1}, & \text{if } n \text{ is odd} \end{cases}.$$

For all $z \in \mathcal{Z}$, $P(z) \in \mathbb{R}^{n \times n}$ and $\mathcal{T} = \{z \in \mathcal{Z} \,|\, P(z) \succeq 0\}$.

Proof. Let $z \in \mathbb{C}^n$ and set $c_i := c_i(z)$ for $1 \leq i \leq n$.

To show "$\subseteq$", assume that $z \in \mathcal{T}$. Then there exists $x \in \mathbb{T}^n$, such that $\theta_i(x) = z_i$ for $1 \leq i \leq n$. Furthermore, we have $z \in \mathcal{Z}$ and $c_i \in \mathbb{R}$. By Proposition 2.30 and Lemma 1.43, the solution of the symmetric polynomial system

$$\text{(II)} \quad \sigma_i\left(\frac{y_1 + y_1^{-1}}{2}, \ldots, \frac{y_n + y_n^{-1}}{2}\right) = (-1)^i\, \tilde{c}_i \quad \text{for} \quad 1 \leq i \leq n$$

is $y = \psi(x) \in \mathbb{T}^n$, where ψ is the map from Proposition 2.31. Applying Corollary 2.16 yields $P(z) \succeq 0$.

For "$\supseteq$" on the other hand, assume $z \in \mathcal{Z}$ with $P(z) \succeq 0$. Hence, $c_i \in \mathbb{R}$ and by Corollary 2.16, the solution y of the above system (II) is contained in $\mathbb{T}^n$. According to Proposition 2.31, y has two distinct preimages $x, x' \in \mathbb{T}^n$. We have $z_i = \theta_i(x) = \theta_i(x')$ for $1 \leq i \leq n-2$ and $\theta_{n-1}(x) = -\theta_{n-1}(x'), \theta_n(x) = -\theta_n(x')$. Furthermore, $z_{n-1}^2 + z_n^2 = \theta_{n-1}(x)^2 + \theta_n(x)^2 = \theta_{n-1}(x')^2 + \theta_n(x')^2$ and $z_{n-1}\, z_n = \theta_{n-1}(x)\, \theta_n(x) = \theta_{n-1}(x')\, \theta_n(x')$. Therefore, $\{z_{n-1}, z_n\} \in \{\{\theta_{n-1}(x), \theta_n(x)\}, \{\theta_{n-1}(x'), \theta_n(x')\}\}$. If $z_{n-1} = \theta_{n-1}(x), z_n = \theta_n(x)$, then $z = \vartheta(x)$. Otherwise by Proposition 2.31, there exists $\tilde{x}$, such that $z_{n-1} = \theta_{n-1}(\tilde{x}), z_n = \theta_n(\tilde{x})$ and $z = \vartheta(\tilde{x})$. An analogous argument applies to x' and thus, z is contained in $\mathcal{T}$. □

8 Type G_2

In this section, we give a closed formula for the matrix polynomial from Theorem 2.19 in the standard monomial basis for G_2. This is a root system of rank 2. Hence, the ring of Laurent polynomials is $\mathbb{R}[x^\pm] = \mathbb{R}[x_1, x_1^{-1}, x_2, x_2^{-1}]$ and the polynomial ring is $\mathbb{R}[z] = \mathbb{R}[z_1, z_2]$.

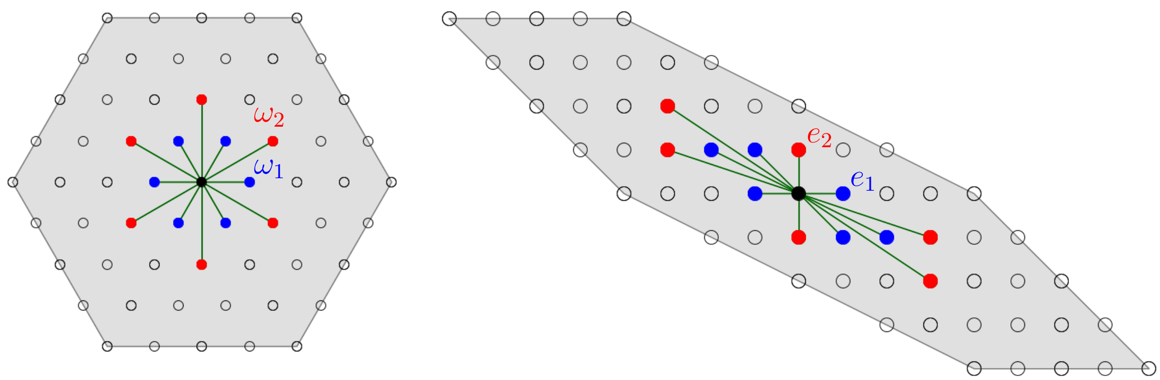


Figure 2.8: The root system G_2 and the weight lattice in the usual orthogonal representation and the integer representation. The orbits of the fundamental weights are the blue and red lattice elements.

8.1 Orbit polynomials

We denote by $\mathcal{G} \in \mathrm{GL}_2(\mathbb{Z})$ the integer representation of $\mathfrak{S}_3 \ltimes \{\pm 1\}$ with respect to the fundamental weights in Equation (1.11). Then the orbit $\mathcal{G} \cdot x_1 = \{x^\alpha \in \mathbb{R}[x^\pm] \,|\, \exists\, B \in \mathcal{G} :\, \alpha = B e_1\}$ consists of 6 distinct monomials, given by

$$y_1 = x_1, \quad y_2 = x_1\, x_2^{-1}, \quad y_3 = x_1^{-2}\, x_2 \tag{2.1}$$

and their inverses. For $1 \leq i \leq 3$, let σ_i be the i–th elementary symmetric function in 3 indeterminates and recall that, for $i \leq 2$, θ_i is the $\mathcal{G}$–invariant orbit polynomial associated to $e_i \in \mathbb{Z}^2$.

Proposition 2.33. *For $x \in (\mathbb{C}^*)^2$, we have*

$$\begin{aligned}
\sigma_1\left(\frac{y_1(x)+y_1(x)^{-1}}{2}, \frac{y_2(x)+y_2(x)^{-1}}{2}, \frac{y_3(x)+y_3(x)^{-1}}{2}\right) &= 3\,\theta_1(x),\\
\sigma_2\left(\frac{y_1(x)+y_1(x)^{-1}}{2}, \frac{y_2(x)+y_2(x)^{-1}}{2}, \frac{y_3(x)+y_3(x)^{-1}}{2}\right) &= \frac{3(\theta_1(x)+\theta_2(x))}{2},\\
\sigma_3\left(\frac{y_1(x)+y_1(x)^{-1}}{2}, \frac{y_2(x)+y_2(x)^{-1}}{2}, \frac{y_3(x)+y_3(x)^{-1}}{2}\right) &= \frac{9\,\theta_1(x)^2 - 3\,\theta_1(x) - 3\,\theta_2(x) - 1}{2}.
\end{aligned}$$

Proof. In principle, this can be checked by hand, but we give a constructive proof to show how to obtain the equations. From Equation (2.1), it follows that $x_1 = y_1(x)$, $x_1^{-1} = y_2(x)\, y_3(x)$ and $x_2 = y_1^2(x)\, y_3(x)$,

$x_2^{-1} = y_2^2(x)\, y_3(x)$. Thus, after computing the orbits $\mathcal{G}\cdot x_1, \mathcal{G}\cdot x_2$, we can express $\theta_1, \theta_2 \in \mathbb{R}[x^\pm]$ as polynomials $g_1, g_2 \in \mathbb{R}[y_1, y_2, y_3]$. Define the ideal

$$\mathcal{I} := \langle \theta_1 - g_1(y), \theta_2 - g_2(y), 1 - y_1\, y_2\, y_3 \rangle \subseteq \mathbb{R}[y_1, y_2, y_3, \theta_1, \theta_2].$$

With respect to the lexicographical ordering $y_1 \succeq_{\mathrm{lex}} y_2 \succeq_{\mathrm{lex}} y_3 \succeq_{\mathrm{lex}} \theta_1 \succeq_{\mathrm{lex}} \theta_2$, let G_{lex} be the reduced Gröbner basis of $\mathcal{I}$. Since $\succeq_{\mathrm{lex}}$ is an elimination ordering and the left–hand side is $\mathcal{G}$–invariant, one finds the normal form of $\sigma_i(y_1 + y_2\, y_3, y_2 + y_1\, y_3, y_3 + y_1\, y_2)/2^i$ with respect to G_{lex} for $1 \leq i \leq 3$ to be the right–hand side of the claimed equation. □

Proposition 2.34. *The map*

$$\begin{array}{rccl} \psi: & (\mathbb{C}^*)^2 & \to & (\mathbb{C}^*)^3, \\ & x & \mapsto & (y_1(x), y_2(x), y_3(x)) \end{array}$$

is injective and the image contains $\mathbb{T}_1^3 = \{x \in \mathbb{T}^3 \,|\, x_1\, x_2\, x_3 = 1\}$. *The preimage of* $\mathbb{T}_1^3$ *is* $\mathbb{T}^2$.

Proof. This follows immediately from Equation (2.1). □

8.2 Hermite characterization with standard monomials

We give a Hermite characterization of the $\mathbb{T}$–orbit space.

Theorem 2.35. *Define the matrix* $H \in \mathbb{R}[z]^{3\times 3}$ *by*

$$H(z)_{ij} = \mathrm{Trace}((C(z))^{i+j-2} - (C(z))^{i+j}) \quad \textit{with}$$

$$C(z) = \begin{bmatrix} 0 & 0 & (9\, z_1^2 - 3\, z_1 - 3\, z_2 - 1)/2 \\ 1 & 0 & -3(z_1 + z_2)/2 \\ 0 & 1 & 3\, z_1 \end{bmatrix}.$$

Then $\mathcal{T} = \{z \in \mathbb{R}^2 \,|\, H(z) \succeq 0\}$.

Proof. With Proposition 2.34, the proof is analogous to Theorem 2.26. □

Example

Let $z = (z_1, z_2) \in \mathbb{R}^2$. The Hermite matrix polynomial from Theorem 2.35 is $4\, H(z) =$

$$\begin{bmatrix} -12\, z_1^2 + 4\, z_1 + 4\, z_2 + 4 & \cdots \\ -36\, z_1^3 + 18\, z_1\, z_2 + 10\, z_1 + 6\, z_2 + 2 & \cdots \\ -108\, z_1^4 + 72\, z_1^2\, z_2 + 30\, z_1^2 + 12\, z_1\, z_2 - 6\, z_2^2 + 4\, z_1 - 4\, z_2 & \cdots \end{bmatrix}$$

$$\begin{bmatrix} \cdots & -36\, z_1^3 + 18\, z_1\, z_2 + 10\, z_1 + 6\, z_2 + 2 & \cdots \\ \cdots & -108\, z_1^4 + 72\, z_1^2\, z_2 + 30\, z_1^2 + 12\, z_1\, z_2 - 6\, z_2^2 + 4\, z_1 - 4\, z_2 & \cdots \\ \cdots & -324\, z_1^5 + 270\, z_1^3\, z_2 + 126\, z_1^3 + 45\, z_1^2\, z_2 - 45\, z_1\, z_2^2 + 15\, z_1^2 - 48\, z_1\, z_2 - 15\, z_2^2 - 11\, z_1 - 11\, z_2 - 2 & \cdots \end{bmatrix}$$

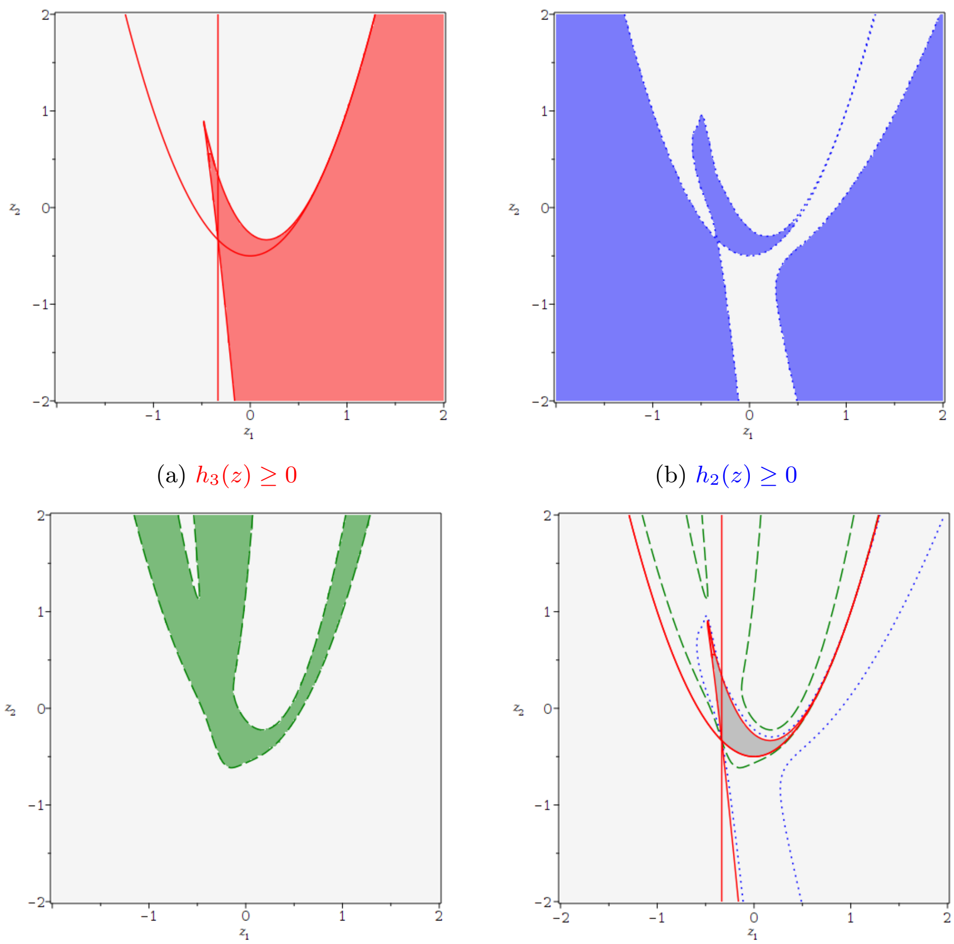
$$\begin{bmatrix} \cdots & -108\, z_1^4 + 72\, z_1^2\, z_2 + 30\, z_1^2 + 12\, z_1\, z_2 - 6\, z_2^2 + 4\, z_1 - 4\, z_2 \\ \cdots & -324\, z_1^5 + 270\, z_1^3\, z_2 + 126\, z_1^3 + 45\, z_1^2\, z_2 - 45\, z_1\, z_2^2 + 15\, z_1^2 - 48\, z_1\, z_2 - 15\, z_2^2 - 11\, z_1 - 11\, z_2 - 2 \\ \cdots & -972\, z_1^6 + 972\, z_1^4\, z_2 + 432\, z_1^4 + 162\, z_1^3\, z_2 - 243\, z_1^2\, z_2^2 + 63\, z_1^3 - 207\, z_1^2\, z_2 - 81\, z_1\, z_2^2 + 9\, z_2^3 - 45\, z_1^2 - 66\, z_1\, z_2 - 3\, z_2^2 - 14\, z_1 - 6\, z_2 - 1 \end{bmatrix}$$

and shall have characteristic polynomial

$$\mathrm{Det}(x\, I_3 - H(z)) = x^3 - h_1(z)\, x^2 + h_2(z)\, x - h_3(z) \in (\mathbb{R}[z])[x].$$

Again, we have $z \in \mathcal{T}$ if and only if $h_i(z) \geq 0$ for $1 \leq i \leq 3$ and

$$\begin{aligned}
h_3(z) &= -\mathrm{Coeff}(x^0, \mathrm{Det}(x\, I_3 - H(z))) \quad \text{(solid)}\\
&= 81/16\,(24\, z_1^3 - 12\, z_1\, z_2 - z_2^2 - 6\, z_1 - 4\, z_2 - 1)\,(3\, z_1^2 - 2\, z_2 - 1)^2\,(3\, z_1 + 1)^2,\\
h_2(z) &= \;\;\mathrm{Coeff}(x^1, \mathrm{Det}(x\, I_3 - H(z))) \quad \text{(dots)}\\
&= 27/16\,(3\, z_1^2 - 2\, z_2 - 1)\,(648\, z_1^6 - 540\, z_1^5 - 972\, z_1^4\, z_2 - 216\, z_1^3\, z_2^2 - 648\, z_1^4 + 36\, z_1^3\, z_2\\
&\quad +369\, z_1^2\, z_2^2 + 126\, z_1\, z_2^3 + 9\, z_2^4 - 18\, z_1^3 + 480\, z_1^2\, z_2 + 246\, z_1\, z_2^2 + 36\, z_2^3 + 129\, z_1^2 + 202\, z_1\, z_2\\
&\quad +37\, z_2^2 + 44\, z_1 + 28\, z_2 + 4),\\
h_1(z) &= -\mathrm{Coeff}(x^2, \mathrm{Det}(x\, I_3 - H(z))) \quad \text{(dash)}\\
&= 9/4 - 729\, z_1^6 + 243\, z_1^4 + 729\, z_1^4\, z_2 - 729/4\, z_1^2\, z_2^2 + 243/2\, z_1^3\, z_2 + 189/4\, z_1^3 - 405/4\, z_1^2\, z_2\\
&\quad -243/4\, z_1\, z_2^2 + 27/4\, z_2^3 - 81/4\, z_1^2 - 81/2\, z_1\, z_2 - 27/4\, z_2^2 - 9/2\, z_1 - 9/2\, z_2.
\end{aligned}$$



(a) $h_3(z) \geq 0$ (b) $h_2(z) \geq 0$

(c) $h_1(z) \geq 0$ (d) $h_1(z), h_2(z), h_3(z) \geq 0$

Figure 2.9: Vanishing points and positivity regions for the coefficients of $\mathrm{Det}(x\, I_3 - H(z))$.

The vertices are

$$\text{Vertex}_1 := \vartheta(\exp(-2\pi\mathrm{i}\,\langle\omega_1,\omega_1/3\rangle),\exp(-2\pi\mathrm{i}\,\langle\omega_2,\omega_1/3\rangle)) = \vartheta\left(-\frac{1}{2}+\mathrm{i}\frac{\sqrt{3}}{2},1\right) = \left(-\frac{1}{2},1\right),$$

$$\text{Vertex}_2 := \vartheta(\exp(-2\pi\mathrm{i}\,\langle\omega_1,\omega_2/6\rangle),\exp(-2\pi\mathrm{i}\,\langle\omega_2,\omega_2/6\rangle)) = \vartheta(-1,1) = \left(-\frac{1}{3},-\frac{1}{3}\right),$$

$$\text{Vertex}_3 := \vartheta(\exp(-2\pi\mathrm{i}\,\langle\omega_1,0\rangle),\exp(-2\pi\mathrm{i}\,\langle\omega_2,0\rangle)) = \vartheta(1,1) = (1,1).$$

9 Alternative fundamental invariants

Let R be a root system with Weyl group $\mathcal{W}$. Denote by $\mathcal{G}$ the integer representation of $\mathcal{W}$. We have given a description for the $\mathbb{T}$–orbit space of $\mathcal{G}$ through orbit polynomials and the identity

$$\mathbb{R}[x^{\pm}]^{\mathcal{G}} = \mathbb{R}[\theta_1,\ldots,\theta_n],$$

where $\theta_i = \Theta_{e_i}$ is the invariant character polynomial associated to e_i. One could therefore argue that this approach only leads to a particular description. Hence, a valid question is the following. How do we obtain a polynomial description of $\mathcal{T}$, if the θ_i are replaced by other fundamental invariants? We answer this question explicitly for character polynomials.

9.1 $\mathbb{T}$–orbit spaces through characters

Recall that we also have the identity

$$\mathbb{R}[x^{\pm}]^{\mathcal{G}} = \mathbb{R}[\Xi_{e_1},\ldots,\Xi_{e_n}], \tag{2.2}$$

given by the character polynomials from Definition 1.29. By Theorem 2.4, the image of $\mathbb{T}^n$ under the Ξ_{e_i} is a $\mathbb{T}$–orbit space of $\mathcal{G}$. Furthermore, there exist polynomial maps U and P, such that $U(\Theta_{e_1},\ldots,\Theta_{e_n}) = (\Xi_{e_1},\ldots,\Xi_{e_n})$ and $P(\Xi_{e_1},\ldots,\Xi_{e_n}) = (\Theta_{e_1},\ldots,\Theta_{e_n})$. Hence, $U\circ P$ is, essentially, the identity on $\mathbb{T}^n/\mathcal{G}$. Indeed, those maps are given by the generalized Chebyshev polynomials of the second and their counterparts from Equation (2.2). Recall that the second kind was defined via the property $U_\alpha(\Theta_{e_1},\ldots,\Theta_{e_n}) = \Xi_\alpha$. On the other hand, we can introduce the following family of polynomials.

Definition 2.36. *For $\alpha\in\mathbb{N}^n$, we define $P_\alpha\in\mathbb{R}[z]$ via $P_\alpha(\Xi_{e_1},\ldots,\Xi_{e_n}) = \Theta_\alpha$.*

Remark 2.37. *In the univariate case, we have $\Xi_1 = \frac{x^2-x^{-2}}{x-x^{-1}} = x+x^{-1} = 2\Theta_1$. Thus, P_α is a generalization of $P_\ell(2\cos(2\pi\,u)) = \cos(2\pi\,\ell\,u)$. Other generalizations of Chebyshev polynomials are for example to be found in [LU13], but are not treated in this thesis.*

Define the maps

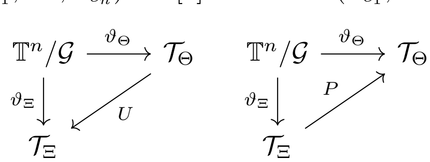
$$\begin{array}{rccl} \vartheta_\Theta: & (\mathbb{C}^*)^n & \to & \mathbb{C}^n, \\ & x & \mapsto & (\Theta_{e_1}(x),\ldots,\Theta_{e_n}(x)) \end{array}$$

and

$$\begin{array}{rccl} \vartheta_\Xi: & (\mathbb{C}^*)^n & \to & \mathbb{C}^n, \\ & x & \mapsto & (\Xi_{e_1}(x),\ldots,\Xi_{e_n}(x)). \end{array}$$

We write $\mathcal{T}_\Theta := \vartheta_\Theta(\mathbb{T}^n)$ and $\mathcal{T}_\Xi := \vartheta_\Xi(\mathbb{T}^n)$ for the respective $\mathbb{T}$–orbit spaces of $\mathcal{G}$.

Proposition 2.38. *With $U = (U_{e_1},\ldots,U_{e_n})\in\mathbb{R}[z]^n$ and $P = (P_{e_1},\ldots,P_{e_n})\in\mathbb{R}[z]^n$, the diagrams*



commute.

Proof. By Theorem 2.4, ϑ_Θ and ϑ_Ξ are bijections between $\mathbb{T}^n/\mathcal{G}$ and the respective $\mathbb{T}$–orbit spaces. By the definitions of the generalized Chebyshev polynomials of the second and P, we obtain $U \circ \vartheta_\Theta = \vartheta_\Xi$ and $P \circ \vartheta_\Xi = \vartheta_\Theta$. □

Assume that we have an explicit polynomial description of the $\mathbb{T}$–orbit space $\mathcal{T}_\Theta$, for example by Theorem 2.19. We can then describe $\mathcal{T}_\Xi$ as follows.

Corollary 2.39. [of Proposition 2.38] *Assume that there exists a symmetric matrix polynomial $H \in \mathbb{R}[z]^{n\times n}$, such that*

$$\mathcal{T}_\Theta = \{z \in \mathbb{R}^n \,|\, H(z) \succeq 0\}.$$

Then, with U and P as in Proposition 2.38, we have

$$\mathcal{T}_\Xi = \{U(z) \,|\, z \in \mathbb{R}^n,\, H(z) \succeq 0\} = \{z \in \mathbb{R}^n \,|\, H(P(z)) \succeq 0\}.$$

Proof. We have

$$\begin{aligned}\mathcal{T}_\Xi &= \vartheta_\Xi(\mathbb{T}^n) = U \circ \vartheta_\Theta(\mathbb{T}^n) = \{U(z) \,|\, z \in \mathbb{R}^n,\, H(z) \succeq 0\}\\ &= \{U(z) \,|\, z \in \mathbb{R}^n,\, H(P(U(z))) \succeq 0\} \subseteq \{z \in \mathbb{R}^n \,|\, H(P(z)) \succeq 0\}.\end{aligned}$$

To show "$\supseteq$", let $z \in \mathbb{R}^n$ with $H(P(z)) \succeq 0$. Then $P(z) \in \mathcal{T}_\vartheta = P \circ \vartheta_\Xi(\mathbb{T}^n)$ and thus $z = U(P(z)) \in \vartheta_\Xi(\mathbb{T}^n) = \mathcal{T}_\Xi$. □

9.2 Linear and diagonal transformations

The maps U and P from Proposition 2.38 define polynomial transformations and are inverse to each other. The question in this section is, when this transformation is linear or even diagonal. We give an answer for the case of orbit and character polynomials.

Definition 2.40. *We call $\alpha \in \mathbb{N}^n$* ***minuscule****, if, for all $\beta \in \mathbb{N}^n$, $\beta \preceq \alpha$ implies $\beta = \alpha$.*

The background to this definition is given in Appendix A. It gives us a way to characterize the diagonality of the transformations U and P.

Lemma 2.41. *U and P are diagonal if and only if all the $e_1, \ldots, e_n$ are minuscule.*

Proof. It suffices to show the statement for U. Note that U is diagonal if and only if, for all $1 \leq i \leq n$, the generalized Chebyshev polynomials of the second kind U_{e_i} is a scalar multiple of z_i. By Proposition 1.36, we have

$$U_{e_i}(z) = \sum_{\beta \preceq e_i} u_\beta\, z^\beta,$$

where the sums ranges over $\beta \in \mathbb{N}^n$. Hence, for U_{e_i} to have the desired property, we require that $\beta \preceq e_i$ implies $\beta = e_i$. If e_i is minuscule, this is true by definition. Thus, U is diagonal. Since P is inverse to U, P is also diagonal. The converse is true by the theorem of the highest weight Theorem A.11 and the characterization of minuscule weights Theorem A.14. □

The only irreducible root system, where all the e_i are minuscule, is A_{n-1}, see for example [Hum72, §13.4].

Corollary 2.42. [of Lemma 2.41] *If R is a root system of type A_{n-1}, then U and P are diagonal.*

Denote by Cartan(R) the Cartan matrix of R.

Definition 2.43. *Let $1 \leq i \leq n$. We say that* R *is i–**linear**, if, for all $\beta \in \mathbb{N}^n$, the following holds.*

$$\text{If there exists } \alpha \in \mathbb{N}^n\text{, such that } \beta + \mathrm{Cartan}(\mathrm{R})^t \alpha = e_i\text{, then } \beta \in \{e_1, \ldots, e_n\}.$$

Hence, checking U and P for linearity comes down to properties of the Cartan matrix.

Lemma 2.44. *U and P are linear if and only if, for all $1 \leq i \leq n$,* R *is i–linear.*

Proof. Assume that R is i–linear for all i. Similar to the proof of Lemma 2.41, we need to show that $\beta \preceq e_i$ implies $\beta \in \{e_1, \ldots, e_n\}$. Indeed, if $\beta \preceq e_i$, then there exists $\alpha \in \mathbb{N}^n$, such that

$$e_i - \beta = \sum_{i=1}^{n} \alpha_i \, W^{-1} \rho_i = \sum_{i=1}^{n} \alpha_i \begin{bmatrix} \langle \rho_i, \rho_1^\vee \rangle \\ \vdots \\ \langle \rho_i, \rho_n^\vee \rangle \end{bmatrix} = \sum_{i=1}^{n} \alpha_i \, (\mathrm{Cartan}(\mathrm{R})_{i \cdot})^t = \mathrm{Cartan}(\mathrm{R})^t \alpha.$$

By i–linearity, $\beta \in \{e_1, \ldots, e_n\}$. The converse is shown analogously. □

Example 2.45. *For* $\mathrm{R} = \mathrm{C}_3$*, the Chebyshev polynomials of the second kind associated to the e_i are*

$$U_{e_1} = 6\, z_1, \quad U_{e_2} = 12\, z_2 + 2, \quad \text{and} \quad U_{e_3} = 6\, z_1 + 8\, z_3.$$

The matrix $H(P(z))$ from Corollary 2.39 yields the constraints for $\mathcal{T}_\Xi$, where $P : z \mapsto A^{-1} \cdot (z - b)$ with

$$A := \begin{bmatrix} 6 & 0 & 0 \\ 0 & 12 & 0 \\ 6 & 0 & 8 \end{bmatrix} \quad \text{and} \quad b := \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix}.$$

Note that e_1 is the only minuscule element and C_3 *is 1– and 3–linear, but not 2–linear.*

Chapter 3

Global optimization in terms of generalized Chebyshev polynomials

The optimization of

- trigonometric polynomials on $\mathbb{R}^n$ with Weyl symmetry,
- multiplicative invariants on the compact torus,
- classical polynomials on $\mathbb{T}$–orbit spaces

are three equivalent problems. The first two are addressed by solving the third one with techniques from polynomial optimization on basic semi–algebraic sets. We adapt Lasserre's hierarchy. In particular, we study sums of squares representations with Chebyshev polynomials and Chebyshev moments with respect to weighted degrees. This leads to two converging dual hierarchies of lower bounds for the optimal value of the objective function. These hierarchies are semi–definite programs and can be solved numerically. We implement a procedure to compute the associated matrices and compare our technique with an established one from trigonometric optimization.

The results are based on joint work with Evelyne Hubert (Inria), Philippe Moustrou (Toulouse) and Cordian Riener (Tromsø) [HMMR22].

Public availability:
https://hal.archives-ouvertes.fr/hal-03768067v1

Implementation:
https://www-sop.inria.fr/members/Tobias.Metzlaff/GeneralizedChebyshev.zip

1 Optimization of trigonometric polynomials

Trigonometric polynomials as real linear combinations of complex exponential functions are ubiquitous in applied mathematics and physics. In this chapter, we consider multivariate trigonometric polynomials, which are sign–symmetric and invariant under the multiplicative action of a Weyl group. The goal is to find the optimal value, that is, the maximum or minimum. This problem can be reformulated to a polynomial optimization problem and subsequently solved with Lasserre's hierarchy.

Let $n \in \mathbb{N}$ and denote the Euclidean scalar product on $\mathbb{R}^n$ by $\langle \cdot, \cdot \rangle$. For a lattice $\Omega \subseteq \mathbb{R}^n$, consider a sequence $c = (c_\mu)_{\mu\in\Omega} \in \mathbb{R}^\Omega$ with finite **support** $S := \{\mu \in \Omega \,|\, c_\mu \neq 0\}$. A **trigonometric polynomial** f is a multivariate map

$$\begin{array}{rccl} f: & \mathbb{R}^n & \to & \mathbb{C} \\ & u & \mapsto & \sum\limits_{\mu\in S} c_\mu \, \mathfrak{e}^\mu(u), \end{array} \tag{3.1}$$

where $\mathfrak{e}^\mu(u) = \exp(-2\pi\mathrm{i}\, \langle \mu, u \rangle)$. Since this is essentially an element of the group algebra of Ω as a function on $\mathbb{R}^n$, the set of all trigonometric polynomials with support in Ω is denoted by $\mathbb{R}[\Omega]$. If the coefficients are sign–symmetric, that is, if $S = -S$ and $c_\mu = c_{-\mu}$ for $\mu \in S$, then f is real–valued. The problem considered in this section is to find

$$f^* = \inf_{u\in\mathbb{R}^n} \sum_{\mu\in S} c_\mu \, \mathfrak{e}^\mu(u). \tag{3.2}$$

Since f is by definition periodic with respect to the dual lattice Λ of Ω, f^* is a minimum and assumed on the Voronoï cell $\mathrm{Vor}(\Lambda)$ of the dual lattice.

The theory that we have recalled in Chapter 1 and advanced in Chapter 2 comes into play, when we consider trigonometric polynomials with crystallographic symmetry. In this section, let R be an irreducible root system of rank n with Weyl group $\mathcal{W}$. The weight lattice Ω is spanned by fundamental weights $\omega_1, \ldots, \omega_n$. The dual lattice of Ω, that is, the lattice of coroots, is denoted by Λ. Recall from Proposition 1.14 that, if the affine Weyl group $\mathcal{W} \ltimes \Lambda$ has fundamental domain $\triangle$, then the Voronoï cell of Λ is $\mathcal{W}\triangle$.

The multiplicative action of the Weyl group on the group algebra of Ω from Equation (1.16) carries over naturally to the trigonometric polynomials. For $A \in \mathcal{W}$, we have

$$A \cdot \mathfrak{e}^\mu(u) = \mathfrak{e}^{A\mu}(u) = \mathfrak{e}^\mu(A^t u) = \mathfrak{e}^\mu(A^{-1}u).$$

The trigonometric polynomials, which are invariant under this action, are called $\mathcal{W}$–**invariant**.

1.1 Generalized cosine functions

Note that every trigonometric polynomial f as in Equation (3.1) with support $S \subseteq \Omega$ is periodic with respect to translation by coroots, that is $\mathfrak{e}^\mu(u+\lambda) = \mathfrak{e}^\mu(u)$ for $\mu \in \Omega$, $\lambda \in \Lambda$ and $u \in \mathbb{R}^n$. Thus, a periodicity domain is $\mathcal{W}\triangle$.

Proposition 3.1. [Fug74, §5] *The set* $\{\mathfrak{e}^\mu \,|\, \mu \in \Omega\}$ *is an orthonormal basis for both*

- *the* Λ*–periodic locally square integrable functions* $\mathrm{L}^2(\mathbb{R}^n/\Lambda)$ *and*
- *the square integrable functions on* $\mathcal{W}\triangle$

with respect to the inner product

$$(f, g) \mapsto \frac{1}{|\mathcal{W}|\,\mathrm{Vol}(\triangle)} \int\limits_{\mathcal{W}\triangle} f(u)\,\overline{g(u)}\,\mathrm{d}u,$$

where $\mathrm{Vol}(\triangle)$ *is the Lebesgue volume of* $\triangle$ *in* $\mathbb{R}^n$.

Definition 3.2. *The* ***generalized cosine*** *associated to $\mu \in \Omega$ is the $\mathcal{W}$–invariant Λ–periodic function*

$$\begin{array}{rccl} \mathfrak{c}_\mu: & \mathbb{R}^n & \to & \mathbb{C}, \\ & u & \mapsto & \dfrac{1}{|\mathcal{W}|} \sum\limits_{A \in \mathcal{W}} \mathfrak{e}^{A\mu}(u). \end{array}$$

The ***generalized sine*** *associated to $\mu \in \Omega$ is the $\mathcal{W}$–anti–invariant Λ–periodic function*

$$\begin{array}{rccl} \mathfrak{s}_\mu: & \mathbb{R}^n & \to & \mathbb{C}, \\ & u & \mapsto & \dfrac{1}{|\mathcal{W}|} \sum\limits_{A \in \mathcal{W}} \mathrm{Det}(A)\, \mathfrak{e}^{A\mu}(u). \end{array}$$

Example 3.3. *Let* R *be a root system of type* C_n*. Then, for $1 \leq i \leq n$, we have*

$$\binom{n}{i} \mathfrak{c}_i(u) = \sigma_i(\cos(2\pi u_1), \ldots, \cos(2\pi u_n)).$$

This follows immediately from Proposition 2.24.

Denote by $\mathcal{G}$ the integer representation of $\mathcal{W}$ and by $W : \mathbb{Z}^n \to \Omega$ the change of basis. Assume that $\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\theta_1, \ldots, \theta_n]$ as in Theorem 1.30 with $\theta_i = \Theta_{e_i}$ the orbit polynomial associated to e_i. The $\mathbb{T}$–orbit space of $\mathcal{G}$ shall be $\mathcal{T} = \{(\theta_1(x), \ldots, \theta_n(x)) \,|\, x \in \mathbb{T}^n\}$.

The generalized cosine and sine functions are those trigonometric polynomials in $\mathbb{R}[\Omega]$, which correspond to the $\mathcal{W}$–invariant orbit polynomials Θ_{e_i} and the $\mathcal{G}$–anti–invariant orbit polynomials Υ_{e_i} in $\mathbb{R}[x^\pm]$. Therefore, the $\mathbb{T}$–orbit space is also the image of the generalized cosines associated to the fundamental weights.

Lemma 3.4. *For $u \in \mathbb{R}^n$, define $\mathfrak{c}(u) := (\mathfrak{c}_{\omega_1}(u), \ldots, \mathfrak{c}_{\omega_n}(u)) \in \mathbb{C}^n$. Then $\mathfrak{c}(\mathbb{R}^n) = \mathfrak{c}(\triangle) = \mathcal{T}$.*

Proof. For $\alpha \in \mathbb{Z}^n$ and $\mu = W\alpha \in \Omega$, we have $\mathfrak{c}_\mu = \Theta_\alpha \circ (\mathfrak{e}^{\omega_1}, \ldots, \mathfrak{e}^{\omega_n})$, where W is the matrix with columns given by the fundamental weights. The map

$$\begin{array}{ccl} \mathbb{R}^n & \to & \mathbb{T}^n, \\ u & \mapsto & (\mathfrak{e}^{\omega_1}(u), \ldots, \mathfrak{e}^{\omega_n}(u)) \end{array}$$

is surjective, because the fundamental weights form a basis of $\mathbb{R}^n$. Hence, $\mathfrak{c}(\mathbb{R}^n) = \mathcal{T}$. Since $\mathfrak{c}$ is $\mathcal{W}$–invariant Λ–periodic and $\triangle$ is a fundamental domain for $\mathcal{W} \ltimes \Lambda$, we have $\mathfrak{c}(\mathbb{R}^n) = \mathfrak{c}(\triangle)$. □

If $-I_n \notin \mathcal{G}$, then the real $\mathbb{T}$–orbit space is denoted by $\mathcal{T}_\mathbb{R}$.

Remark 3.5. *The following statements hold.*

1. *The orbit spaces $\mathbb{T}^n/\mathcal{G}$ of $\mathcal{G}$ and $\mathbb{R}^n/(\mathcal{W} \ltimes \Lambda)$ of the affine Weyl group can both be embedded in $\mathbb{R}^n$ as the compact basic semi–algebraic set $\mathcal{T}_\mathbb{R}$, see Equation (2.1).*

2. *For $\alpha \in \mathbb{Z}^n$, we have defined the generalized Chebyshev polynomials of the first kind associated to α as the unique $T_\alpha \in \mathbb{R}[z]$, such that $T_\alpha(\theta_1, \ldots, \theta_n) = \Theta_\alpha$. For $\mu = W\alpha$, we subsequently have*

$$T_\alpha \circ (\mathfrak{c}_{\omega_1}, \ldots, \mathfrak{c}_{\omega_n}) = \Theta_\alpha \circ (\mathfrak{e}^{\omega_1}, \ldots, \mathfrak{e}^{\omega_n}) = \mathfrak{c}_\mu.$$

Thus, Definition 3.2 is a generalization of the univariate case $T_\ell(\cos(2\pi\, u)) = \cos(2\pi\, \ell\, u)$ for $\ell \in \mathbb{N}$, which corresponds to the root system A_1.

3. *Analogously, for the generalized Chebyshev polynomials of the second kind, we have*

$$U_\alpha \circ (\mathfrak{c}_{\omega_1}, \ldots, \mathfrak{c}_{\omega_n}) = \frac{\Upsilon_{\alpha+\delta}}{\Upsilon_\delta} \circ (\mathfrak{e}^{\omega_1}, \ldots, \mathfrak{e}^{\omega_n}) = \frac{\mathfrak{s}_{\mu+\omega_0}}{\mathfrak{s}_{\omega_0}},$$

where $\delta := [1, \ldots, 1]^t \in \mathbb{N}^n$ *and* $\omega_0 := W\delta = \omega_1 + \ldots + \omega_n$. *In the classical univariate case, this implies*

$$\Xi_\ell(x) = \frac{x^{\ell+1} - x^{-\ell-1}}{x - x^{-1}} = x^\ell + x^{\ell-1} + \ldots + x^{1-\ell} + x^{-\ell}.$$

Thus, $U_\ell(\cos(2\pi\, u)) = \sin(2\pi\, (\ell+1)\, u)/\sin(2\pi\, u)$ *for* $\ell \in \mathbb{N}$.

The generalized sine and cosine functions appear in many other applications. For example, one can show that $\mathfrak{c}_\mu$ and $\mathfrak{s}_\mu$ are orthogonal eigenfunctions of Laplacian operators [MKNR12, Lemma 1.22]. Orthogonality is easy to prove with Fuglede's result.

Remark 3.6. *Let* $\mu, \nu \in \Omega$.

1. *By Proposition 3.1 and the* $\mathcal{W}$*–invariance, we have*

$$\frac{1}{\mathrm{Vol}(\triangle)} \int\limits_{\triangle} \mathfrak{c}_\mu(u)\, \overline{\mathfrak{c}_\nu(u)}\, \mathrm{d}u = \begin{cases} \dfrac{|\mathrm{Stab}_{\mathcal{W}}(\mu)|}{|\mathcal{W}|}, & \text{if} \quad \mu \in \mathcal{W}\,\nu \\ 0, & \text{otherwise} \end{cases}.$$

2. *Let* $\delta := [1, \ldots, 1]^t \in \mathbb{N}^n$. *For* $\alpha \in \mathbb{N}^n \setminus (\delta + \mathbb{N}^n)$, *the weight* $\mu = W\alpha$ *lies on a wall of a Weyl chamber. In this case, due to the anti–invariance, we have* $\mathfrak{s}_\mu = 0$. *For* $\alpha \in \delta + \mathbb{N}^n$ *on the other hand,* $\mu = W\alpha$ *is strongly dominant and we have* $|\mathrm{Stab}_{\mathcal{W}}(\mu)| = 1$. *Hence, if* μ *and* ν *are strongly dominant, then*

$$\frac{1}{\mathrm{Vol}(\triangle)} \int\limits_{\triangle} \mathfrak{s}_\mu(u)\, \overline{\mathfrak{s}_\nu(u)}\, \mathrm{d}u = \begin{cases} \dfrac{1}{|\mathcal{W}|}, & \text{if} \quad \mu \in \mathcal{W}\,\nu \\ 0, & \text{otherwise.} \end{cases}$$

With these facts, one can show that the generalized Chebyshev polynomials of the first and second kind are two orthogonal families on the $\mathbb{T}$–orbit space of $\mathcal{G}$. We prove this in Appendix B.

1.2 Rewriting the optimization problem

In the case of crystallographic symmetry, we can now solve the problem in Equation (3.2) by studying invariant trigonometric polynomials via invariant Laurent polynomials on the compact torus and generalized Chebyshev polynomials. This is summarized here.

Corollary 3.7. [of Lemma 3.4] *Let* $(c_\mu)_{\mu\in\Omega} \in \mathbb{R}^\Omega$ *with finite support* S, *so that*

1. $\mathcal{W}S = -S = S$ *and*
2. $c_{A\mu} = c_{-\mu} = c_\mu$ *for* $A \in \mathcal{W}$, $\mu \in S$.

We write $c_\alpha := c_\mu$ *if* $W\alpha = \mu \in S$. *Then*

$$\sum_{\mu\in S} c_\mu\, \mathfrak{e}^\mu(\mathbb{R}^n) = \sum_{\mu\in S\cap\Omega^+} |\mathcal{W}\mu|\, c_\mu\, \mathfrak{c}_\mu(\triangle) = \sum_{W\alpha\in S\cap\Omega^+} |\mathcal{G}\alpha|\, c_\alpha\, \Theta_\alpha(\mathbb{T}^n) = \sum_{W\alpha\in S\cap\Omega^+} |\mathcal{G}\alpha|\, c_\alpha\, T_\alpha(\mathcal{T}) \subseteq \mathbb{R}.$$

Due to the $\mathcal{W}$–invariance and Λ–periodicity, one can replace $\mathbb{R}^n$ with $\triangle$ on the left–hand side. Therefore, the maximal and minimal value on $\mathbb{R}$ are assumed in a compact subset of $\mathbb{C}^n$. If the root system is of type A_{n-1}, B_n, C_n, D_n or G_2, then $\mathcal{T}$ can be replaced with $\{z \in \mathbb{R}^n \mid P(z) \succeq 0\}$, where P is the Hermite matrix polynomial from Chapter 2.

Corollary 3.8. [of Lemma 3.4 and Corollary 3.7] *Consider the trigonometric optimization problem*

$$f^* = \inf_{u \in \mathbb{R}^n} \sum_{\mu \in S} c_\mu \, \mathfrak{e}^{\mu}(u),$$

where $S \subseteq \Omega$ satisfies the assumptions of Corollary 3.7. Denote by

$$S(\mathbb{N}) := \{W^{-1}\mu \,|\, \mu \in S \text{ dominant}\} \subseteq \mathbb{N}^n$$

the coordinates of dominant weights in S with respect to the basis of fundamental weights.

1. *If $-I_n \in \mathcal{G}$, then*

$$f^* = \inf_{z \in \mathcal{T}} \sum_{\alpha \in S(\mathbb{N})} |\mathcal{G}\alpha| \, c_\alpha \, T_\alpha(z).$$

2. *If $-I_n \notin \mathcal{G}$, then*

$$f^* = \inf_{z \in \mathcal{T}_\mathbb{R}} \sum_{\substack{\alpha \in S(\mathbb{N}) \\ -\alpha \in \mathcal{G}\alpha}} |\mathcal{G}\alpha| \, c_\alpha \, \widehat{T}_\alpha(z) + 2 \sum_{\substack{\{\alpha \neq \widehat{\alpha}\} \subseteq S(\mathbb{N}) \\ -\widehat{\alpha} \in \mathcal{G}\alpha}} |\mathcal{G}\alpha| \, c_\alpha \, \widehat{T}_\alpha(z),$$

where the second sum ranges over all pairs $\alpha \neq \widehat{\alpha}$ with $\widehat{T}_\alpha(\mathfrak{c}_\mathbb{R}(u)) = \Re(T_\alpha(\mathfrak{c}(u))) = \Re(T_{\widehat{\alpha}}(\mathfrak{c}(u)))$.

Example 3.9. *The group $\mathcal{W} := \mathfrak{S}_3 \ltimes \{\pm 1\}$ of order $6 \cdot 2 = 12$ acts on $\mathbb{R}^3$ by permutation of coordinates and scalar multiplication with ± 1. Consider the set*

$$S := \mathcal{W} \left\{ \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ -1 \\ 2 \end{bmatrix}, \begin{bmatrix} -1 \\ -2 \\ 3 \end{bmatrix}, \begin{bmatrix} 0 \\ -3 \\ 3 \end{bmatrix} \right\} \subseteq \mathbb{R}^3 / \langle \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \rangle.$$

$\mathcal{W}$ is the Weyl group of the root system G_2 and $S \subseteq \Omega$ satisfies the assumptions of Corollary 3.7 with $S(\mathbb{N}) = \{e_1, e_2, e_1 + e_2, 3\,e_1\}$. Consider the trigonometric polynomial

$$f(u) = \frac{1}{|\mathcal{W}|} \sum_{A \in \mathcal{W}} 2\,\mathfrak{e}^{A\omega_1}(u) + \mathfrak{e}^{A\omega_2}(u) + \mathfrak{e}^{A(\omega_1+\omega_2)}(u) + 4\,\mathfrak{e}^{3\,A\omega_1}(u).$$

Then f is supported by S and thus

$$f(u) = 2\,T_{10}(\mathfrak{c}(u)) + T_{01}(\mathfrak{c}(u)) + T_{11}(\mathfrak{c}(u)) + 4\,T_{30}(\mathfrak{c}(u)).$$

In particular, the minimum is

$$f^* = \inf_{z \in \mathcal{T}} 2\,T_{10}(z) + T_{01}(z) + T_{11}(z) + 4\,T_{30}(z) = \inf_{z \in \mathcal{T}} 144\,z_1^3 - 6\,z_1^2 - 69\,z_1\,z_2 - 33\,z_1 - 21\,z_2 - 7,$$

where the feasible region is the compact basic semi–algebraic set $\mathcal{T} = \{z \in \mathbb{R}^2 \,|\, P(z) \succeq 0\}$. Here,

$$P = \begin{bmatrix} T_{00} - T_{20} & T_{10} - T_{30} & T_{00} - T_{40} \\ T_{10} - T_{30} & T_{00} - T_{40} & 2\,T_{10} - T_{30} - T_{50} \\ T_{00} - T_{40} & 2\,T_{10} - T_{30} - T_{50} & 2\,T_{00} + T_{20} - 2\,T_{40} - T_{60} \end{bmatrix} \in \mathbb{R}[z]^{3 \times 3}$$

is obtained from Theorem 2.19 in the Chebyshev basis or from Theorem 2.35 in the standard monomial basis. The function f is periodic with respect to translation by the hexagonal lattice.

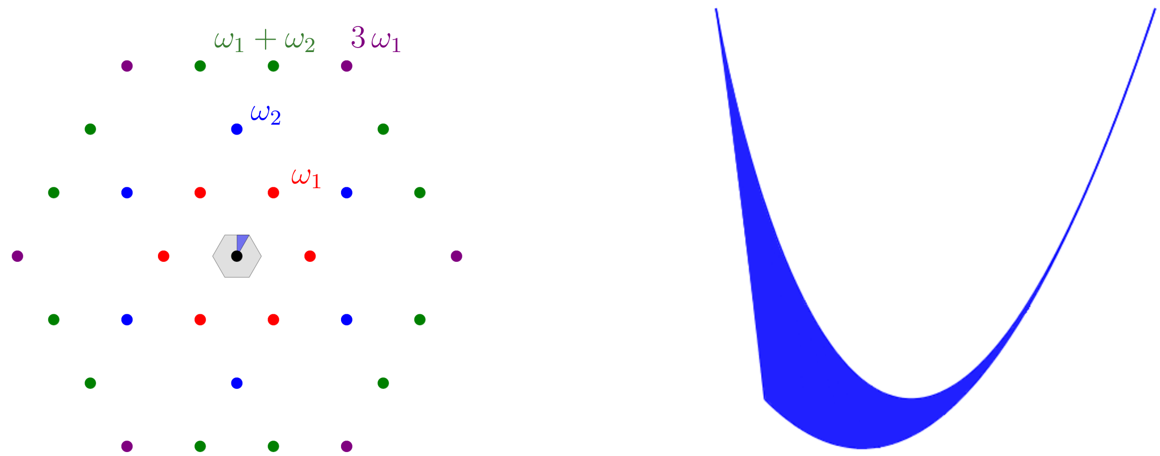


Figure 3.1: The support of f and the feasible region $\mathcal{T}$ of the polynomial optimization problem.

2 Chebyshev moments in polynomial optimization

In the previous section, we introduced the problem of finding the optimal value of a trigonometric polynomial with Weyl group symmetry. Following Corollary 3.8, this is equivalent to optimizing a linear combination of generalized Chebyshev polynomials

$$f = \sum_{\alpha \in \mathbb{N}^n} c_\alpha \, T_\alpha \tag{3.3}$$

on the associated $\mathbb{T}$–orbit space, which is assumed to be real. Note that f is naturally represented in the Chebyshev basis, when the original objective function is a trigonometric polynomial. The goal of the present section is to solve this polynomial optimization problem numerically with a hierarchy of semi–definite programs.

Let $\mathcal{W}$ be the Weyl group of a rank n irreducible root system R with integer representation $\mathcal{G}$. We assume that the $\mathbb{T}$–orbit space of $\mathcal{G}$ is given by

$$\mathcal{T} = \{(\Theta_{e_1}(x), \ldots, \Theta_{e_n}(x)) \,|\, x \in \mathbb{T}^n\} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$$

with $P \in \mathbb{R}[z]^{n\times n}$ and Θ_{e_i} the $\mathcal{G}$–invariant orbit polynomials from Definition 1.24. If $-I_n \notin \mathcal{G}$, then we have to work with the real $\mathbb{T}$–orbit space $\mathcal{T}_\mathbb{R}$.

Remark 3.10. *If the root system is irreducible of type* A_{n-1}, C_n, B_n, D_n *or* G_2, *then* P *is the Hermite matrix polynomial from Theorem 2.19. If we are in the special cases* $\mathrm{E}_{6,7,8}$ *or* F_4, *then such a description can be obtained with* [PS85, §4].

On the other hand, the root system may not be irreducible, that is, $\mathrm{R} = \mathrm{R}^{(1)} \times \ldots \times \mathrm{R}^{(k)}$ *with* $k \in \mathbb{N}$ *and* $\mathrm{R}^{(i)} \neq \emptyset$. *Hence, we can write the Weyl group as* $\mathcal{W} = \mathcal{W}^{(1)} \times \ldots \times \mathcal{W}^{(k)}$ *and the fundamental domain of the affine Weyl group as* $\triangle = \triangle^{(1)} \times \ldots \times \triangle^{(k)}$. *Since* $\mathcal{T} = \mathfrak{c}(\triangle)$ *is the* $\mathbb{T}$*–orbit space of* $\mathcal{W}$, *we have* $P(z^{(1)}, \ldots, z^{(k)}) = \mathrm{diag}(P^{(1)}(z^{(1)}), \ldots, P^{(k)}(z^{(k)})) \in \mathbb{R}[z^{(1)}, \ldots, z^{(k)}]^{n\times n}$, *where the* $P^{(i)}$ *are matrix polynomials corresponding to the irreducible* $\mathrm{R}^{(i)}$.

As an example, we consider k *copies* $\mathrm{R} = \mathrm{A}_1 \times \ldots \times \mathrm{A}_1$. *Then* $\mathcal{T} = [-1, 1]^k$. *This is not a simplex in* $\mathbb{R}^k$ *but the product of* k *identical* 1*–dimensional ones. In particular,* $\mathcal{T}$ *is the positivity locus of the matrix polynomial* $P = \mathrm{diag}(1 - z_1^2, \ldots, 1 - z_k^2)$.

The polynomial f from Equation (3.3) has coefficients given by a sequence $(c_\alpha)_{\alpha \in \mathbb{N}^n} \in \mathbb{R}^{\mathbb{N}^n}$. The support of

f is the finite set S of all $\alpha \in \mathbb{N}^n$, such that $c_\alpha \neq 0$. Consider the polynomial optimization problem

$$f^* = \begin{array}{ll} \inf & f(z), \\ \text{s.t.} & z \in \mathcal{T} \end{array} \quad = \begin{array}{ll} \inf & \sum\limits_{\alpha \in S} c_\alpha \, T_\alpha(z), \\ \text{s.t.} & z \in \mathbb{R}^n, \, P(z) \succeq 0. \end{array} \tag{3.4}$$

Lasserre proposed a hierarchy of dual moment–sums of squares relaxations in [Las01] to solve such problems. We make the following adjustments to this hierarchy. Instead of the standard monomial basis, we use the basis of generalized Chebyshev polynomials from Definition 1.32 to obtain a semi–definite problem. We replace degrees by weighted degrees from Definition 1.39, so that we can relax the problem to a finite dimensional space. Furthermore, we use a positivity certificate of Hol and Scherer [HS05, HS06] to exploit the matrix constraint. This result has already lead to advances in optimization, see [HL06] or [ALRT13]. Finally, we ensure convergence of the hierarchy. Our motivation is a computational problem from algebraic combinatorics, which we consider later in Chapter 4.

2.1 Putinar's theorem and Lasserre's hierarchy

Before we go into the technical details, we shall revisit the cornerstones of Lasserre's hierarchy. For further details, we refer to [Las09, Chapter 2 and 3] and [Lau09, Chapter 6]. The classical polynomial optimization problem asks to compute

$$f^* = \begin{array}{ll} \inf & f(z), \\ \text{s.t.} & z \in \mathbb{R}^n, \, p_1(z), \ldots, p_m(z) \geq 0, \end{array} \tag{3.5}$$

where the polynomial matrix constraint $0 \preceq P(z) \in \mathbb{R}[z]^{n \times n}$ from Equation (3.4) is replaced by finitely many scalar constraints $0 \leq p_i(z) \in \mathbb{R}[z]$. In fact, our problem falls in this category with $n = m$ thanks to Remark 2.17. On the other hand, writing the p_i in a diagonal matrix brings us back to the matrix constraint.

To avoid confusion, let us write the feasible region in this section as the basic closed semi–algebraic set $K := \{z \in \mathbb{R}^n \,|\, p_1(z), \ldots, p_m(z) \geq 0\}$, not necessarily compact. A **probability measure on** K is a finite Borel measure on $\mathbb{R}^n$ with support in K and mass 1. We observe that

$$f^* = \begin{array}{ll} \inf & \int\limits_K f(z) \, \mathrm{d}\eta(z), \\ \text{s.t.} & \eta \text{ is a probability measure on } K \end{array} \quad = \begin{array}{ll} \sup & \lambda \\ \text{s.t.} & \lambda \in \mathbb{R}, \, \forall \, z \in K : \\ & f(z) - \lambda \geq 0. \end{array}$$

The first equality follows from the fact that η can be chosen as the Dirac measure in a minimizer, assuming that f has a global minimum. The second equality is clear. Lasserre then uses a result due to Putinar. Denote by

$$\mathrm{QM}(p_1, \ldots, p_m) := \left\{ \sum_{i=0}^{m} q_i \, p_i \,|\, \forall \, 0 \leq i \leq m : \, q_i \in \mathrm{SOS}(\mathbb{R}[z]) \right\}$$

the **quadratic module of** $p_1, \ldots, p_m$. Here, $p_0 := 1$ and $q_i \in \mathrm{SOS}(\mathbb{R}[z])$ means that $q_i \in \mathbb{R}[z]$ can be written as a sum of squares. The quadratic module is said to be **Archimedean**, if there exists $f \in \mathrm{QM}(p_1, \ldots, p_m)$, such that $\{z \in \mathbb{R}^n \,|\, f(z) \geq 0\}$ is compact.

Theorem 3.11. [Put93] *Assume that* $\mathrm{QM}(p_1, \ldots, p_m)$ *is Archimedean. Then the following statements hold.*

1. *A linear functional* $\mathscr{L} \in \mathbb{R}[z]^*$ *has a representing probability measure on* K *if and only if* $\mathscr{L}(1) = 1$ *and* $\mathscr{L}$ *is nonnegative on* $\mathrm{QM}(p_1, \ldots, p_m)$.

2. *If* $f \in \mathbb{R}[z]$ *is strictly positive on* K*, then* $f \in \mathrm{QM}(p_1, \ldots, p_m)$.

Remark 3.12. *We add some comments to this result.*

1. *If* K *is compact, then the Archimedean property can be achieved by adding a ball constraint to the* p_i*. Archimedean implies compact, but not vice versa.*

2. *A linear functional is a linear map from* $\mathbb{R}[z]$ *to* $\mathbb{R}$ *and thus defined on any basis* $b = (b_\alpha)_{\alpha\in\mathbb{N}^n}$ *of* $\mathbb{R}[z]$. *If* $\mathscr{L} \in \mathbb{R}[z]^*$ *has a representing probability measure* η *on* K, *then* $\mathscr{L}(b_\alpha) = \int_K b_\alpha(z)\,\mathrm{d}\eta(z)$. *These values are called the moments of* η. *Furthermore,* $\mathscr{L}(1) = \int_K 1\,\mathrm{d}\eta(z) = \eta(K) = 1$.

3. *For* $\mathscr{L} \in \mathbb{R}[z]^*$ *and* $0 \le i \le m$, *an infinite symmetric matrix, indexed by* $\alpha, \beta \in \mathbb{N}^n$, *is defined through* $\mathcal{H}^{\mathscr{L}*p_i}_{\alpha\,\beta} := \mathscr{L}(p_i\, b_\alpha\, b_\beta)$.

4. *Under the Archimedean assumption, Putinar showed that* $\mathscr{L} \in \mathbb{R}[z]^*$ *has a representing probability measure on* K *if and only if all the* $\mathcal{H}^{\mathscr{L}*p_i}$ *are positive semi–definite.*

This allows to formulate the following relaxations. For $d \in \mathbb{N}$, $\mathbb{R}[z]_{2d}$ denotes the ring of polynomials up to degree $2d$. For $\mathscr{L} \in \mathbb{R}[z]^*_{2d}$, $\mathcal{H}^{\mathscr{L}*p_i}_{d-D_i}$ is the finite matrix with rows and columns indexed by monomials up to degree $d - D_i$, where $D_i := \lceil \deg(p_i)/2 \rceil$. Moreover, $\mathrm{QM}(p_1, \dots, p_m)_{2d}$ is the truncated quadratic module, where only sums of squares q_i are allowed, such that $q_i\, p_i$ has degree at most $2d$. Then

$$\begin{array}{lll} \inf & \mathscr{L}(f), & =: \tilde{f}^d_{\mathrm{mom}} \le f^* \ge \tilde{f}^d_{\mathrm{sos}} := \;\sup \quad \lambda, \\ \text{s.t.} & \mathscr{L} \in \mathbb{R}[z]^*_{2d},\ \mathscr{L}(1) = 1, & \qquad\qquad\qquad\quad \text{s.t.} \quad \lambda \in \mathbb{R},\ \forall\, z \in K: \\ & \mathcal{H}^{\mathscr{L}*p_i}_{d-D_i} \succeq 0 & \qquad\qquad\qquad\qquad\qquad f(z) - \lambda \in \mathrm{QM}(p_1, \dots, p_m)_{2d}. \end{array} \tag{3.6}$$

The two relaxations $\tilde{f}^d_{\mathrm{mom}}$ and $\tilde{f}^d_{\mathrm{mom}}$ are dual finite–dimensional semi–definite programs and can therefore be solved numerically as in [BV96]. It remains to show that the two relaxations converge to the original optimal value.

Theorem 3.13. [Las01] *The following statements hold.*

1. *The sequence* $(\tilde{f}^d_{\mathrm{sos}})_{d\in\mathbb{N}}$ *is monotonously non–decreasing.*

2. *The sequence* $(\tilde{f}^d_{\mathrm{mom}})_{d\in\mathbb{N}}$ *is monotonously non–decreasing.*

3. *For* $d \in \mathbb{N}$, *we have* $\tilde{f}^d_{\mathrm{sos}} \le \tilde{f}^d_{\mathrm{mom}}$.

4. *If* $\mathrm{QM}(p_1, \dots, p_m)$ *is Archimedean, then* $\lim\limits_{d\to\infty} \tilde{f}^d_{\mathrm{sos}} = \lim\limits_{d\to\infty} \tilde{f}^d_{\mathrm{mom}} = f^*$.

If $\{p_1, \dots, p_m\}$ contains an explicit ball constraint, then strong duality holds, that is, for $d \in \mathbb{N}$, we have $\tilde{f}^d_{\mathrm{sos}} = \tilde{f}^d_{\mathrm{mom}}$. This assumption is slightly stronger than Archimedean [JH16].

2.2 Matrix version of Putinar's theorem

As we have mentioned already, our problem from Equation (3.4) can be formulated as Equation (3.5) by using Remark 2.17. We would prefer to avoid this formulation, because the degrees of the p_i are much larger than those of the entries of P. Since the feasible region in our optimization problem is given by a polynomial matrix inequality, it is reasonable to use the following notion, generalizing the concept of sums of squares from scalar to matrix polynomials.

Definition 3.14. *A matrix polynomial* $Q \in \mathbb{R}[z]^{n\times n}$ *is said to be a* ***sum of squares****, if there exist* $k \in \mathbb{N}$ *and* $Q_1, \dots, Q_k \in \mathbb{R}[z]^n$, *such that*

$$Q(z) = \sum_{i=1}^{k} Q_i(z)\, Q_i(z)^t.$$

We write $Q \in \mathrm{SOS}(\mathbb{R}[z]^{n\times n})$.

The property Archimedean can be generalized to the matrix case as well. Denote by

$$\mathrm{QM}(P) := \{q + \mathrm{Trace}(P\, Q) \mid q \in \mathrm{SOS}(\mathbb{R}[z]),\ Q \in \mathrm{SOS}(\mathbb{R}[z]^{n\times n})\}$$

the **quadratic module of** P. We say that it is **Archimedean**, if there exists $f \in \mathrm{QM}(P)$, such that $\{z \in \mathbb{R}^n \mid f(z) \ge 0\}$ is compact. With this notation, Putinar's Theorem 3.11 can be extended to polynomial matrix inequalities.

Theorem 3.15. [HS06] *Assume that* $\mathrm{QM}(P)$ *is Archimedean. If* $f \in \mathbb{R}[z]$ *is strictly positive on the* $\mathbb{T}$*–orbit space* $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$ *of* $\mathcal{G}$*, then* $f \in \mathrm{QM}(P)$*.*

We can now relax Equation (3.4) to

$$f^* = \begin{array}{rl} \sup & \lambda \\ \text{s.t.} & \lambda \in \mathbb{R},\, \forall\, z \in \mathcal{T}: \\ & \sum\limits_{\alpha\in S} c_\alpha\, T_\alpha(z) - \lambda \geq 0. \end{array} \quad \geq \quad \begin{array}{rl} \sup & \lambda \\ \text{s.t.} & \lambda \in \mathbb{R},\, q \in \mathrm{SOS}(\mathbb{R}[z]),\, Q \in \mathrm{SOS}(\mathbb{R}[z]^{n\times n}), \\ & \sum\limits_{\alpha\in S} c_\alpha\, T_\alpha - \lambda = q + \mathrm{Trace}(P\, Q). \end{array} \tag{3.7}$$

Here, the quadratic module from Putinar's theorem is replaced by a scalar and a matrix sum of squares. For our application in optimization, we obtain the following statement.

Theorem 3.16. [HS05] *If* $\mathrm{QM}(P)$ *is Archimedean, then equality holds in Equation (3.7).*

In our case, the Archimedean property can always be enforced by adding an explicitly known ball constraint.

Proposition 3.17. *Set* $\widehat{P} := \mathrm{diag}(P, p) \in \mathbb{R}[z]^{(n+1)\times(n+1)}$*, where* $p(z) := n - \|z\|^2 \in \mathbb{R}[z]$*. Then* $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, \widehat{P}(z) \succeq 0\}$ *and* $\mathrm{QM}(\widehat{P})$ *is Archimedean.*

Proof. By Proposition 2.6, the $\mathbb{T}$–orbit space $\mathcal{T}$ of $\mathcal{G}$ is contained in the cube $[-1,1]^n$. Thus, for all $z \in \mathcal{T}$, $n - \|z\|^2 \geq 0$. With $Q = \mathrm{diag}(0, \ldots, 0, 1) \in \mathrm{SOS}(\mathbb{R}[z]^{(n+1)\times(n+1)})$, we have $\mathrm{Trace}(\widehat{P}\, Q) \in \mathrm{QM}(\widehat{P})$. The set

$$\{z \in \mathbb{R}^n \,|\, \mathrm{Trace}(\widehat{P}(z)\, Q(z))\}$$

is the Euclidean ball of radius $\sqrt{n}$ and thus compact. □

Remark 3.18. *In the basis of generalized Chebyshev polynomials of the first kind, we obtain*

$$p(z) = n - \|z\|^2 = n - z_1^2 - \ldots - z_n^2 = n - T_{e_1}(z)^2 - \ldots - T_{e_n}(z)^2 = n - \frac{1}{|\mathcal{G}|} \sum_{i=1}^{n} \sum_{B \in \mathcal{G}} T_{(e_i + B e_i)'}(z)$$

through Proposition 1.25, where α' *denotes the unique element in* $\mathbb{N}^n$ *contained in the* $\mathcal{G}$*–orbit of* α*.*

Positivity certificates go hand in hand with Archimedean polynomial descriptions of orbit spaces, as they allow us to characterize positive invariants via invariant sums of squares. This appears for example in [Pro78, §1] and [PS85, §7]. With our characterization of $\mathcal{T}$ as a compact basic semi–algebraic set, we can benefit from theorems such as Putinar's and its matrix version to deal with multiplicative invariants.

Example 3.19. *In the univariate case* A_1*, where* $\mathcal{G} = \{\pm 1\}$ *and*

$$\mathcal{T} = \{z \in \mathbb{R} \,|\, P(z) := 1 - z^2 \geq 0\} = [-1, 1],$$

we consider $f := x + x^{-1} + 3 \in \mathbb{R}[x^{\pm}]^{\mathcal{G}}$*. Then* $f(x) = g((x + x^{-1})/2)$ *with* $g := 2\,z + 3 \in \mathbb{R}[z]$*. Furthermore, we have* $f(x) > 0$ *on* $\mathbb{T}$ *or equivalently* $g(z) > 0$ *on* $[-1,1]$*, but* g *can not be written as a sum of squares. However, we have*

$$g(z) = 2\,z + 3 = (z+1)^2 + 2 - z^2 = (z+1)^2 + 1 + P(z).$$

Thus, g *is an element of* $\mathrm{QM}(P)$*.*

2.3 Hankel operators

The goal of the following sections is to obtain a hierarchy of semi–definite programs approximating the optimal value f^* of our problem Equation (3.4). Therefore, we shall review the dual formulation of Theorem 3.15 with measures and linear functionals as in Putinar's Theorem 3.11. In principle, Lasserre's relaxation can be formulated in any polynomial basis of $\mathbb{R}[z]$ containing 1. Since our original problem arises from trigonometric optimization, we choose the basis of generalized Chebyshev polynomials $\{T_\alpha \,|\, \alpha \in \mathbb{N}^n\}$. Explicitly, this means to replace the truncated moment matrices $\mathcal{H}^{p_i * \mathscr{L}}$ from Equation (3.6) with a matrix $\mathcal{H}^{P*\mathscr{L}}$ and to show convergence as in Theorem 3.13.

Definition 3.20. *A linear functional $\mathscr{L} \in \mathbb{R}[z]^*$ is said to have a **representing measure on** $\mathcal{T}$, if there exists a finite Borel measure η on $\mathbb{R}^n$ with support in $\mathcal{T}$, such that, for all $f \in \mathbb{R}[z]$, $\int_{\mathcal{T}} f(z)\,\mathrm{d}\eta(z) = \mathscr{L}(f)$.*

Borel measures with mass 1 are called probability measures. Hence, since Dirac measures are probability measures, we have

$$f^* = \begin{array}{ll} \inf & \int_{\mathcal{T}} f(z)\,\mathrm{d}\eta(z), \\ \text{s.t.} & \eta \text{ is a probability measure on } \mathcal{T} \end{array} = \begin{array}{ll} \inf & \mathscr{L}(f), \\ \text{s.t.} & \mathscr{L} \in \mathbb{R}[z]^*,\ \mathscr{L}(1) = 1, \\ & \mathscr{L} \text{ has a representing measure on } \mathcal{T}. \end{array} \tag{3.8}$$

To obtain a relaxation, that can be solved numerically, our first step is to find a necessary condition for $\mathscr{L}$ to have a representing measure on $\mathcal{T}$.

Definition 3.21. *The **Hankel operator** associated to a linear functional $\mathscr{L} \in \mathbb{R}[z]^*$ is*

$$\begin{array}{rcl} \mathbb{H}^{\mathscr{L}}: \ \mathbb{R}[z] & \to & \mathbb{R}[z]^*, \\ f & \mapsto & \mathscr{L}_f : \begin{cases} \mathbb{R}[z] & \to \mathbb{R}, \\ g & \mapsto \mathscr{L}(f\,g). \end{cases} \end{array}$$

For the basis $\{T_\alpha \,|\, \alpha \in \mathbb{N}^n\}$ of $\mathbb{R}[z]$ and the corresponding dual basis of $\mathbb{R}[z]^*$, the infinite symmetric matrix of $\mathbb{H}^{\mathscr{L}}$ is denoted by $\mathcal{H}^{\mathscr{L}} := \mathscr{L}(\mathbf{T}\,\mathbf{T}^t)$, where $\mathscr{L}$ applies entry–wise and $\mathbf{T}$ is the vector of basis elements T_α with $\alpha \in \mathbb{N}^n$. The entries are therefore $\mathcal{H}^{\mathscr{L}}_{\alpha\,\beta} = \mathscr{L}(T_\alpha T_\beta)$.

From now on, assume that the semi–algebraic constraints of our optimization problem are given by

$$P(z) = \sum_{\gamma \in \mathbb{N}^n} P_\gamma\, T_\gamma(z) \in \mathbb{R}[z]^{n\times n},$$

where $P_\gamma \in \mathbb{R}^{n\times n}$ is the coefficient matrix of the generalized Chebyshev polynomial $T_\gamma(z)$ in $P(z)$. We define the infinite symmetric block matrix $\mathcal{H}^{P*\mathscr{L}} := \mathscr{L}(P \otimes (\mathbf{T}\,\mathbf{T}^t))$. Again, $\mathscr{L}$ applies entry–wise and $\otimes$ denotes the Kronecker product. The entries of this matrix, indexed by $\alpha, \beta \in \mathbb{N}^n$, are symmetric blocks of size n.

As in [HL06], one can now show the following necessary condition. For $\alpha \in \mathbb{Z}^n$, α' denotes the unique element in $\mathbb{N}^n$ contained in the $\mathcal{G}$–orbit of α.

Proposition 3.22. *Let $\mathscr{L} \in \mathbb{R}[z]^*$. For $\alpha, \beta \in \mathbb{N}^n$, we have*

$$\mathcal{H}^{\mathscr{L}}_{\alpha\,\beta} = \frac{1}{|\mathcal{G}|} \sum_{A \in \mathcal{G}} \mathscr{L}(T_{(A\,\alpha+\beta)'}) \in \mathbb{R} \quad \textit{and} \quad \mathcal{H}^{P*\mathscr{L}}_{\alpha\,\beta} = \frac{1}{|\mathcal{G}|^2} \sum_{\gamma \in \mathbb{N}^n} P_\gamma \sum_{A,B \in \mathcal{G}} \mathscr{L}(T_{(A\alpha+B\beta+\gamma)'}) \in \mathbb{R}^{n\times n}.$$

If $\mathscr{L}$ has a representing measure on $\mathcal{T}$, then $\mathcal{H}^{\mathscr{L}} \succeq 0$ and $\mathcal{H}^{P*\mathscr{L}} \succeq 0$.

Proof. We have

$$\mathcal{H}^{\mathscr{L}}_{\alpha\,\beta} = \mathscr{L}(T_\alpha\, T_\beta) \in \mathbb{R} \quad \text{and} \quad \mathcal{H}^{P*\mathscr{L}}_{\alpha\,\beta} = \sum_{\gamma \in \mathbb{N}^n} P_\gamma\, \mathscr{L}(T_\alpha\, T_\beta\, T_\gamma) \in \mathbb{R}^{n\times n}.$$

Then the formula follows from the linearity of $\mathscr{L}$ and the recurrence relation of generalized Chebyshev polynomials Proposition 1.25.

Assume that $\mathscr{L}$ has a representing measure η on $\mathcal{T}$. Then, for all $p \in \mathbb{R}[z]$ with coordinate vector $\mathrm{vec}(p)$ in the Chebyshev basis, we have

$$\mathrm{vec}(p)^t\, \mathcal{H}^{\mathscr{L}}\, \mathrm{vec}(p) = \mathscr{L}((\mathrm{vec}(p)^t\, \mathbf{T})^2) = \mathscr{L}(p^2) = \int_{\mathcal{T}} p(z)^2\, \mathrm{d}\eta(z) \geq 0.$$

Hence, $\mathcal{H}^{\mathscr{L}} \succeq 0$. In particular, since $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$, we obtain $\mathcal{H}^{P*\mathscr{L}} \succeq 0$. □

In combination with Equation (3.8), this gives us

$$\begin{array}{rlll} f^* = & \inf & \sum\limits_{\alpha\in S} c_\alpha\, \mathscr{L}(T_\alpha) & \geq \quad \inf \quad \sum\limits_{\alpha\in S} c_\alpha\, \mathscr{L}(T_\alpha) \\ & \text{s.t.} & \mathscr{L} \in \mathbb{R}[z]^*,\ \mathscr{L}(1) = 1, & \qquad \text{s.t.} \quad \mathscr{L} \in \mathbb{R}[z]^*,\ \mathscr{L}(1) = 1, \\ & & \mathscr{L} \text{ has a representing measure on } \mathcal{T} & \qquad\qquad\ \ \mathcal{H}^{\mathscr{L}},\ \mathcal{H}^{P*\mathscr{L}} \succeq 0. \end{array} \tag{3.9}$$

Remark 3.23. *To enforce that the quadratic module of P is Archimedean, we can replace the matrix polynomial P with $\widehat{P}$ from Proposition 3.17. Then the blocks of $\mathcal{H}^{\widehat{P}*\mathscr{L}}$ corresponding to $p(z) = n - \|z\|^2$ have entries*

$$\mathcal{H}^{p*\mathscr{L}}_{\alpha\,\beta} = n - \frac{1}{|\mathcal{G}|^3} \sum_{i=1}^{n} \sum_{A,B,C\in\mathcal{G}} \mathscr{L}(T_{(A\alpha+B\beta+Ce_i+e_i)'}) \in \mathbb{R}.$$

As a corollary of Proposition 3.22, if a linear functional $\mathscr{L}$ has a representing measure on $\mathcal{T}$, then $\mathcal{H}^{p*\mathscr{L}} \succeq 0$.

2.4 Truncation

In order to solve Equation (3.9) numerically, the next step is to restrict to a finite–dimensional space. A suitable choice is given by the notion of weighted degrees. From now on, assume that $\mathbb{R}[z] = \bigcup_d \mathcal{F}_d$ is a filtration of $\mathbb{R}[z]$ as an $\mathbb{R}$–algebra, such that, if $T_{\mu_1} \in \mathcal{F}_{d_1}$ and $T_{\mu_2} \in \mathcal{F}_{d_2}$, then $T_{\mu_1} T_{\mu_2} \in \mathcal{F}_{d_1+d_2}$. If R is irreducible, then we can take

$$\mathcal{F}_d := \bigoplus_{\ell=0}^{d} \langle \{T_\mu \,|\, \mu \in \Omega^+,\, \deg_W(T_\mu) = \ell\} \rangle_{\mathbb{R}}$$

from Proposition 1.40. Otherwise, a product order can be constructed.

Example 3.24. *As in Example 1.38, we consider the root system B_3. Let $\mathscr{L} \in \mathbb{R}[z]^*$ and, for $\alpha \in \mathbb{N}^3$, set $y_\alpha := \mathscr{L}(T_\alpha)$. Then the Hankel operator $\mathbb{H}^{\mathscr{L}}$, restricted to the linear subspace $\langle 1, T_{001} = z_3, T_{010} = z_2, T_{100} = z_1\rangle_{\mathbb{R}}$ of degree 1 polynomials in $\mathbb{R}[z]$, has matrix*

$$\begin{bmatrix} y_{000} & y_{001} & y_{010} & y_{100} \\ y_{001} & (3y_{100}+3y_{010}+y_{002}+y_{000})/8 & (2y_{101}+y_{011}+y_{001})/4 & (y_{101}+y_{001})/2 \\ y_{010} & (2y_{101}+y_{011}+y_{001})/4 & (2y_{200}+4y_{102}+y_{020}+4y_{010}+y_{000})/12 & (y_{110}+y_{100}+y_{002})/3 \\ y_{100} & (y_{101}+y_{001})/2 & (y_{110}+y_{100}+y_{002})/3 & (y_{200}+4y_{010}+y_{000})/6 \end{bmatrix}.$$

Hence, $\mathscr{L}$ must be defined on T_{102}, which has degree 3. When $\mathbb{H}^{\mathscr{L}}$ is restricted to $\mathcal{F}_1$ on the other hand, the largest degree is 2 and it suffices to choose $\mathscr{L} \in \mathcal{F}_2^*$.

For a linear functional $\mathscr{L} \in \mathcal{F}_{2d}^*$, the operator

$$\begin{array}{rccl} \mathbb{H}_d^{\mathscr{L}} : & \mathcal{F}_d & \to & \mathcal{F}_d^*, \\ & f & \mapsto & \mathscr{L}_f : \begin{cases} \mathcal{F}_d & \to \mathbb{R} \\ g & \mapsto \mathscr{L}(f\,g) \end{cases} \end{array} \tag{3.10}$$

is well–defined thanks to Proposition 1.40. The matrix of $\mathbb{H}_d^{\mathscr{L}}$ is $\mathcal{H}_d^{\mathscr{L}}$, which has rows and columns indexed by those $\alpha \in \mathbb{N}^n$ with $T_\alpha \in \mathcal{F}_d$. The size of $\mathcal{H}_d^{\mathscr{L}}$ is $\dim(\mathcal{F}_d)$. Analogously, the matrix $\mathcal{H}_{d-D}^{P*\mathscr{L}}$ is well–defined, when

$$d \geq D := \min\{\lceil \ell/2 \rceil \mid \ell \in \mathbb{N},\, P \in (\mathcal{F}_\ell)^{n\times n}\}.$$

2.5 Chebyshev moment and SOS hierarchy

We have reviewed that our optimization problem Equation (3.4) has a formulation with sums of squares Equation (3.7) and with linear functionals Equation (3.9). Furthermore, we have shown that the $\mathcal{F}_d$ are suitable finite–dimensional linear subspace for truncation of Hankel operators when using Chebyshev polynomials. This comes now together in two hierarchies of finite–dimensional optimization problems, which are later shown to be dual.

For $f = \sum_{\alpha\in S} c_\alpha T_\alpha$ our objective function and P our constraining matrix polynomial, fix a **relaxation order** $d \in \mathbb{N}$, such that

$$d \geq \max\{\min\{\lceil \ell/2 \rceil \mid \ell \in \mathbb{N},\, f \in \mathcal{F}_\ell\},\, \underbrace{\min\{\lceil \ell/2 \rceil \mid \ell \in \mathbb{N},\, P \in (\mathcal{F}_\ell)^{n\times n}\}}_{=:D}\}. \tag{3.11}$$

When we write $d \in \mathbb{N}$, we automatically assume that d is large enough in the above sense.

The **Chebyshev moment relaxation of order** d is

$$\begin{aligned} f_{\mathrm{mom}}^d := \quad \inf \quad & \sum_{\alpha\in S} c_\alpha \mathscr{L}(T_\alpha) \\ \text{s.t.} \quad & \mathscr{L} \in \mathcal{F}_{2d}^*,\, \mathscr{L}(1) = 1, \\ & \mathcal{H}_d^{\mathscr{L}},\, \mathcal{H}_{d-D}^{p*\mathscr{L}} \succeq 0. \end{aligned} \tag{3.12}$$

The **Chebyshev SOS relaxation of order** d is

$$\begin{aligned} f_{\mathrm{sos}}^d := \quad \sup \quad & \lambda \\ \text{s.t.} \quad & \lambda \in \mathbb{R},\, q \in \mathrm{SOS}(\mathcal{F}_d),\, Q \in \mathrm{SOS}(\mathcal{F}_{d-D}^{n\times n}), \\ & \sum_{\alpha\in S} c_\alpha T_\alpha - \lambda = q + \mathrm{Trace}(P\,Q). \end{aligned} \tag{3.13}$$

Theorem 3.25. *The following statements hold.*

1. *The sequence $(f_{\mathrm{sos}}^d)_{d\in\mathbb{N}}$ is monotonously non–decreasing.*
2. *The sequence $(f_{\mathrm{mom}}^d)_{d\in\mathbb{N}}$ is monotonously non–decreasing.*
3. *For $d \in \mathbb{N}$, we have $f_{\mathrm{sos}}^d \leq f_{\mathrm{mom}}^d$.*
4. *If $\mathrm{QM}(P)$ is Archimedean, then $\lim_{d\to\infty} f_{\mathrm{sos}}^d = \lim_{d\to\infty} f_{\mathrm{mom}}^d = f^*$.*

Proof. *1.* and *2.* follow from the fact that $\mathcal{F}_d \subseteq \mathcal{F}_{d+1} \subseteq \ldots$ is an ascending chain.

3. Let $\mathscr{L}$ be optimal for Equation (3.12) and (λ, q, Q) be optimal for Equation (3.13). Then

$$\sum_{\alpha\in S} c_\alpha \mathscr{L}(T_\alpha) - \lambda = \mathscr{L}(q) + \mathscr{L}(\mathrm{Trace}(P\,Q)).$$

The right–hand side is nonnegative, because q, Q are sums of squares and $\mathcal{H}_d^{\mathscr{L}}, \mathcal{H}_{d-D}^{P*\mathscr{L}} \succeq 0$. Thus, $\lambda \leq \sum_\alpha c_\alpha \mathscr{L}(T_\alpha)$.

4. By Theorem 3.15, for any $\varepsilon > 0$, there exist sums of squares q, Q, such that

$$\sum_{\alpha\in S} c_\alpha T_\alpha - f^* + \varepsilon = q + \mathrm{Trace}(P\,Q).$$

Since ε is arbitrary and $\bigcup_{d\in\mathbb{N}} \mathcal{F}_d = \mathbb{R}[z]$, we obtain $\lim_{d\to\infty} f^d_{\mathrm{sos}} = f^*$. With *3.*, the same holds for f^d_{mom}. □

Remark 3.26. *In particular, we obtain the first assertion of Putinar's theorem in the matrix case: If* $\mathrm{QM}(P)$ *is Archimedean, then equality holds in Equation (3.9).*

3 Implementation

We want to solve the two optimization problems from the Chebyshev moment and SOS hierarchy numerically with solvers such as [MOS] in practice. To do this, we translate the problems in a standard form for semi–definite programs (SDP), that is, optimization problems on the cone of semi–definite matrices, and show duality. This translation is implemented in a Maple package with more tools for root systems and Chebyshev polynomials[1].

3.1 SDP formulation

By Proposition 3.22, for a linear functional $\mathscr{L} \in \mathcal{F}^*_{2d}$ and $d \in \mathbb{N}$, we can write

$$\begin{pmatrix} \mathcal{H}^{\mathscr{L}}_d & 0 \\ 0 & \mathcal{H}^{P*\mathscr{L}}_{d-D} \end{pmatrix} = \sum_{\alpha\in\mathbb{N}^n} \mathscr{L}(T_\alpha)\, A_\alpha, \tag{3.14}$$

where A_α is the symmetric coefficient matrix of $\mathscr{L}(T_\alpha)$. For $d \geq D$, $\mathscr{L}(T_\alpha)$ is well–defined whenever $A_\alpha \neq 0$. We write $\mathrm{Sym}^N := \mathrm{Sym}^{N_d} \times \mathrm{Sym}^{n\, N_{d-D}}$ for the space of block–diagonal symmetric matrices with two blocks of size $N_d := \dim(\mathcal{F}_d)$ and $n\, N_{d-D}$. The positive semi–definite elements are denoted by $\mathrm{Sym}^N_{\succeq 0}$.
Now, we consider the optimization problems

$$\begin{array}{llll} \text{(P)} & \inf & \sum_{\alpha\in S} c_\alpha\, \mathscr{L}(T_\alpha) \\ & \text{s.t.} & \mathscr{L} \in \mathcal{F}^*_{2d},\ Z \in \mathrm{Sym}^N_{\succeq 0}, \\ & & \mathscr{L}(1) = 1,\ Z = \sum_{\alpha\in\mathbb{N}^n} \mathscr{L}(T_\alpha)\, A_\alpha \end{array} \quad \text{and} \quad \begin{array}{lll} \text{(D)} & \sup & c_0 - \mathrm{Trace}(A_0\, X) \\ & \text{s.t.} & X \in \mathrm{Sym}^N_{\succeq 0},\ \forall\, \alpha \neq 0 : \\ & & \mathrm{Trace}(A_\alpha\, X) = c_\alpha. \end{array} \tag{3.15}$$

Proposition 3.27. *Fix a relaxation order $d \in \mathbb{N}$. The following statements hold.*

1. *The optimal value of* (P) *is* f^d_{mom}.
2. *The optimal value of* (D) *is* f^d_{sos}.
3. (P) *and* (D) *are dual with respect to the trace inner products on* Sym^N *and the induced Euclidean scalar product on* $\mathcal{F}^*_{2d}$.
4. *If* $(X, \mathscr{L}, Z)$ *are optimal for* (P) *and* (D)*, then the duality gap is*

$$f^d_{\mathrm{mom}} - f^d_{\mathrm{sos}} = \mathrm{Trace}(X\, Z).$$

Proof. *1.* Let $\mathscr{L}$ be optimal for (P). Then $\sum_\alpha c_\alpha\, \mathscr{L}(T_\alpha) = f^d_{\mathrm{mom}}$ by definition.

2. Let $\lambda \in \mathbb{R}$, $q \in \sum(\mathcal{F}_d)^2$ and $Q \in \sum(\mathcal{F}^{n\times n}_{d-D})^2$ be optimal for Equation (3.13). Then

$$\sum_{\alpha\in S} c_\alpha\, \mathscr{L}(T_\alpha) - \lambda = \mathscr{L}(q) + \mathscr{L}(\mathrm{Trace}(P\, Q)).$$

[1] GeneralizedChebyshev: https://www-sop.inria.fr/members/Tobias.Metzlaff/GeneralizedChebyshev.zip

Assume that $Q = \sum_{i=1}^{k} Q_i\, Q_i^t$ and let $\mathbf{T}_{d-D}$ be the vector of generalized Chebyshev polynomials in $\mathcal{F}_{d-D}$. For $1 \leq i \leq k$, write $Q_i = \mathrm{mat}(Q_i)\, \mathbf{T}_{d-D}$, where $\mathrm{mat}(Q_i)$ is the coordinate matrix of Q_i with n rows and $N_{d-D})$ columns. We have

$$\begin{aligned} \mathrm{Trace}(P\, Q) &= \sum_{i=1}^{k} \mathrm{Trace}(P\, \mathrm{mat}(Q_i)\, \mathbf{T}_{d-D}\, \mathbf{T}_{d-D}^t\, \mathrm{mat}(Q_i)^t) \\ &= \mathrm{Trace}((\mathbf{T}_{d-D}^t\, \mathbf{T}_{d-D} \otimes P) \underbrace{\sum_{i=1}^{k} \mathrm{vec}(\mathrm{mat}(Q_i))\, \mathrm{vec}(\mathrm{mat}(Q_i))^t}_{=:X_2}), \end{aligned}$$

where $\mathrm{vec}(\mathrm{mat}(Q_i)) := ((\mathrm{mat}(Q_i)_{\cdot 1})^t, \ldots, (\mathrm{mat}(Q_i)_{\cdot N_{d-D}})^t)^t$ are the stacked columns of $\mathrm{mat}(Q_i)$. The matrix X_2 is symmetric of size $n\, N_{d-D}$ and positive semi–definite. Hence, $\mathscr{L}(\mathrm{Trace}(P\, Q)) = \mathrm{Trace}(\mathcal{H}_{d-D}^{P*\mathscr{L}}\, X_2)$. In particular, there exists $X_1 \in \mathrm{Sym}_{\succeq 0}^{N_d}$ with $\mathscr{L}(q) = \mathrm{Trace}(\mathcal{H}_d^{\mathscr{L}}\, X_1)$. When we fix $X := \mathrm{diag}(X_1, X_2) \in \mathrm{Sym}_{\succeq 0}^{N}$ and A_α as in Equation (3.14), we obtain

$$\lambda = c_0\, \mathscr{L}(1) - \mathscr{L}(q(0)) - \mathscr{L}(\mathrm{Trace}(P(0)\, Q(0))) = c_0 - \mathrm{Trace}(A_0\, X)$$

and, for $\alpha \neq 0$, $c_\alpha = \mathrm{Trace}(A_\alpha\, X)$. Thus, $c_0 - \mathrm{Trace}(A_0\, X) = f_{\mathrm{sos}}^d$.

3. Define the linear operators

$$\begin{array}{rccl} \mathbb{A}: & \mathcal{F}_{2d}^* & \to & \mathrm{Sym}^N, \\ & \mathscr{L} & \mapsto & \sum\limits_{\alpha \in \mathbb{N}^n} \mathscr{L}(T_\alpha)\, A_\alpha, \\[2ex] \mathbb{A}^*: & \mathrm{Sym}^N & \to & \mathcal{F}_{2d}^*, \\ & X & \mapsto & \begin{cases} \mathcal{F}_{2d} & \to \mathbb{R}, \\ T_\alpha & \mapsto \mathrm{Trace}(A_\alpha\, X). \end{cases} \end{array}$$

We have

$$\mathrm{Trace}(\mathbb{A}(\mathscr{L})\, X) = \sum_{\alpha \in \mathbb{N}^n} \mathscr{L}(T_\alpha)\, \mathbb{A}^*(X)(T_\alpha).$$

Thus $\mathbb{A}$ and $\mathbb{A}^*$ are adjoint and (P) and (D) are dual.

4. We have

$$\begin{aligned} \mathrm{Trace}(X\, Z) &= \mathrm{Trace}(X\, \mathbb{A}(\mathscr{L})) + \mathrm{Trace}(X\, A_0) - c_0 = \sum_{\alpha \in S} \mathbb{A}^*(X)_\alpha\, \mathscr{L}(T_\alpha) + \mathrm{Trace}(X\, A_0) - c_0 \\ &= \sum_{\alpha \in S} \mathbb{A}^*(X)_\alpha\, \mathscr{L}(T_\alpha) - (c_0 - \mathrm{Trace}(X\, A_0)) = f_{\mathrm{mom}}^d - f_{\mathrm{sos}}^d. \end{aligned}$$

This completes the proof. □

Remark 3.28. *For fixed order d, we define*

1. *the* ***number of matrices*** *A_α as $m + 1 := \dim(\mathcal{F}_{2d})$ and*

2. *the* ***overall matrix size*** *as $N := \dim(\mathcal{F}_d) + n\, \dim(\mathcal{F}_{d-D})$.*

Then Equation (3.15) is a semi–definite program with primal formulation (P) over the cone $\mathcal{F}_{2d}^* \cong \mathbb{R}^{m+1}$ with dual cone 0 and with dual formulation (D) over the self–dual cone $\mathrm{Sym}_{\succeq 0}^N$.

$\mathrm{R}\backslash d$	2	3	4	5	6	7	8	9	10
$\mathrm{B}_2, \mathrm{C}_2$	$6+2, 14$	$10+6, 27$	$15+12, 44$	$21+20, 65$	$28+30, 90$	$36+42, 119$	$45+56, 152$	$55+72, 189$	$66+90, 230$
G_2	–	$6+3, 15$	$9+6, 24$	$12+12, 35$	$16+18, 48$	$20+27, 63$	$25+36, 80$	$30+48, 99$	$36+60, 120$
A_2	–	$10+3, 27$	$15+9, 44$	$21+18, 65$	$28+30, 90$	$36+45, 119$	$45+63, 152$	$55+84, 189$	$66+108, 230$
B_3	–	$13+3, 49$	$22+9, 94$	$34+21, 160$	$50+39, 251$	$70+66, 371$	$95+102, 524$	$125+150, 714$	$161+210, 945$
C_3	–	$20+3, 83$	$35+12, 164$	$56+30, 285$	$84+60, 454$	$120+105, 679$	$165+168, 968$	$220+252, 1329$	$286+360, 1770$
A_3	–	–	$35+4, 164$	$56+16, 285$	$84+40, 454$	$120+80, 679$	$165+140, 968$	$220+224, 1329$	$286+336, 1770$
B_4	–	–	$30+4, 174$	$50+12, 335$	$80+32, 587$	$120+64, 959$	$175+120, 1484$	$245+200, 2199$	$336+320, 3145$
C_4	–	–	$70+4, 494$	$126+20, 1000$	$210+60, 1819$	$330+140, 3059$	$495+280, 4844$	$715+504, 7314$	$1001+840, 10625$
D_4	–	–	$46+4, 294$	$80+16, 580$	$130+44, 1035$	$200+96, 1715$	$295+184, 2684$	$420+320, 4014$	$581+520, 5785$

Table 3.1: SDP parameters (N, m) for Equation (3.15).

If we took the standard monomial basis and applied the moment relaxation from [HL06], the number of obtained matrices for the SDP would be the same as in the case of A_{n-1} and C_n, because the weighted degree is the classical degree in those cases. Here we see an immediate advantage when using B_n, D_n or G_2 instead. The number of matrices and their overall size is significantly smaller. Numerical examples follow in the next chapter.

The downside of using Chebyshev polynomials instead of standard monomials is that the matrices of the SDP take longer to compute, because one has to apply the recurrence formula Proposition 1.25. This computation is not numerical, but exact. Hence, this technique is more efficient, if the numerical effort to solve a larger SDP in the standard monomial basis is bigger than the effort to solve a smaller SDP in the Chebyshev basis plus matrix computation. Furthermore, since the matrices only depend on the objective function in terms of the weighted degree, the same matrices can be used to solve several problems.

If one adds the constraint $p(z) = n - \|z\|^2$ from Proposition 3.17, one adds a block of size $N_{d-\tilde{D}} = \dim(\mathcal{F}_{d-\tilde{D}})$, where $\tilde{D} := \min\{\lceil \ell/2 \rceil \mid \ell \in \mathbb{N},\, p \in \mathcal{F}_\ell\}$. Otherwise, the semi–definite program is not necessarily feasible for small orders of relaxation. The additional block size is listed below.

$\mathrm{R}\backslash d$	2	3	4	5	6	7	8	9	10
$\mathrm{B}_2, \mathrm{C}_2$	3	6	10	15	21	28	36	45	55
G_2	–	2	4	6	9	12	16	20	25
A_2	–	6	10	15	21	28	36	45	55
B_3	–	3	7	13	22	34	50	70	95
C_3	–	10	20	35	56	84	120	165	220
A_3	–	–	20	35	56	84	120	165	220
B_4	–	–	8	16	30	50	80	120	175
C_4	–	–	35	70	126	210	330	495	715
D_4	–	–	11	24	46	80	130	200	295

Table 3.2: Block size $N_{d-\tilde{D}}$ for the additional constraint $p(z) = n - \|z\|^2$.

3.2 A case study

We apply the Chebyshev moment and SOS hierarchy to solve a trigonometric polynomial optimization problem and compare with other techniques. One approach is to study positivity as in the left hand side of Equation (3.7), but adapted to trigonometric polynomials via sums of Hermitian squares (SOHS). The Riesz–Fejér theorem states that a univariate ($n = 1$, $\Omega = \mathbb{Z}$) trigonometric polynomial with sign–symmetric coefficients is nonnegative on $\mathbb{R}$ if and only if it has a spectral factorization. In this case, complex coefficients are admissible and the factorization reads

$$f = h\, h^*,$$

where h is causal with support in $\mathbb{N}$ and h^* is obtained from h by complex conjugation of coefficients and inversion of monomials [Dum07, Theorem 1.1]. Algorithms to compute a spectral factorization are known, see for example [KS01, MW02, MDSV22]. The Riesz–Fejér theorem can be generalized to the multivariate case for strictly positive polynomials [Dum07, Theorem 4.11]. Such positivity certificates benefit us in problems of optimization, which to solve is the primary goal of this chapter.

Now, [Dum07, §3] proposes to approximate the minimum of a trigonometric polynomial f as in Equation (3.1) by solving the semi–definite program

$$f_{\mathrm{rf}}^{S} = \begin{array}{ll} \sup & \lambda \\ \text{s.t.} & f-\lambda \in \mathrm{SOHS}(S) \end{array} \tag{3.16}$$

as in Riesz–Fejér, where $S \subseteq \Omega$ is a finite set of exponents containing the support of f up to central symmetry. This can be translated into standard form with Kronecker products of elementary Toeplitz matrices, yielding a hierarchy of lower bounds.

Example 3.29. *We search the minima f^*, g^*, h^* and k^* of the following trigonometric polynomials with graphs depicted in Figure 3.2.*

1. $f(u) = ((-23\cos(2\pi(u_1-u_2))-23\cos(2\pi(u_1-u_3))-23\cos(2\pi(u_2-u_3))-21)\cos((4u_1-2u_2-2u_3)\pi))/3+((-23\cos(2\pi(u_1-u_2))-23\cos(2\pi(u_1-u_3))-23\cos(2\pi(u_2-u_3))-21)\cos(2\pi(u_1-2u_2+u_3)))/3+((-23\cos(2\pi(u_1-u_2))-23\cos(2\pi(u_1-u_3))-23\cos(2\pi(u_2-u_3))-21)\cos(2\pi(u_1+u_2-2u_3)))/3+(16\cos(2\pi(u_1-u_2))^3)/3+((48(\cos(2\pi(u_1-u_3))+\cos(2\pi(u_2-u_3)))-2)\cos(2\pi(u_1-u_2))^2)/3+((48\cos(2\pi(u_1-u_3))^2+(96\cos(2\pi(u_2-u_3))-4)\cos(2\pi(u_1-u_3))+48\cos(2\pi(u_2-u_3))^2-4\cos(2\pi(u_2-u_3))-33)\cos(2\pi(u_1-u_2)))/3+(16\cos(2\pi(u_1-u_3))^3)/3+((48\cos(2\pi(u_2-u_3))-2)\cos(2\pi(u_1-u_3))^2)/3+((48\cos(2\pi(u_2-u_3))^2-4\cos(2\pi(u_2-u_3))-33)\cos(2\pi(u_1-u_3)))/3+(16\cos(2\pi(u_2-u_3))^3)/3-(2\cos(2\pi(u_2-u_3))^2)/3-11\cos(2\pi(u_2-u_3))-7$
   with $u \in \mathbb{R}^3/[1,1,1]^t$ is invariant under $\mathcal{W} = \mathfrak{S}_3 \ltimes \{\pm 1\}$ and can be written as
   $f(u) = \frac{1}{|\mathcal{W}|}\sum\limits_{A\in\mathcal{W}} 2\,\mathfrak{e}^{A\omega_1}(u)+\mathfrak{e}^{A\omega_2}(u)+\mathfrak{e}^{A(\omega_1+\omega_2)}(u)+4\,\mathfrak{e}^{3A\omega_1}(u) = 144\,z_1^3-6\,z_1^2-69\,z_1z_2-33\,z_1-21\,z_2-7|_{z=\mathfrak{c}(u)}$
   with $\omega_1=[0,-1,1]^t$, $\omega_2=[-1,-1,2]^t$ the weights associated to G_2.

2. $g(u) = (2(\cos(2\pi(u_1-u_2))+\cos(2\pi(u_1-u_3))+\cos(2\pi(u_2-u_3)))^2)/3-(2\cos(2\pi(u_1-u_2)))/3-(2\cos(2\pi(u_1-u_3)))/3-(2\cos(2\pi(u_2-u_3)))/3-1$
   with $u \in \mathbb{R}^3/[1,1,1]^t$ is invariant under $\mathcal{W} = \mathfrak{S}_3 \ltimes \{\pm 1\}$ and can be written as
   $g(u) = \frac{1}{|\mathcal{W}|}\sum\limits_{A\in\mathcal{W}} \mathfrak{e}^{2A\omega_1}(u)+2\,\mathfrak{e}^{A\omega_2}(u) = 6\,z_1^2-2\,z_1-1|_{z=\mathfrak{c}(u)}$
   with $\omega_1=[0,-1,1]^t$, $\omega_2=[-1,-1,2]^t$ the weights associated to G_2.

3. $h(u) = ((-8\cos(2\pi u_2)^2-6\cos(2\pi u_2)+4)\cos(2\pi x)^2)/2+((-6\cos(2\pi u_2)^2+2\cos(2\pi u_2)+5)\cos(2\pi u_1))/2+2\cos(2\pi u_2)^2+(5\cos(2\pi u_2))/2-1$
   with $u \in \mathbb{R}^2$ is invariant under $\mathcal{W} = \mathfrak{S}_2 \ltimes \{\pm 1\}^2$ and can be written as
   $h(u) = \frac{1}{|\mathcal{W}|}\sum\limits_{A\in\mathcal{W}} 2\,\mathfrak{e}^{A\omega_1}(u)+\mathfrak{e}^{A\omega_2}(u)-\mathfrak{e}^{2A\omega_2}(u)-3\,\mathfrak{e}^{A(\omega_1+\omega_2)}(u) = 8\,z_1^2-6\,z_1z_2-4\,z_2^2+5\,z_1-3\,z_2-1|_{z=\mathfrak{c}(u)}$
   with $\omega_1=[1,0]^t$, $\omega_2=[1,1]^t$ the weights associated to C_2.

4. $k(u) = 4\cos(2\pi u_1)^2\cos(2\pi u_2)^2-1$
   with $u \in \mathbb{R}^2$ is invariant under $\mathcal{W} = \mathfrak{S}_2 \ltimes \{\pm 1\}^2$ and can be written as
   $k(u) = \frac{1}{|\mathcal{W}|}\sum\limits_{A\in\mathcal{W}} 2\,\mathfrak{e}^{2A\omega_1}(u)+\mathfrak{e}^{2A\omega_2}(u) = 4\,z_2^2-1|_{z=\mathfrak{c}(u)}$
   with $\omega_1=[1,0]^t$, $\omega_2=[1,1]^t$ the weights associated to C_2.

Here, ω_1, ω_2 span a weight lattice Ω of a root system with Weyl group $\mathcal{W}$ as in Definition 1.1 and $\mathfrak{S}_n$ denotes the symmetric group of order $n!$. In practice, the exact optimal value is usually unknown. However, since we compare lower bounds, it suffices to check which bound is larger and therefore closer to the actual optimum.

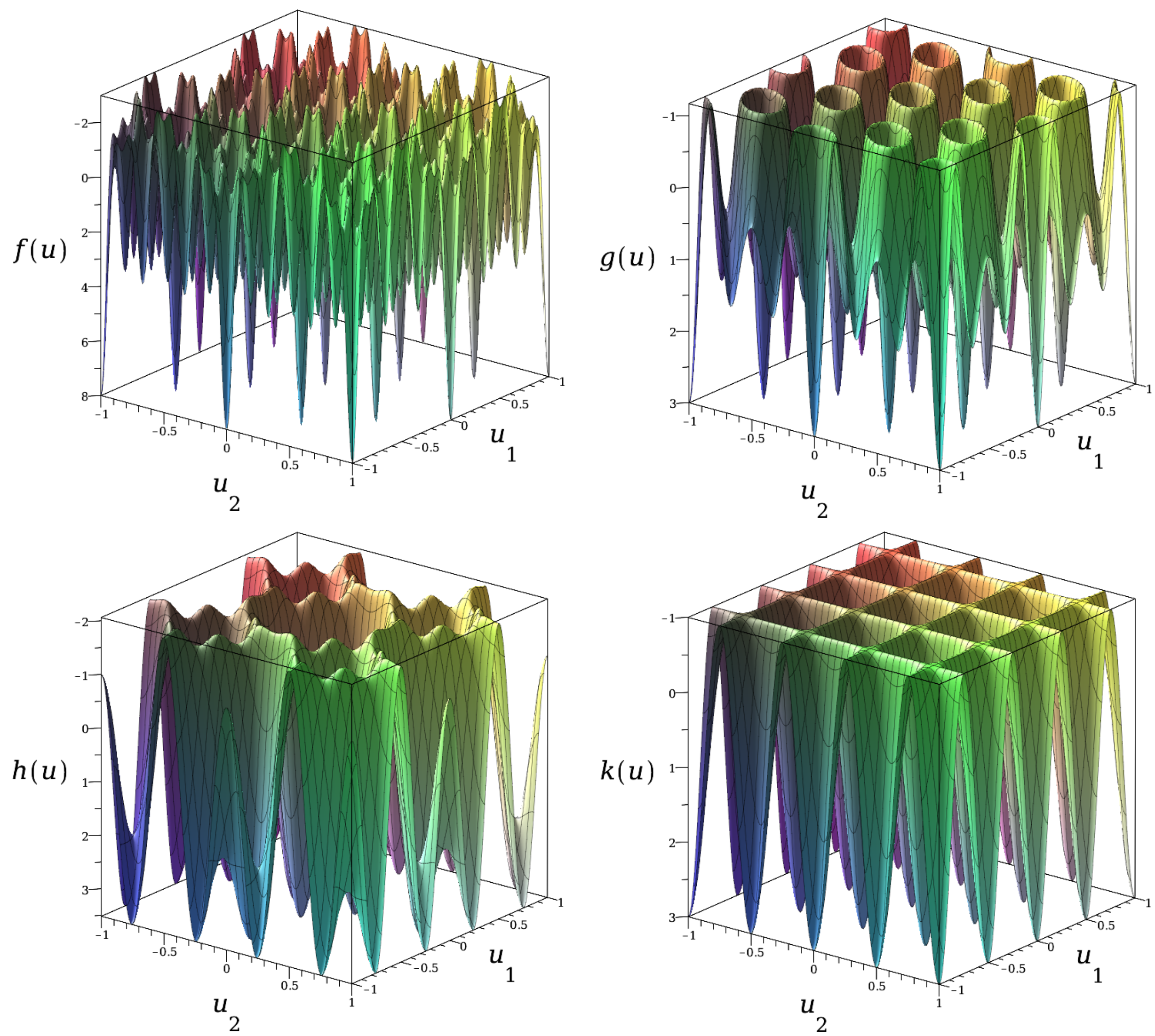


Figure 3.2: The graphs of f, g, h and k with $u \in \mathbb{R}^3/[1,1,1]^t \cong \mathbb{R}^2$.

For $3 \leq d \leq 7$, *we choose* $\tilde{S}$ *to be the set of all dominant weights* $\alpha \in \Omega^+ \cong \mathbb{N}^2$ *with* $\deg_W(T_\alpha) \leq d$. *In* Equation (3.16), $S = (\tilde{S} - \tilde{S}) \cap (H \setminus \{0\})$ *is an admissible choice for any halfspace* H, *since* S *contains all exponents of the objective functions up to central symmetry. In this case, we denote the optimal value by* f_{rf}^d. *On the other hand, we apply the Chebyshev SOS hierarchy* f_{sos}^d *from Equation* (3.13), *where we only need to take exponents up to Weyl group symmetry, that is,* $\tilde{S}$. *With the two techniques, we obtain the results in Table 3.3.* N *denotes the matrix size and* $m+1$ *the number of matrices, depending on* d. *To solve the semi–definite programs, we rely on* [MOS].

We observe that the lower bounds f_{sos}^d *are always larger or equal and therefore closer to the exact optimal value, while the parameters* N, m *that indicate the size of the semi–definite program are smaller compared to* f_{rf}^d *from Equation* (3.16). *The size difference becomes more relevant for larger dimension* n. *Sparsity was not exploited in either case.*

d	3	4	5	6	7
f_{rf}^d	-3.50118	-3.40372	-3.31195	-3.25383	-3.22049
N,m	$49,33$	$81,58$	$121,90$	$169,129$	$225,175$
f_{sos}^d	-3.20499	-3.10220	-2.98718	-2.98718	-2.98718
N,m	$9,15$	$15,24$	$24,35$	$34,48$	$47,63$
g_{rf}^d	-1.18824	-1.180240	-1.17058	-1.16970	-1.16719
N,m	$49,33$	$81,58$	$121,90$	$169,129$	$225,175$
g_{sos}^d	-1.16667	-1.16667	-1.16667	-1.16667	-1.16667
N,m	$9,15$	$15,24$	$24,35$	$34,48$	$47,63$
h_{rf}^d	-2.12159	-2.10672	-2.1012	-2.09959	-2.09073
N,m	$25,24$	$49,54$	$81,96$	$121,150$	$169,217$
h_{sos}^d	-2.27496	-2.06250	-2.06250	-2.06250	-2.06250
N,m	$16,27$	$27,44$	$41,65$	$58,90$	$78,119$
k_{rf}^d	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
N,m	$25,24$	$49,54$	$81,96$	$121,150$	$169,217$
k_{sos}^d	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
N,m	$16,27$	$27,44$	$41,65$	$58,90$	$78,119$

Table 3.3: Comparison of the two techniques in terms of approximation and SDP size.

Other optimization techniques for trigonometric polynomials are for example studied in [JM18]. There, the Lasserre hierarchy is applied for complex polynomials without symmetry reduction. Our original problem Equation (3.2) can also be solved with this approach by introducing equality constraints, which might influence the convergence of the hierarchy, see [Lau09, §6]. We do not do this in practice and can therefore not compare the quality. The size of the semi–definite program can be expected to be larger without the exploitation of symmetry.

3.3 Optimizing on coefficients

Finally, we apply the Chebyshev moment and SOS hierarchy to bilevel optimization. For $S \subseteq \mathbb{N}^n \setminus \{0\}$ finite, consider the problem

$$\begin{aligned} F(S) := \sup_c \inf_z \quad & \sum_{\alpha \in S} c_\alpha \, T_\alpha(z) \\ \text{s.t.} \quad & c \in \mathbb{R}^S_{\geq 0},\ z \in \mathcal{T} \\ & \sum_{\alpha \in S} c_\alpha = 1. \end{aligned} \tag{3.17}$$

This was studied in [Las09, Chapter 13]. For a fixed relaxation order $d \in \mathbb{N}$ sufficiently large, define

$$\begin{aligned} f_{\mathrm{mix}}^d := \sup \quad & -\mathrm{Trace}(A_0 \, X) \\ \text{s.t.} \quad & X \in \mathrm{Sym}^N_{\succeq 0},\ \sum_{\alpha \in S} \mathrm{Trace}(A_\alpha \, X) = 1, \\ & \mathrm{Trace}(A_\alpha \, X) \geq 0 \quad \text{for} \quad \alpha \in S, \\ & \mathrm{Trace}(A_\beta \, X) = 0 \quad \text{for} \quad \beta \notin S \cup \{0\}, \end{aligned} \tag{3.18}$$

where the A_α and A_β are defined as in Equation (3.14). We follow the proof of [Las09, Theorem 13.1] to show convergence.

Theorem 3.30. *Assume that* $\mathrm{QM}(P)$ *is Archimedean. Then the sequence* $(f_{\mathrm{mix}}^d)_{d \in \mathbb{N}}$ *is monotonously non–decreasing and converges to* $F(S)$*.*

Proof. Let (λ, c, q, Q) be optimal for Equation (3.18). Then $f_{\mathrm{mix}}^d = \lambda \leq (f_c)^* \leq F(S)$, where $(f_c)^*$ denoted the minimum of $f_c(z) := \sum_{\alpha \in S} c_\alpha \, T_\alpha(z) \in \mathbb{R}[z]$ on $\mathcal{T}$.

On the other hand, $\mathcal{T} = \{z \in \mathbb{R}^n \,|\, P(z) \succeq 0\}$ is compact and the T_α are continuous. Hence, the map $g : c \mapsto (f_c)^*$ is continuous on a compact set. Thus, there exists a feasible $c^* \in \mathbb{R}^S_{\geq 0}$, such that $F(S) = g(c^*)$.

For any $\varepsilon > 0$, the polynomial $\sum_{\alpha\in S} c_\alpha^* \, T_\alpha - F(S) + \varepsilon$ is strictly positive on $\mathcal{T}$. Thus, by Theorem 3.15, there exist sums of squares q and Q, such that

$$\sum_{\alpha\in S} c_\alpha^* \, T_\alpha - (F(S) - \varepsilon) = q + \mathrm{Trace}(P\,Q).$$

For $d \in \mathbb{N}$ sufficiently large, we can follow our proof of Proposition 3.27 to construct a matrix $X \in \mathrm{Sym}^N_{\succeq 0}$ with $-\mathrm{Trace}(A_0\,X) = c_0^*$, $-\mathrm{Trace}(A_0\,X) = F(S) - \varepsilon$, $\mathrm{Trace}(A_\alpha\,X) = c_\alpha^*$ for $\alpha \in S$ and $\mathrm{Trace}(A_\beta\,X) = 0$ for $0 \neq \beta \notin S$. Then X is feasible for Equation (3.18), and therefore $f^d_{\mathrm{mix}} \geq F(S) - \varepsilon$. Since $\varepsilon > 0$ is arbitrary, the statement follows. □

In particular, we can obtain the optimal coefficients as follows.

Lemma 3.31. *Assume that the following statements hold for some $d \in \mathbb{N}$ sufficiently large.*

1. $X \in \mathrm{Sym}^N_{\succeq 0}$ *is optimal for Equation (3.18). Define $c \in \mathbb{R}^S_{\geq 0}$ through* $c_\alpha = \mathrm{Trace}(A_\alpha\,X)$.
2. $(f_c)^* = (f_c)^d_{\mathrm{sos}}$ *and* $\mathscr{L} \in \mathcal{F}^*_{2d}$, $Z \in \mathrm{Sym}^N_{\succeq 0}$ *are such that* $(X, \mathscr{L}, Z)$ *is optimal for Equation (3.15).*

Then $F(S) = f^d_{\mathrm{mix}}$ and c is optimal for Equation (3.17).

Proof. We have $F(S) = \sup\limits_c (f_c)^* = \sup\limits_c (f_c)^d_{\mathrm{sos}} = f^d_{\mathrm{mix}}$. □

If $-I_n \notin \mathcal{G}$, we add the additional constraints $\mathrm{Trace}(A_{\widehat{\alpha}}\,X) = \mathrm{Trace}(A_\alpha\,X)$ for $-\alpha \in \mathcal{G}\,\widehat{\alpha}$ to Equation (3.18).

Chapter 4

The chromatic number of geometric graphs for symmetric polytopes

We study the problem of computing chromatic numbers of lattices in $\mathbb{R}^n$ and $\mathbb{R}^n$ itself for distance graphs with respect to polytope norms. Spectral lower bounds for chromatic numbers were generalized from the finite to the infinite setting. These bounds involve the optimization of a trigonometric polynomial and can therefore be computed with the techniques established in this thesis under the assumption of Weyl group symmetry. We target polytope norms, which are related to Voronoï cells of coroot lattices, and formulate the spectral bound in terms of generalized Chebyshev polynomials. This allows us to prove sharpness in several cases analytically. We then introduce a hierarchy of semi–definite programs, whose optimal solution converges to the spectral bound. We compute these bounds for several instances numerically and compare with known results.

The results are based on joint work with Evelyne Hubert (Inria), Philippe Moustrou (Toulouse) and Cordian Riener (Tromsø) [HMMR22].

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1 The spectral bound for geometric graphs

In the final chapter, we study a natural application of the theory with the goal to give lower bounds for chromatic numbers of geometric graphs. This number can be estimated with so–called spectral bounds. Computing these bounds involves the optimization of Fourier transformation of discrete measures, that is, of trigonometric polynomials. If the support of the measure is invariant under a Weyl group, then optimizing its Fourier transform over $\mathbb{R}^n$ falls within Chapter 3. After a recap on the spectral bound for infinite graphs, we explain the connection and provide several examples. First, we review definitions and results about the spectral bound for graphs, taken from [BDFV14], [BBMP19] and [DSMMV19].

1.1 The spectral bound for finite graphs

All graphs are assumed to be undirected. We denote vertices by V and edges by $E \subseteq \binom{V}{2}$.

Definition 4.1. *Let $G = (V, E)$ be a finite graph.*

1. *A subset $I \subseteq V$ is said to be* ***independent****, if no pair of vertices in I are connected by an edge in E, that is, if $u \neq v \in I$, then $\{u, v\} \notin E$.*

2. *The* ***independence number*** *of G is*

$$\alpha(G) = \max\{|I| \,|\, I \text{ is independent}\}.$$

3. *The* ***independence ratio*** *of G is*

$$\overline{\alpha}(G) = \frac{\alpha(G)}{|V|}$$

4. *A* ***coloring*** *X of G is a partition of V in independent sets, that is, if $I \neq J \in X$, then I and J are independent, $I \cap J = \emptyset$ and $V = \bigcup_{I \in X} I$.*

5. *The* ***chromatic number*** *of G is*

$$\chi(G) = \min\{|X| \,|\, X \text{ is a coloring}\}.$$

The chromatic number is by definition the minimal number of colors needed, to paint V, such that no two vertices of the same color are connected by an edge. Furthermore, it follows immediately from the definition that

$$\alpha(G)\,\chi(G) \geq |V| \quad \text{and} \quad \chi(G) \geq \frac{1}{\overline{\alpha}(G)}. \tag{4.1}$$

Hence, any upper bound on $\overline{\alpha}(G)$ gives a lower bound on $\chi(G)$. Historically, the spectral bound for finite graphs goes back to Hoffman and Lovász.

Theorem 4.2. *Denote by $A = A(G)$ the adjacency matrix of G with largest and smallest eigenvalue $M(A)$ and $m(A)$. The following statements hold.*

1. [Hof70] $\chi(G) \geq \frac{M(A)-m(A)}{-m(A)}$.

2. [Lov79] $\overline{\alpha}(G) \leq \frac{-m(A)}{M(A)-m(A)}$.

1.2 The spectral bound for infinite graphs

Going from finite to infinite graphs, these notions and bounds have been generalized in [BNFV09, BDFV14] and can be specified for geometric graphs.

Let $S \subseteq \mathbb{R}^n$ be centrally symmetric, that is, $S = -S$, and bounded, such that $0 \notin \overline{S}$. We define $G(V, S)$ as the graph with vertices $V = \mathbb{R}^n$ or $V \subseteq \mathbb{R}^n$ a lattice and edges connecting u and v whenever $u - v \in S$. In this setup, the definition of an independent set is still valid, but the independence number is not well–defined, since an independent set might be infinite, or even of infinite Lebesgue measure.

Definition 4.3. *For $I \subseteq \mathbb{R}^n$ Lebesgue–measurable, we define the* ***upper density*** *of I as*

$$\delta(I) = \limsup_{r \to \infty} \frac{\operatorname{Vol}(I \cap [-r, r]^n)}{\operatorname{Vol}([-r, r]^n)}.$$

For $S \subseteq \mathbb{R}^n$ centrally symmetric and bounded with $0 \notin \overline{S}$, the ***independence ratio*** *of $G(\mathbb{R}^n, S)$ is*

$$\overline{\alpha}(\mathbb{R}^n, S) = \sup\{\delta(I) \,|\, I \text{ is independent}\}.$$

Regarding the chromatic number, the definition via colorings is the same, even if $\chi(\mathbb{R}^n, S)$ might be infinite. We would expect a similar relation between $\overline{\alpha}$ and χ as in the finite framework, but this relation only holds with the **measurable chromatic number** $\chi_m(\mathbb{R}^n, S)$, where the color classes are required to be measurable. We then have

$$\chi_m(\mathbb{R}^n, S) \geq \frac{1}{\overline{\alpha}(\mathbb{R}^n, S)}. \tag{4.2}$$

Now, one can show that the convolution operator on the Hilbert space $L^2(\mathbb{R}^n)$ is self–adjoint and use the spectral bound for such operators from [BDFV14, §2] to obtain the following spectral bounds for $\overline{\alpha}(\mathbb{R}^n, S)$ and $\chi_m(\mathbb{R}^n, S)$, see [BDFV14, §3.1 and 3.2]. Denote by $\langle \cdot, \cdot \rangle$ the Euclidean scalar product on $\mathbb{R}^n$.

Theorem 4.4. [BDFV14] *Let $S \subseteq \mathbb{R}^n$ be centrally symmetric and bounded, such that $0 \notin \overline{S}$. For any signed Borel measure ν with support S, the independence ratio of $G(\mathbb{R}^n, S)$ satisfies*

$$\overline{\alpha}(\mathbb{R}^n, S) \leq \frac{-\inf\limits_{u \in \mathbb{R}^n} \hat{\nu}(u)}{\sup_{u \in \mathbb{R}^n} \hat{\nu}(u) - \inf\limits_{u \in \mathbb{R}^n} \hat{\nu}(u)},$$

where $\hat{\nu}$ denotes the Fourier transform

$$\hat{\nu}(u) = \int_{\mathbb{R}^n} \exp(-2\pi \mathrm{i} \langle u, v \rangle) \mathrm{d}\nu(v)$$

with $u \in \mathbb{R}^n$.

As a consequence, one obtains a bound for the measurable chromatic number, which is our main tool in this chapter.

Corollary 4.5. [of Equation (4.2) and Theorem 4.4] *Let $S \subseteq \mathbb{R}^n$ be centrally symmetric and bounded, such that $0 \notin \overline{S}$. For any signed Borel measure ν with support S, the measurable chromatic number of $G(\mathbb{R}^n, S)$ satisfies*

$$\chi_m(\mathbb{R}^n, S) \geq 1 - \frac{\sup\limits_{u \in \mathbb{R}^n} \hat{\nu}(u)}{\inf\limits_{u \in \mathbb{R}^n} \hat{\nu}(u)}.$$

We will now compute such bounds for special instances of forbidden sets S.

1.3 Sets avoiding distance 1 in $\mathbb{R}^n$

A type of graph of the form $G(\mathbb{R}^n, S)$ consists of so–called distance graphs. Let $\|\cdot\|$ be a norm in $\mathbb{R}^n$, not necessarily induced by $\langle \cdot, \cdot \rangle$. If we take S as the unit sphere $\{y \in \mathbb{R}^n \mid \|y\| = 1\}$, then S satisfies the assumptions of Corollary 4.5. The corresponding graph $G(\mathbb{R}^n, S)$ is called the **unit–distance graph** associated to $\|\cdot\|$ and is sometimes denoted by $G(\mathbb{R}^n, \|\cdot\|)$.

The computation of the parameters $\overline{\alpha}(\mathbb{R}^n, \|\cdot\|)$ and $\chi_m(\mathbb{R}^n, \|\cdot\|)$ have been extensively studied for the Euclidean norm, see [Soi09] and the recent advances [Gre18, BPS21, AM22, ACM+22], but also for other norms such as p–norms

$$\|u\|_p = \left(\sum_{i=1}^{n} |u_i|^p \right)^{1/p}$$

or polytope norms [BR19, BBMP19]. Indeed, if $\mathcal{P}$ is a centrally symmetric convex polytope, then the function

$$\|u\|_{\mathcal{P}} = \inf\{r \in \mathbb{R} \mid u \in r\,\mathcal{P}\}$$

defines a norm with unit sphere $S = \partial\mathcal{P}$.

Lemma 4.6. [BBMP19] *Let $\mathcal{P}$ be a centrally symmetric convex polytope that tiles $\mathbb{R}^n$. Then*

$$\chi_m(\mathbb{R}^n, \partial\mathcal{P}) \leq 2^n$$

Equality in the previous statement is conjectured and proved in several cases. While the spectral bound has been computed and strengthened for the case of the Euclidean norm [BDFV14, BPT15, AM22], it has not been used as a tool for other norms.

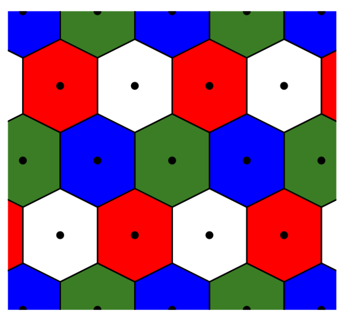


Figure 4.1: The chromatic number of $\mathbb{R}^2$ for the hexagon norm is $\chi(\mathbb{R}^2, \|\cdot\|_{\text{hex}}) = 2^2 = 4$.

2 Analytical bounds

In the computation of the spectral bound for chromatic numbers from Corollary 4.5, we a priori have some freedom regarding the choice of the measure. Given a forbidden set S, which is invariant under a subgroup $\mathcal{W}$ of the orthogonal group $\mathrm{O}_n(\mathbb{R})$, we consider measures, which are also $\mathcal{W}$–invariant. For the Euclidean norm for instance, the unit sphere is invariant under the entire orthogonal group $\mathrm{O}_n(\mathbb{R})$. We shall focus on those norms with a finite symmetry group. More precisely, we will consider norms whose unit sphere is a polytope $\mathcal{P}$ with Weyl group symmetry.

In this section, R is a root system with Weyl group $\mathcal{W}$ and weight lattice Ω.

2.1 Relaxation to discrete subgraphs

Before going into the details, we present our strategy. Assume that a given polytope $\mathcal{P}$ is symmetric with respect to the reflections of a crystallographic root system, that is, $\mathcal{W}(\mathcal{P}) = \mathcal{P}$. We will consider discrete measures supported on $\mathcal{W}$–orbits of points on the boundary $\partial\mathcal{P}$. In fact, these points will be closely related to the weight lattice Ω, which is dual to the lattice of coroots Λ. For some integers r, we will consider orbits of points of the weight lattice Ω that lie on the boundary of $r\,\partial\mathcal{P}$. After rescaling by $1/r$, this indeed gives a measure invariant under $\mathcal{W}$ and supported on the boundary of $\mathcal{P}$. In addition to the choice of points, we have freedom on the choice of the coefficients attributed to supporting points and we will optimize over the possible coefficient distributions. With this strategy, we are actually computing spectral bounds for the chromatic number of discrete graphs $G(\Omega, \Omega \cap \partial(r\,\mathcal{P}))$.

Lemma 4.7. *Let $r \in \mathbb{N}$ and $\mathcal{P}$ be a centrally symmetric convex polytope, such that $S_r := \Omega \cap \partial(r\,\mathcal{P}) \neq \emptyset$. Then*

$$\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathcal{P}}) \geq \chi(\Omega, S_r).$$

Proof. Since $\mathbb{R}^n$ is invariant under scaling with $1/r$, we have $\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathcal{P}}) = \chi_m(\mathbb{R}^n, \partial(r\,\mathcal{P}))$. The latter is at least $\chi(\Omega, S_r)$, because Ω with forbidden set S_r is a subgraph. □

This makes the problem of computing chromatic numbers of discrete subgraphs interesting in itself and motivates our strategy. We assume that the polytope has Weyl group symmetry. Let $\mathcal{G}$ by the integer representation of $\mathcal{W}$ and write $\mathcal{T}$ for the $\mathbb{T}$–orbit space of $\mathcal{G}$. The generalized Chebyshev polynomials of the first kind are denoted by T_α. For $S \subseteq \Omega$, the set

$$S(\mathbb{N}) := \{W^{-1}\mu \mid \mu \in S \text{ dominant weight}\} \subseteq \mathbb{N}^n$$

contains the coordinates of dominant weights in S with respect to the basis of fundamental weights. Here, $W : \mathbb{Z}^n \to \Omega$ is the corresponding change of basis from Equation (1.14).

Theorem 4.8. *Let $r \in \mathbb{N}$ and $\mathcal{P}$ be a centrally symmetric convex polytope with $\mathcal{W}(\mathcal{P}) = \mathcal{P}$, such that $S_r := \Omega \cap \partial(r\,\mathcal{P}) \neq \emptyset$. Then*

$$\chi(\Omega, S_r) \geq 1 - \frac{1}{F(r)},$$

where

$$F(r) := \max\left\{ \min\left\{ \sum_{\alpha \in S_r(\mathbb{N})} c_\alpha\, T_\alpha(z) \,\middle|\, z \in \mathcal{T} \right\} \,\middle|\, \sum_{\alpha \in S_r(\mathbb{N})} c_\alpha = 1, c_\alpha \geq 0 \right\}$$

Furthermore, if r divides $\tilde{r} \in \mathbb{N}$, then $S_{\tilde{r}} \neq \emptyset$ and $F(r) \leq F(\tilde{r})$.

Proof. Consider the centrally symmetric signed Borel measure

$$\nu = \sum_{\mu \in S_r} \frac{c_\mu}{|\mathcal{W}\mu|}\, \delta_\mu$$

with δ_μ Dirac and $c_\mu \in \mathbb{R}_{\geq 0}$. We assume that, for $A \in \mathcal{W}$, $c_{A\mu} = c_\mu$. The Fourier transformation $\hat{\nu}$ is a trigonometric polynomial and assumes only real values on $\mathbb{R}^n$ due to central symmetry. We show that this measure yields the bound in question. For $u \in \mathbb{R}^n$, we have

$$\begin{aligned}\hat{\nu}(u) &= \sum_{\{\pm\mu\} \subseteq S} \frac{c_\mu}{|\mathcal{W}\mu|} \left(\exp(2\pi \mathrm{i} \langle \mu, u\rangle) + \exp(-2\pi \mathrm{i}\, \langle \mu, u\rangle)\right) \\ &= \sum_{\{\pm\mu\} \subseteq S} 2\, \frac{c_\mu}{|\mathcal{W}\mu|} \cos(2\pi \langle \mu, u\rangle) = \sum_{\mu \in S} \frac{c_\mu}{|\mathcal{W}\mu|} \cos(2\pi \langle \mu, u\rangle) \leq \sum_{\mu \in S} \frac{c_\mu}{|\mathcal{W}\mu|}\end{aligned}$$

and equality holds for $u = 0$. Thus, $\sup_u \widehat{\nu}(u) = \sum_\mu c_\mu / |\mathcal{W}\mu|$. Fixing the sum of coefficients to be 1 gives us the numerator.

Since ν is $\mathcal{W}$–invariant, we can write $\inf_u \widehat{\nu}(u)$ as a polynomial optimization problem on the $\mathbb{T}$–orbit space $\mathcal{T}$. For the basis of generalized Chebyshev polynomials, the coefficients are $c_\alpha = \frac{c_\mu}{|\mathcal{W}\mu|}$ for $W\alpha = \mu$. This gives us the spectral bound from Corollary 4.5 and we obtain $F(r)$ by optimizing on the coefficients.

It remains to show that this is in fact a bound for the discrete subgraph with vertices Ω and not just for the larger graph $\mathbb{R}^n$. To do this, we follow [DSMMV19, §5.1], which involves the chromatic number of operators from [BDFV14, §2]. Consider the Hilbert space $\ell^2(\Omega)$ of discrete functions $f : \Omega \to \mathbb{C}$ with $(f, f)_{\ell^2} < \infty$, where $(\cdot, \cdot)_{\ell^2}$ is the usual ℓ^2–inner product

$$(f, g)_{\ell^2} := \sum_{\mu\in\Omega} f(\mu)\,\overline{g(\mu)}.$$

We have $\nu \in \ell^2(\Omega)$ and define the convolution operator

$$\begin{array}{rccl} \mathrm{Conv}_\nu : & \ell^2(\Omega) & \to & \ell^2(\Omega), \\ & f & \mapsto & f * \nu : \begin{cases} \Omega \to \mathbb{C}, \\ \tilde{\mu} \mapsto \sum\limits_{\mu\in S_r} f(\mu - \tilde{\mu})\,\nu(\tilde{\mu}) \end{cases} . \end{array}$$

Then Conv_ν is bounded and self–adjoint. Furthermore, if $I \subset \Omega$ is an independent set of $G(\Omega, S_r)$, then, for all $f \in \ell^2(\Omega)$ with $f(\Omega \setminus I) = 0$, we have $(\mathrm{Conv}_\nu(f), f)_{\ell^2} = 0$. Hence, the chromatic number of $G(\Omega, S_r)$ is at least that of Conv_ν. In other words, we have to determine the numerical range of Conv_ν. To do this, denote by $\Lambda := \Omega^*$ the dual lattice of Ω. Let $L^2(\mathrm{Vor}(\Lambda))$ be the Hilbert space of Lebesgue measurable functions $F : \mathrm{Vor}(\Lambda) \to \mathbb{C}$ with $(F, F)_{L^2} < \infty$, where $(\cdot, \cdot)_{L^2}$ is the usual L^2–inner product

$$(F, G)_{L^2} := \frac{1}{\mathrm{Vol}(\mathrm{Vor}(\Lambda))} \int\limits_{\mathrm{Vor}(\Lambda)} F(u)\,\overline{G(u)}\,\mathrm{d}u.$$

As in Proposition 3.1, we consider $\widehat{\nu}$ as an element of $L^2(\mathrm{Vor}(\Lambda))$. We then have

$$(\mathrm{Conv}_\nu(f), f)_{\ell^2} = (f * \nu, f)_{\ell^2} = (\widehat{f}\,\widehat{\nu}, \widehat{f})_{L^2} = \frac{1}{\mathrm{Vol}(\mathrm{Vor}(\Lambda))} \int\limits_{\mathrm{Vor}(\Lambda)} \widehat{\nu}(u)\,|\widehat{f}(u)|^2\,\mathrm{d}u.$$

Thus, the numerical range of Conv_ν is the interval in $\mathbb{R}$, given by the supremum and infimum of $\widehat{\nu}$ divided by $\mathrm{Vol}(\mathrm{Vor}(\Lambda))$ which cancels out.

For the last statement, set $\ell := \tilde{r}/r$. Then $\ell\, S_r \subseteq S_{\tilde{r}}$. For any admissible choice of coefficients c for $F(r)$, set $c'_{\ell\alpha} = c_\alpha$, if $\alpha \in S_r$, and $c'_\gamma = 0$, otherwise. Then c' is admissible for $F(\tilde{r})$ and yields the same bound. □

A natural polytope to consider in the presence of crystallographic symmetries is the Voronoï cell of the coroot lattice Λ. In this case, $\mathcal{P}$ tiles $\mathbb{R}^n$ by translation, see Proposition 1.14.

Remark 4.9. *If* R *is irreducible and* $\mathcal{P} = \mathrm{Vor}(\Lambda) = \{u \in V \,|\, \forall \lambda \in \Lambda : \, \|u\| \leq \|u - \lambda\|\}$ *is the Voronoï cell in Theorem 4.8, then* $S_r(\mathbb{N}) = \{\alpha \in \mathbb{N}^n \,|\, \langle W\alpha, \rho_0 \rangle = r\}$*, where* ρ_0 *is the highest root.*

2.2 Computing analytical bounds on $\chi_m(\mathbb{R}^n, \|\cdot\|_\infty)$

The cube $\mathcal{P} = [-1/2, 1/2]^n$ is the Voronoï cell of the coroot lattice Λ for the root system C_n and $\partial(2\,\mathcal{P})$ is the unit sphere of the maximum norm, also known as the infinity norm $\|\cdot\|_\infty$. In this case, the chromatic number is known to be 2^n, see for example [BBMP19] for a counting argument that does not involve spectral bounds. We reprove this fact to illustrate our reformulation method with generalized Chebyshev polynomials and show that it is easily applicable to find exact optimal values.

Proposition 4.10. *Let* R *be a root system of type* C_n *with coroot lattice* Λ*. Then the spectral bound is sharp for*

$$\chi_m(\mathbb{R}^n,\, \partial \mathrm{Vor}(\Lambda)) = 2^n.$$

Proof. Define $c_1, \ldots, c_n \geq 0$ by $(2^n - 1)\, c_i = \binom{n}{i}$. In Theorem 4.8, we have $S_2^+ = \{\omega_1, \ldots, \omega_n\}$ and thus

$$\sum_{\mu \in S_2^+} c_\mu \, T_\mu(z) = \sum_{i=1}^{n} c_i \, z_i.$$

We substitute the generalized cosines $z_i = \mathfrak{c}_i(u)$ and obtain

$$(2^n - 1) \sum_{i=1}^{n} c_i \mathfrak{c}_i(u) = \sum_{i=1}^{n} \sigma_i(\cos(2\pi u_1), \ldots, \cos(2\pi u_n)) = \prod_{k=1}^{n} (1 + \cos(2\pi u_k)) - 1 \geq -1$$

with Proposition 2.24 and Vieta's formula. Equality holds when $u = 1/2\, \omega_j$ for some $1 \leq j \leq n$, that is, when $z = \mathfrak{c}(u)$ is a nontrivial vertex of $\mathcal{T}$. We have $c_1 + \ldots + c_n = 1$, and thus

$$2^n \geq \chi_m(\mathbb{R}^n,\, \partial \mathrm{Vor}(\Lambda)) \geq 1 - \frac{1}{F(2)} = 1 - \frac{1}{-1/(2^n - 1)} = 2^n.$$

□

Remark 4.11. *We have shown that the optimal bound* 2^n *for the measurable chromatic number of* $\mathbb{R}^n$ *is obtained from the discrete graph in Theorem 4.8 with* $r = 2$*. Since the fundamental weights of* C_n *are* $\omega_i = e_1 + \ldots + e_i$*, the orbit of* ω_i *under the Weyl group consists of the centers of the* $(n - i)$*–dimensional faces of* $2\, \partial \mathrm{Vor}(\Lambda)$ *(facets, ..., faces, edges, vertices). Those are the forbidden points* S_2 *and thus, for this particular case, equality holds in Lemma 4.7 with*

$$\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathcal{P}}) = \chi(\Omega, S_2).$$

2.3 Computing analytical bounds on $\chi(\Lambda)$

The spectral bound Theorem 4.8 also applies for the discrete geometric graphs considered in [DSMMV19]. Let Λ be an n–dimensional lattice in $\mathbb{R}^n$ with Voronoï cell $\mathrm{Vor}(\Lambda)$. A vector $\lambda \in \Lambda \setminus \{0\}$ is called a **strict Voronoï vector** or a **relevant vector**, if the intersection $(\lambda + \mathrm{Vor}(\Lambda)) \cap \mathrm{Vor}(\Lambda)$ is a facet of $\mathrm{Vor}(\Lambda)$, that is, a face of dimension $n - 1$. Let S be the set of strict Voronoï vectors of Λ. Then the chromatic number of the lattice Λ is the chromatic number of the graph $G(\Lambda) := G(\Lambda, S)$.

This is a subgraph of $G(\mathbb{R}^n, \mathrm{Vor}(\Lambda))$. In particular, a lower bound for the chromatic number $\chi(\Lambda)$ of $G(\Lambda)$ gives a bound for the chromatic number of $\mathbb{R}^n$, where we color all the points in the interior of the Voronoï cell $\lambda + \mathrm{Vor}(\Lambda)$ with the color of λ (let us not care about the boundaries here).

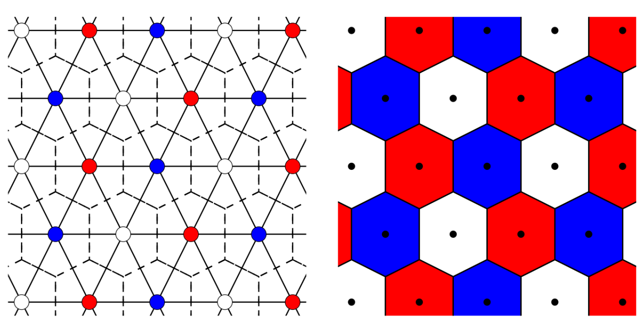


Figure 4.2: The chromatic number of the hexagon lattice is $\chi(\Lambda) = 3 \leq \chi(\mathbb{R}^2, \|\cdot\|_{\text{hex}})$.

For a root system R in $\mathbb{R}^n$ with base $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$, we consider the lattice $\Lambda = \mathbb{Z}\,\rho_1^\vee \oplus \ldots \oplus \mathbb{Z}\,\rho_n^\vee$ spanned by the coroots. The dual of Λ is the weight lattice $\Lambda^* = \Omega = \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_n$. The set S of strict Voronoï vectors for Λ consists of the short roots of $\mathrm{R}^\vee$ and is a generating set for Λ, see [CS99, Chapter 4, §2 and Chapter 21, §3].

In the case of the four infinite families of irreducible root systems, the coroot lattice is

$$\Lambda = \begin{cases} \mathbb{Z}^n, & \text{if} \quad \mathrm{R} = \mathrm{C}_n \\ \{\mu \in \mathbb{Z}^n \,|\, \mu_1 + \ldots + \mu_n = 0\}, & \text{if} \quad \mathrm{R} = \mathrm{A}_{n-1} \\ \{\mu \in \mathbb{Z}^n \,|\, \mu_1 + \ldots + \mu_n \text{ is even}\}, & \text{if} \quad \mathrm{R} = \mathrm{B}_n \quad \text{or} \quad \mathrm{R} = \mathrm{D}_n \end{cases}.$$

The case G_2, respectively F_4, is obtained from A_2, respectively B_4, by rescaling. We do not list $\mathrm{E}_{6,7,8}$ here. The coroot lattice for E_8 is a self–dual extension of B_8. E_6 and E_7 yield sublattices of E_8, see [Bou68, Planche I – IX].

Lemma 4.12. *If* R *is irreducible,* S *the set of strict Voronoï vectors for* Λ *and* $\rho_0^\vee = 2/\langle \rho_0, \rho_0\rangle\, \rho_0$ *the coroot of the highest root, then* $S = \mathcal{W}\rho_0^\vee$*.*

Proof. By Proposition 1.17, there are at most two distinct root lengths and two roots have the same length if and only if they are in the same $\mathcal{W}$–orbit. If $\rho \in \mathrm{R}$, then $\langle \rho_0, \rho_0\rangle \geq \langle \rho, \rho\rangle$ and so

$$\langle \rho_0^\vee, \rho_0^\vee\rangle = \frac{4}{\langle \rho_0, \rho_0\rangle} \leq \frac{4}{\langle \rho, \rho\rangle} = \langle \rho^\vee, \rho^\vee\rangle.$$

Thus, $\rho_0^\vee$ is a short root of $\mathrm{R}^\vee$ and the short roots are the strict Voronoï vectors. As $\mathcal{W}(\mathrm{R}) = \mathcal{W}(\mathrm{R}^\vee)$, the statement follows. □

When $\rho_0^\vee \in \Omega$ is a weight, then $\rho_0^\vee = \beta_1\,\omega_1 + \ldots + \beta_n\,\omega_n$ for some $\beta \in \mathbb{N}^n$. In particular, if S is the set of strict Voronoï vectors, we have $S(\mathbb{N}) = \{\beta\}$. Therefore,

$$\chi(\Lambda) \geq 1 - \frac{1}{\min\limits_{z \in \mathcal{T}} T_\beta(z)}.$$

In the basis of fundamental weights, the highest root has the following representation, see [Bou68, Planche I – IX].

R	A_{n-1}	B_2	$\mathrm{B}_n,\, n \geq 3$	C_n	D_3	$\mathrm{D}_n,\, n \geq 4$	E_6	E_7	E_8	F_4	G_2
$\rho_0^\vee$	$\omega_1 + \omega_{n-1}$	$2\omega_2$	ω_2	ω_1	$\omega_2 + \omega_3$	ω_2	ω_2	ω_1	ω_8	ω_1	$1/3\,\omega_2$

Table 4.1: The coroot of the highest root in the basis of fundamental weights.

The exceptional case is G_2, where $\rho_0 = \omega_2 \in \Omega$, but $\rho_0^\vee = 1/3\,\omega_2 \notin \Omega$. In order to compute $\chi(\Lambda)$, we would have to scale by a factor 3. However, this is not necessary as the coroot lattice of G_2 is hexagonal, just as in the A_2 case.

We reprove the bounds from [DSMMV19].

Theorem 4.13. *The following statements hold.*

1. *If* R *is a root system of type* C_n*, then* $\chi(\Lambda) = 2$*.*
2. *If* R *is a root system of type* A_{n-1}*, then* $\chi(\Lambda) \geq n$*.*

3. If R *is a root system of type* B_n *or* D_n*, then*

$$\chi(\Lambda) \geq \begin{cases} n, & \text{if} \quad n \quad \text{is even} \\ n+1, & \text{if} \quad n \quad \text{is odd} \end{cases}.$$

Proof. 1. For $R = C_n$, we have $\Lambda = \mathbb{Z}^n$ and $\rho_0 = \omega_1 = [1, 0, \ldots, 0]^t$. When we partition $\mathbb{Z}^n$ in elements with even and odd 1–norm, then this gives an admissible coloring. To see that the spectral bound is sharp, let us consider the Chebyshev polynomial associated to $\rho_0^\vee$, that is,

$$T_{e_1}(z) = z_1 \geq -1$$

on $\mathcal{T}$. Hence, $2 = \chi(\Lambda) \geq 1 - 1/(-1) = 2$.
2. For $R = A_{n-1}$, we have $\rho_0 = \omega_1 + \omega_{n-1} = [1, 0, \ldots, 0, -1]^t$. The polynomial to be minimized is

$$T_{e_1+e_{n-1}}(z) = |\mathcal{G}\, e_1|\, T_{e_1}(z)\, T_{e_{n-1}(z)} - \sum_{\substack{\alpha \in \mathcal{G}\, e_1 \\ \alpha \neq e_1}} T_{\alpha+e_{n-1}}(z) = n\, z_1\, z_{n-1} - (T_0(z) + (n-2)\, T_{e_1+e_{n-1}}(z))$$

with z in the $\mathbb{T}$–orbit space. By Theorem 2.23, $z_1\, z_{n-1} = z_1\, \overline{z_1} = |z_1|^2 \geq 0$ and thus

$$T_{e_1+e_{n-1}}(z) = \frac{n\, z_1\, z_{n-1} - 1}{n-1} \geq \frac{-1}{n-1}.$$

Equality holds in $z_1 = 0$. Altogether, we obtain

$$\chi(\Lambda) \geq 1 - \frac{1}{\min\limits_{z \in \mathcal{T}} T_{e_1+e_{n-1}}(z)} \geq n.$$

3. For $R = B_2$, we are in the situation of *1.* with $\chi(\Lambda) = 2$. Thus, let $n \geq 3$ and consider B_n. We have $\rho_0 = \omega_2 = [1, 1, 0, \ldots, 0]^t$ and the $\mathcal{W}$–orbit consists of all coordinate–wise permutations and sign changes. Thus, the to be minimized function is $T_{e_2}(z) = z_2$ on $\mathcal{T}$. This is a linear function, hence the minimizer is an extremal point of $\mathcal{T}$. We consider the nontrivial vertices $z = \mathfrak{c}(\omega_i/\alpha_i)$, where $\rho_0 = \alpha_1\, \rho_1^\vee + \ldots + \alpha_n\, \rho_n^\vee$ is the highest root, see Proposition 1.14. We have $\alpha_2 = \ldots = \alpha_{n-1} = 2$ and the second coordinate of z in $\omega_k/2 = (e_1 + \ldots + e_k)/2$ for $2 \leq k \leq n-1$ is

$$z_2 = T_{\omega_2}(\mathfrak{c}(\omega_k/2)) = \frac{2}{n\,(n-1)} \sigma_2(\cos(2\pi u_1), \ldots, \cos(2\pi u_n))|_{u=\omega_k/2} = \frac{2}{n\,(n-1)} \sigma_2(-1, \ldots, -1, 1, \ldots, 1).$$

Now, the Newton identity yields $2\,\sigma_2 = p_1^2 - p_2$, where p_i is the i–th power sum. Hence,

$$z_2 = \frac{1}{n\,(n-1)}\,((n-2\,k)^2 - n) = \frac{1}{n\,(n-1)}\,(n^2 - 4\,n\,k + 4\,k^2 - n).$$

For n even and $k = n/2$, we obtain $1 - 1/z_2 = 1 - 1/(-1/(n-1)) = n$ and this is minimal. For n odd and $k = (n \pm 1)/2$ on the other hand, we obtain $1 - 1/z_2 = 1 - 1/(-1/n) = n+1$ and this is also minimal.

□

2.4 Computing analytical bounds on $\chi(\mathbb{Z}^n, S_r)$

Theorem 4.8 also applies when Ω is replaced by another lattice such as $\mathbb{Z}^n$. We consider the problem of computing the spectral bound for the chromatic number of the graph $G(\mathbb{Z}^n, \mathbb{Z}^n \cap \mathbb{B}_r^1)$. Here, for $r \in \mathbb{N}$, $\mathbb{B}_r^1$ is the sphere of radius r with respect to the 1–norm $\|\cdot\|_1$

$$\mathbb{B}_r^1 := \{u \in \mathbb{R}^n \mid \|u\|_1 = |u_1| + \ldots + |u_n| = r\} = \partial\, \mathrm{ConvHull}(\pm r\, e_1, \ldots, \pm r\, e_n).$$

This problem has been studied in [FK04], giving theoretical bounds for the chromatic number. Implicitly, this gives a bound for $\chi_m(\mathbb{R}^n, \|\cdot\|_1)$. Here we have to be careful as $\mathbb{Z}^n$ is on one hand the considered subgraph of $\mathbb{R}^n$, and on the other the coordinates of weights in Ω.

Let $r \in \mathbb{N}$ and set $S_r := \mathbb{B}_r^1 \cap \mathbb{Z}^n$. If $S_r \subseteq \Omega$, then

$$\chi(\mathbb{Z}^n, S_r) \geq 1 - \frac{1}{F(r)},$$

where $F(r)$ is defined as in Theorem 4.8. Since the associated polytope $\mathcal{P}$, that is, the unit ball of $\|\cdot\|_1$, does not tile $\mathbb{R}^n$ by translation, the conjectured upper bound 2^n from Lemma 4.6 does not apply here.

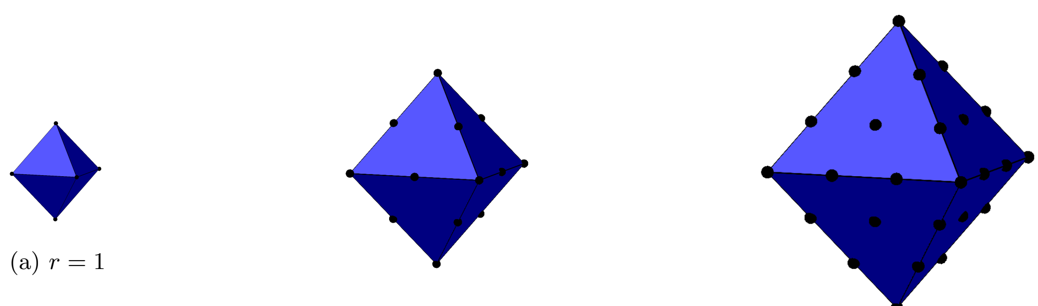
Lemma 4.14. *Let $r \in \mathbb{N}$. If R is a root system of type B_n, C_n or D_n, then $S_r = \mathbb{B}_r^1 \cap \mathbb{Z}^n \subseteq \Omega$ and*

$$S_r(\mathbb{N}) = \begin{cases} \{\alpha \,|\, \alpha \in \mathbb{N}^n,\, \sum\limits_{i=1}^{n} i\,\alpha_i = r\}, & \text{if} \quad \mathrm{R} = \mathrm{C}_n \\ \{\alpha + \alpha_n\, e_n \,|\, \alpha \in \mathbb{N}^n,\, \sum\limits_{i=1}^{n} i\,\alpha_i = r\}, & \text{if} \quad \mathrm{R} = \mathrm{B}_n \\ \{\alpha + \alpha_{n-1}\, e_{n-1} + \alpha_n\, e_n \,|\, \alpha \in \mathbb{N}^n,\, \sum\limits_{i=1}^{n} i\alpha_i + \alpha_{n-1} = r\}, & \text{if} \quad \mathrm{R} = \mathrm{D}_n \end{cases}.$$

Proof. By Equations (1.5), (1.7) and (1.9), we have

$$\mathbb{Z}^n = \bigoplus_{i=1}^{n} \left(\mathbb{Z} \sum_{j=1}^{i} e_j \right) = \bigoplus_{i=1}^{n-2} \mathbb{Z}\,\omega_i \oplus \begin{cases} \mathbb{Z}\,\omega_{n-1} \oplus \mathbb{Z}\,\omega_n, & \text{if} \quad \mathrm{R} = \mathrm{C}_n \\ \mathbb{Z}\,\omega_{n-1} \oplus 2\,\mathbb{Z}\,\omega_n, & \text{if} \quad \mathrm{R} = \mathrm{B}_n \\ \mathbb{Z}\,(\omega_{n-1} + \omega_n) \oplus 2\,\mathbb{Z}\,\omega_n, & \text{if} \quad \mathrm{R} = \mathrm{D}_n \end{cases}.$$

Thus, $\mathbb{Z}^n$ is a sublattice of Ω and the weights in $\mathbb{B}_r^1$ with integer coordinates are precisely S_r. □



(a) $r = 1$

(b) $r = 2$

(c) $r = 3$

Figure 4.3: The ball of radius r with respect to the 1–norm and the weights in $S_r = \mathbb{B}_r^1 \cap \mathbb{Z}^3$.

We can now use Theorem 4.8 to compute spectral bounds on $\chi(\mathbb{Z}^n, \|\cdot\|_1)$. We start with the cases, which we can prove analytically via a Chebyshev rewriting technique.

Lemma 4.15. *Let $r \in \mathbb{N}$ be odd. The spectral bound is sharp for*

$$\chi(\mathbb{Z}^n,\, S_r) = 2.$$

Proof. Since $r \in \mathbb{N}$ is odd, an admissible coloring for $G(\mathbb{Z}^n, \mathbb{B}_1^1)$ admits an admissible coloring for $G(\mathbb{Z}^n, \mathbb{B}_r^1)$. Thus, we have $\chi(\mathbb{Z}^n,\, \mathbb{B}_r^1) = \chi(\mathbb{Z}^n,\, \mathbb{B}_1^1) = 2$, see the proof of Theorem 4.13. Let R be a root system of type C_n. Thanks to Lemma 4.14, we have $S_1 = \mathcal{W}\omega_1$ and $2 = \chi(\mathbb{Z}^n,\, \mathbb{B}_1^1) \geq 1 - 1/F(1) \geq 1 - 1/(-1) = 2$. □

The chromatic number of $\mathbb{Z}^n$ for 1–distance $r = 2$ is $2n$. This was proven in [FK04, Theorem 1] with a purely combinatorial argument by fixing a coloring and showing that is is admissible. We prove that the spectral bound is sharp in this case via our rewriting technique with Chebyshev polynomials.

Theorem 4.16. *The spectral bound is sharp for*

$$\chi(\mathbb{Z}^n,\, S_2) = 2n.$$

Proof. Let R be a root system of type C_n. Thanks to Lemma 4.14, we have $S_2 = \mathcal{W}\,\{2\omega_1, \omega_2\}$. For $c \in [0,1]$, define the trigonometric polynomial $f_c(u) := c\, T_{2e_1}(\mathfrak{c}(u)) + (1-c)\, T_{e_1}(\mathfrak{c}(u))$. We apply Proposition 2.24 to obtain

$$\begin{aligned} f_c(u) &= \tfrac{c}{n}\, \sigma_1(\cos(4\pi u_1), \ldots, \cos(4\pi u_n)) + \tfrac{2\,(1-c)}{n\,(n-1)}\, \sigma_2(\cos(2\pi u_1), \ldots, \cos(2\pi u_n)) \\ &= \tfrac{2c}{n}\, \sigma_1(\cos(2\pi u_1)^2, \ldots, \cos(2\pi u_n)^2) + \tfrac{2\,(1-c)}{n\,(n-1)}\, \sigma_2(\cos(2\pi u_1), \ldots, \cos(2\pi u_n)) - c. \end{aligned}$$

Choose $c = 1/(2n-1)$ and set $X_k := \cos(2\pi u_k)$ for $1 \leq k \leq n$. It follows

$$f_c(u) = \frac{2}{n\,(2n-1)}\, p_2(X) + \frac{2\,(2n-2)}{n\,(n-1)\,(n-2)}\, \sigma_2(X) - \frac{1}{2n-1} = \frac{2}{2n-1}\, (p_2(X) + 2\,\sigma_2(X)) - \frac{1}{2n-1},$$

where $p_i \in \mathbb{R}[z]$ denotes the i–th power sum. By the Newton identity, $p_2(X) + 2\,\sigma_2(X) = \sigma_1(X)\, p_1(X) = \sigma_1(X)^2 \geq 0$. Thus, $f_c(u) \geq -1/(2n-1)$ and finally

$$2n = \chi(\mathbb{Z}^n,\, \mathbb{B}_2^1) \geq 1 - \frac{1}{F(2)} \geq 1 - \frac{1}{\inf\limits_{u \in \mathbb{R}^n} f_c(u)} \geq 1 - \frac{1}{-1/(2n-1)} = 2n$$

completes the proof. □

Corollary 4.17. *Let $r \in \mathbb{N}$ be even. The spectral bound is sharp for*

$$\chi(\mathbb{Z}^2,\, S_r) = 4.$$

Proof. For $n = 2$, $\mathbb{B}_r^1$ is up to rotation and scaling the cube from Proposition 4.10. By Theorem 4.16, $G(\mathbb{Z}^n, S_r)$ being a subgraph of $G(\mathbb{R}^n, \mathbb{B}_r^1)$ and Proposition 4.10, we have

$$4 = \chi(\mathbb{Z}^2,\, S_2) = 1 - 1/F(2) \leq 1 - 1/F(r) \leq \chi(\mathbb{Z}^2,\, S_r) \leq \chi(\mathbb{R}^2,\, \mathbb{B}_r^1) = 4.$$

□

3 Semi–definite bounds

In order to compute a bound for the measurable chromatic number of $\mathbb{R}^n$, we have considered discrete subgraphs and combined the optimization of symmetric trigonometric polynomials from Chapter 3 with the spectral bound from Theorem 4.8 which is due to [BDFV14]. This has allowed us in several cases to prove sharpness analytically.

It is now time to apply our results from Chapter 3, specifically Lasserre's hierarchy of moment and SOS relaxation in the basis of Chebyshev polynomials, to compute bounds numerically.

In this section, let R be a root system with Weyl group $\mathcal{W}$ and weight lattice Ω. Recall from Theorem 4.8 that

$$\chi(\Omega, S_r) \geq 1 - \frac{1}{F(r)}, \tag{4.3}$$

where $r \in \mathbb{N}$, $S_r := \Omega \cap \partial(r\,\mathcal{P}) \neq \emptyset$ for a centrally symmetric convex polytope $\mathcal{P}$ with $\mathcal{W}(\mathcal{P}) = \mathcal{P}$ and

$$F(r) := \max\left\{ \min\left\{ \sum_{\alpha\in S_r(\mathbb{N})} c_\alpha\, T_\alpha(z) \,\middle|\, z \in \mathcal{T} \right\} \,\middle|\, \sum_{\alpha\in S_r(\mathbb{N})} c_\alpha = 1, c_\alpha \geq 0 \right\}.$$

Computing $F(r)$ falls in the context of Equation (3.17), which can be approximated through a hierarchy of semi–definite programs. We fix a relaxation order $d \in \mathbb{N}$ and always assume that it is sufficiently large in the sense of Equation (3.11). This allows us to define the optimization problem

$$\begin{array}{lll} F(r,d) := & \sup & -\mathrm{Trace}(A_0\, X) \\ & \text{s.t.} & X \in \mathrm{Sym}^N_{\succeq 0},\ \sum\limits_{\alpha\in S_r(\mathbb{N})} \mathrm{Trace}(A_\alpha\, X) = 1, \\ & & \mathrm{Trace}(A_\alpha\, X) \geq 0 \quad \text{for} \quad \alpha \in S_r(\mathbb{N}), \\ & & \mathrm{Trace}(A_\beta\, X) = 0 \quad \text{for} \quad \beta \notin S_r(\mathbb{N}) \cup \{0\}, \end{array}$$

where the matrices A_α, A_β and the semi–definite cone $\mathrm{Sym}^N_{\succeq 0}$ are defined as in Equation (3.14). $S_r(\mathbb{N})$ consists of the coordinates in $\mathbb{N}^n$ of the dominant weights in S_r with respect to the basis of fundamental weights $\Omega = \mathbb{Z}\,\omega_1 \oplus \ldots \oplus \mathbb{Z}\,\omega_n$.

Corollary 4.18. [of Theorem 3.30 and Theorem 4.8] *Let $r \in \mathbb{N}$. The sequence $(F(r,d))_{d\in\mathbb{N}}$ is monotonously non–decreasing and converges to $F(r)$. In particular, for $d \in \mathbb{N}$, we have*

$$\chi(\Omega, S_r) \geq 1 - \frac{1}{F(r,d)}.$$

Remark 4.19. *Let $r \in \mathbb{N}$.*

1. *Here, we assume without loss of generality that the quadratic module that appears in Theorem 3.30 is Archimedean. Since this is difficult to prove in general, we make an adjustment according to Proposition 3.17.*

2. *If $\mathcal{P} = \mathrm{Vor}(\Lambda)$ is the Voronoï cell and the relaxation order d is fixed, then r can be at most $2d$.*

3. *By Theorem 4.8, we have $\lim\limits_{d\to\infty} F(r,d) \leq \lim\limits_{d\to\infty} F(\tilde{r},d)$, if r divides $\tilde{r} \in \mathbb{N}$. This is not true without the limit as examples will show.*

4. *To compute $F(r,d)$ numerically, we use the SDP solver [MOS]. If d is too small, either in the sense of Equation (3.11) or so that the problem is infeasible, we denote this by a "–" in the following tables. Further aspects regarding the implementation are discussed at the end of this section.*

3.1 Computing numerical bounds on $\chi(\Omega, S_r)$

We compute $F(r,d)$ for $S_r := \Omega \cap \partial(r\,\mathrm{Vor}(\Lambda))$, where Ω is the weight lattice and Λ the coroot lattice of the root system R. This gives a lower bound for the chromatic number of the graph $G(\Omega, S_r)$ and implicitly also for the measurable chromatic number $\chi_m(\mathbb{R}^n, \|\cdot\|_{\mathrm{Vor}(\Lambda)})$.

We already know what to expect for the root system C_n ($\chi(\mathbb{R}^n, \|\cdot\|_\infty) = 2^n$, Proposition 4.10).

Example: The hexagon in $\mathbb{R}^2$

The hexagon in $\mathbb{R}^2 \cong \mathbb{R}^3/\langle [1,1,1]^t \rangle$, as it has appeared several times now in Figure 1.5, Figure 3.1, Figure 4.1, and Figure 4.2, is the Voronoï cell of the coroot lattice Λ for A_2 and G_2. It has 6 vertices and 6 edges.

For A_2, the vertices of the hexagon are the orbits of the fundamental weights ω_1 and ω_2. The centers of the edges are the orbit of $(\omega_1+\omega_2)/2$. We fix an order of relaxation $d \geq 3$ and consider $F(r,d)$ for $1 \leq r \leq 2d$.

For G_2, the vertices are the orbit of $\omega_1/3$. The centers of edges are the orbit of $\omega_2/6$. If r is not a multiple of 3, then $S_r = \emptyset$. Thus we consider $F(3r,d)$ for $1 \leq r \leq 2d$, but still write $F(r,d)$.

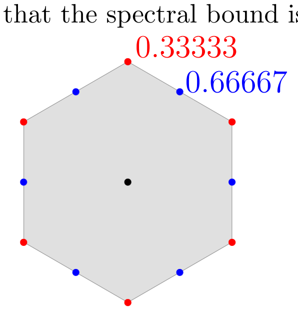
The first column indicates the root system A_2 or G_2. Then the rows are indexed by the relaxation order d and the columns by the radius r.

R	$d \backslash r$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
A_2	3	2.99386	3.57143	3.52451	3.57143	3.37484	3.57143	–	–	–	–	–	–	–	–
	4	3.00000	3.57143	3.52911	3.57143	3.54698	3.57143	3.47461	3.57143	–	–	–	–	–	–
	5	3.00000	3.57143	3.52912	3.57143	3.54789	3.57143	3.54016	3.57143	3.51384	3.57143	–	–	–	–
	6	3.00000	3.57143	3.52912	3.57143	3.54789	3.57143	3.54786	3.57143	3.55920	3.57143	3.47623	3.57143	–	–
	7	3.00000	3.57143	3.52912	3.57143	3.54789	3.57143	3.55183	3.57143	3.55921	3.57143	3.51433	3.57143	3.14739	3.57143
	8	3.00000	3.57143	3.52912	3.57143	3.54789	3.57143	3.55347	3.57143	3.55921	3.57143	3.53571	3.57143	3.25411	3.57143
G_2	3	2.99732	3.57143	3.39930	3.57143	2.47997	3.57143	–	–	–	–	–	–	–	–
	4	2.99962	3.57143	3.52821	3.57143	3.41805	3.57143	2.54024	3.57143	–	–	–	–	–	–
	5	3.00000	3.57143	3.52908	3.57143	3.49102	3.57143	2.76603	3.57143	2.45902	3.57143	–	–	–	–
	6	3.00000	3.57143	3.52912	3.57143	3.52318	3.57143	3.39290	3.57143	2.70265	3.57143	2.98423	3.57143	–	–
	7	3.00000	3.57143	3.52912	3.57143	3.54301	3.57143	3.54780	3.57143	3.53627	3.57143	3.28144	3.57143	2.50993	3.57143
	8	3.00000	3.57143	3.52912	3.57143	3.54656	3.57143	3.55294	3.57143	3.54181	3.57143	3.54139	3.57143	3.13764	3.57143

Table 4.2: The bound $1-1/F(r,d)$ through Chebyshev moment–SOS relaxation of order d for the hexagon.

For $r=1$, there is no choice for the coefficients c_α, as S_1 only contains one element in both cases A_2 and G_2. The value $F(1)$ is the minimum of z_2 on the $\mathbb{T}$–orbit space, see Figure 2.3, and is therefore $-1/2$. This gives spectral bound 3 and is obtained from $F(r,d)$ for $d \geq 4$, respectively $d \geq 5$. Furthermore, this fits with the bound from Theorem 4.13, where $\chi(\Lambda) \geq n$ for A_{n-1}.

For $r \geq 2$, the best possible bound we obtained is already assumed at $r=2$ and $d=3$. We display the optimal coefficients for the corresponding measure below. This bound is assumed in all $F(r,d)$ with r even at lowest possible order. For r odd, the value converges but does not stabilize. This proves a known fact. The chromatic number of $\mathbb{R}^2$ for the hexagon is 4 [BBMP19, Theorem 1], proven analytically via the discrete subgraph $1/2\,\Omega$. However, we see that there is a gap between 4 and the computed value, which indicates that the spectral bound is not sharp in this case.



	A_2		G_2	
r	$1-1/F(r,8)$	$c_\alpha = c_{\widehat{\alpha}}$	$1-1/F(r,8)$	c_α
1	3.00000	$c_{10} = 1.00000$	3.00000	$c_{10} = 1.00000$
2	3.57143	$c_{20} = 0.33333$ $c_{11} = 0.66667$	3.57143	$c_{20} = 0.33333$ $c_{01} = 0.66667$

Figure 4.4: The scaled Voronoï cell and the optimal coefficients for $F(2,8)$. Supporting points α in the same Weyl group orbit and their additive inverse $\widehat{\alpha}$ have the same coefficients, denoted by either red or blue dots.

Let us investigate whether the coefficients 1/3 and 2/3 from the table give the numerically computed bound.

Lemma 4.20. *Let $r \in \mathbb{N}$. The following results can be verified through exact computations.*

1. *For $\mathrm{R} = \mathrm{A}_2$, we have* $f^* := \min_{z \in \mathcal{T}_\mathbb{R}} \frac{2}{3}\widehat{T}_{r\,r}(z) + \frac{1}{3}\widehat{T}_{2r\,0}(z) = -7/18$ *with minimizers* $z \in \{1/6\} \times$

$[-\sqrt{3}/6, \sqrt{3}/6]$.

2. *For* $\mathrm{R} = \mathrm{G}_2$*, we have* $f^* := \min\limits_{z \in \mathcal{T}} \frac{2}{3} T_{0\,r}(z) + \frac{1}{3} T_{2r\,0}(z) = -7/18$ *with minimizers* $z \in \{1/6\} \times [-11/24, -1/3]$.

In both cases, $1 - 1/f^* = 25/7 \approx 3.57143$.

Proof. Let $u \in \mathbb{R}^3$, such that $u_1 + u_2 + u_3 = 0$. With Equation (1.3), one finds that, for $\mathrm{R} = \mathrm{A}_2$, the trigonometric polynomial

$$\left(\frac{2}{3}\,\widehat{T}_{r\,r} + \frac{1}{3}\,\widehat{T}_{2r\,0}\right)(\mathfrak{c}_{\mathbb{R}}(u))$$

has minimum independent of $r \in \mathbb{N}$. Thus, it suffices to consider $r = 1$. In this case,

$$f_{\mathrm{A}}(z) := \frac{2}{3}\,\widehat{T}_{11}(z) + \frac{1}{3}\,\widehat{T}_{20}(z) = 2\,z_1^2 - \frac{2}{3}\,z_1 - \frac{1}{3}$$

is independent of z_2 (Example 2.9). The projection of $\mathcal{T}_{\mathbb{R}} \subseteq \mathbb{R}^2$ on the line "$z_2 = 0$" is the interval $[-1/2, 1]$. Hence, we can simply minimize f_{A} on $\mathcal{T}_{\mathbb{R}}$ as a univariate polynomial to obtain a line of critical points

$$\{z \in \mathcal{T}_{\mathbb{R}} \mid z_1 = 1/6\} = \{1/6\} \times [-\sqrt{3}/6, \sqrt{3}/6]$$

on which f_{A} assumes value $-7/18$. The condition $\mathfrak{c}_{\omega_1,\mathbb{R}}(u) = 1/6$ on $\mathbb{R}^3/\langle[1,1,1]^t\rangle$ defines a family of ovals with centers given by the lattice of coroots Λ.

Analogously for $\mathrm{R} = \mathrm{G}_2$, one finds with Equation (1.11) that it suffices to consider $r = 1$ and

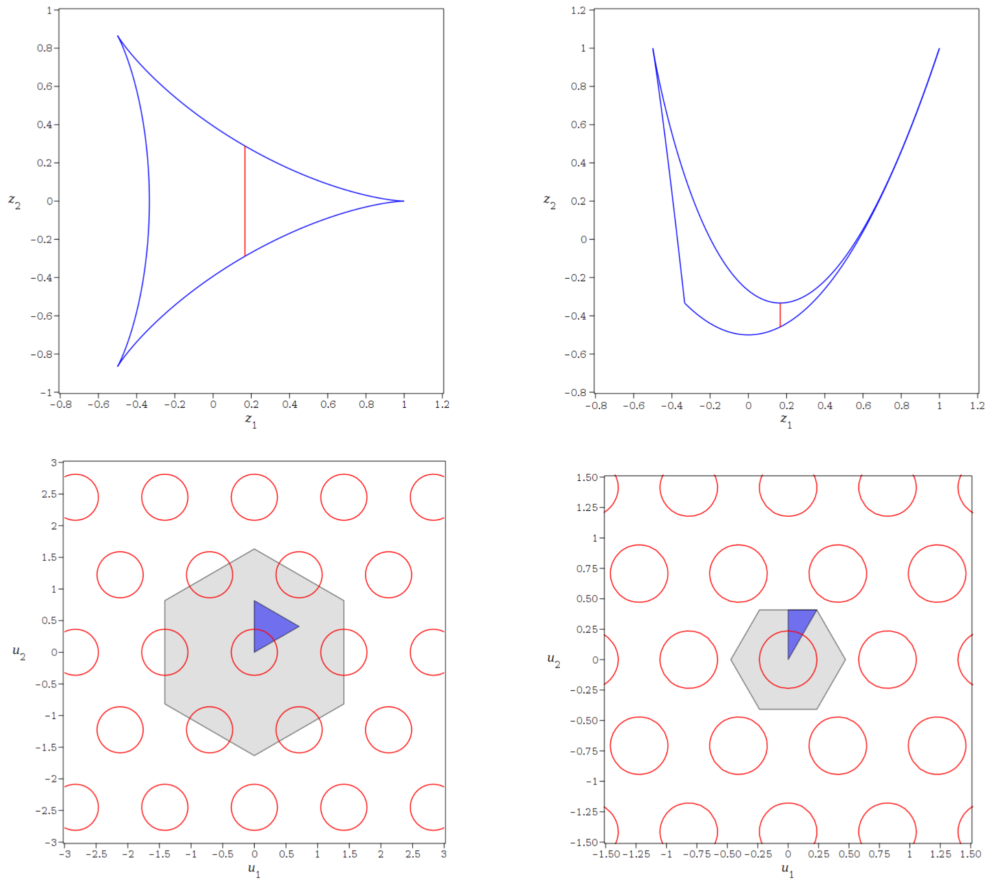
$$f_{\mathrm{G}}(z) := \frac{2}{3}\,T_{01}(z) + \frac{1}{3}\,T_{20}(z) = 2\,z_1^2 - \frac{2}{3}\,z_1 - \frac{1}{3}$$

coincides with f_{A}. In this case, the line of critical points is

$$\{z \in \mathcal{T} \mid z_1 = 1/6\} = \{1/6\} \times [-11/24, -1/3].$$

The condition $\mathfrak{c}_{\omega_1,\mathbb{R}}(u) = 1/6$ on $\mathbb{R}^3/\langle[1,1,1]^t\rangle$ defines a family of ovals (not circles) with centers given by the lattice of coroots Λ (Figure 4.5). $\square$

The minimizers for f^* are in both cases depicted below. One can observe the periodicity with respect to the coroot lattice as well as the Weyl symmetry.



(a) A_2 (b) G_2

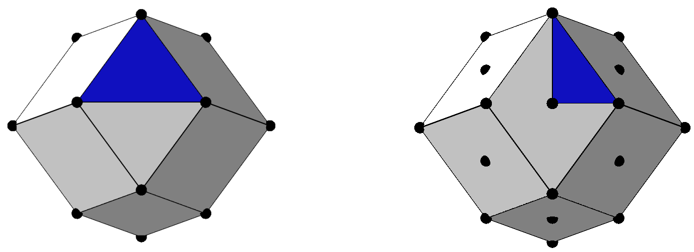
Figure 4.5: The minimizers for f^* in the $\mathbb{T}$–orbit space (lines, above) with preimages (ovals, below).

Example: The rhombic dodecahedron in $\mathbb{R}^3$

The rhombic dodecahedron in $\mathbb{R}^3$ (Figure 4.6) is the Voronoï cell of the coroot lattice Λ for A_3 and B_3. It has 14 vertices, 24 edges and 12 faces.

For A_3, the vertices are the orbits of ω_1, ω_2 and ω_3. The centers of the edges are the orbits of $(\omega_i + \omega_2)/2$ for $i = 1, 2$, and the centers of the faces are the orbit of $(\omega_1 + \omega_3)/2$.

For B_3, the vertices are the orbits of ω_1 and ω_3. The centers of the edges are the orbit of $(\omega_1 + \omega_3)/2$, and the centers of the faces are the orbit of $\omega_2/2$.



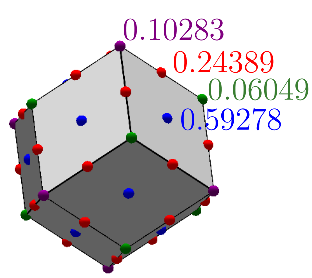
(a) A_3 (b) B_3

Figure 4.6: The rhombic dodecahedron is the Voronoï cell of the lattice of coroots for A_3 and B_3.

R	$d\backslash r$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
A_3	4	3.99424	6.10767	5.86933	6.10766	5.81858	6.10766	4.77576	6.10766	–	–	–	–	–	–
	5	3.99611	6.10767	5.86964	6.10766	5.90988	6.10767	5.85369	6.10766	5.46888	6.10766	–	–	–	–
	6	3.99653	6.10767	5.86972	6.10767	5.93658	6.10767	5.85762	6.10766	5.85825	6.10766	3.78978	6.10766	–	–
	7	3.99702	6.10767	5.86988	6.10767	5.94146	6.10766	5.96334	6.10767	5.85986	6.10766	4.12186	6.10766	–	6.10766
	8	3.99719	6.10767	5.86992	6.10767	5.94327	6.10767	6.05399	6.10767	5.86357	6.10766	5.59839	6.10766	3.88490	6.10766
B_3	3	3.83791	6.10767	3.39918	6.10766	–	6.10766	–	–	–	–	–	–	–	–
	4	3.84571	6.10767	4.11626	6.10766	–	6.10766	–	6.10766	–	–	–	–	–	–
	5	3.98454	6.10767	5.80542	6.10766	5.08174	6.10767	–	6.10766	–	6.10766	–	–	–	–
	6	3.99667	6.10767	5.87057	6.10767	5.86644	6.10767	5.82630	6.10766	–	6.10766	–	6.10766	–	–
	7	3.99872	6.10767	5.87057	6.10767	5.94578	6.10766	5.96989	6.10767	5.88810	6.10766	–	6.10766	–	6.10766
	8	3.99925	6.10767	5.87057	6.10767	5.96374	6.10767	5.99825	6.10767	5.94949	6.10766	5.92157	6.10766	5.31568	6.10766

Table 4.3: The bound $1 - 1/F(r, d)$ through Chebyshev moment–SOS relaxation of order d for the rhombic dodecahedron.

For $r = 1$, the numerically computed bound seems to converge to 4. For $r \geq 2$, the best possible bound we obtained is already assumed at $r = 2$ and $d = 3$, respectively $d = 4$. We display the optimal coefficients for the corresponding measure below. This bound is approximately assumed in all $F(r, d)$ with r even at lowest possible order. For r odd, the value converges but does not stabilize. A_3 and B_3 give the same coefficients for the same supporting points. The chromatic number of $\mathbb{R}^3$ for the rhombic dodecahedron is 8 [BBMP19, Theorem 4], proven analytically via a discrete subgraph and its clique density.



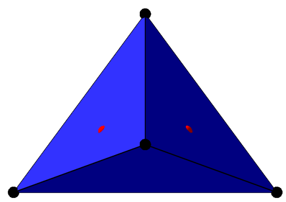
	A_3		B_3	
r	$1 - 1/F(r, 8)$	$c_\alpha = c_{\widehat{\alpha}}$	$1 - 1/F(r, 8)$	c_α
1	3.99719	$c_{010} = 0.33298$ $c_{100} = 0.66702$	3.99925	$c_{100} = 0.33315$ $c_{001} = 0.66685$
2	6.10767	$c_{020} = 0.10282$ $c_{110} = 0.24392$ $c_{200} = 0.06050$ $c_{101} = 0.59276$	6.10767	$c_{200} = 0.10283$ $c_{101} = 0.24389$ $c_{002} = 0.06049$ $c_{010} = 0.59278$

Figure 4.7: The scaled Voronoï cell and the optimal coefficients for $F(2, 8)$. Supporting points α in the same Weyl group orbit and their additive inverse $\widehat{\alpha}$ have the same coefficients, denoted by red, blue, green and purple dots.

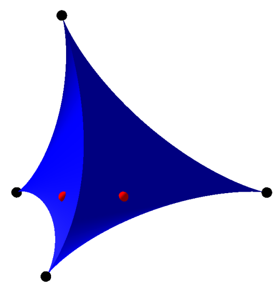
As we can observe, the most weight is put on the center of faces, then on the centers of edges and only small weight is put on the vertices. We investigate the minimizers of the associated sum of generalized Chebyshev polynomials.

Remark 4.21. *Similar to Lemma 4.20, one finds the following.*

1. *For* $\mathrm{R} = \mathrm{B}_3$*, the minimizers for* $F(2,8)$ *are* $z_{\min} \approx (0.059271558, z_2, 0.222115283)$*, where* $z_2 \in \mathbb{R}$ *is such that* $z_{\min} \in \mathcal{T}$*.*
2. *For* $\mathrm{R} = \mathrm{A}_3$*, the real minimizers for* $F(2,8)$ *are* $z_{\min} \approx (0.222089809, 0.059154429, z_3)$*, where* $z_3 \in \mathbb{R}$ *is such that* $z_{\min} \in \mathcal{T}_{\mathbb{R}}$*. The preimage of* $z_{\min}$ *under the generalized cosine is denoted by* $u_{\min} \in \mathbb{R}^4/\langle[1,1,1,1]^t\rangle$*.*



(a) $u_{\min}$



(b) $z_{\min}$

Figure 4.8: The two minimizers for $F(2,8)$ on the boundary of the fundamental domain and their images in the $\mathbb{T}$–orbit space of A_3.

Example: The icositetrachoron in $\mathbb{R}^4$

The icositetrachoron in $\mathbb{R}^4$ is the Voronoï cell of the coroot lattice Λ for B_4 and D_4. It has 24 vertices, 96 edges, 96 faces and 24 facets. The facets are octahedral cells.

For B_4, the vertices are the orbits of ω_1 and ω_4. The centers of edges are the orbits of $(\omega_1+\omega_4)/2$ and $\omega_3/2$. The centers of faces are the orbit of $(\omega_1+\omega_3)/3$. The centers of facets are the orbit of $\omega_2/2$.

For D_4, the vertices are the orbits of ω_1, ω_3 and ω_4. The centers of edges are the orbits of $(\omega_1+\omega_3)/2$, $(\omega_1+\omega_4)/2$ and $(\omega_3+\omega_4)/2$. The centers of faces are the orbit of $(\omega_1+\omega_3+\omega_4)/3$. The centers of facets are the orbit of $\omega_2/2$.

R	$d\backslash r$	1	2	3	4	5	6	7	8	9	10	11	12
B_4	4	3.01160	10.00001	–	10.00000	–	10.0000	–	10.00000	–	–	–	–
	5	3.77462	10.00035	–	10.00000	–	10.00000	–	10.00000	–	10.00000	–	–
	6	3.99453	10.02433	9.10927	10.01295	8.91701	10.00001	4.69147	10.00000	–	10.00000	–	10.00000
	7	3.99961	10.02434	9.12574	10.01902	9.26148	10.00819	9.32108	10.00000	8.35442	10.00000	4.15681	10.00000
D_4	4	3.07035	10.00004	–	10.00000	–	10.00000	–	10.00000	–	–	–	–
	5	3.94031	10.00231	–	10.00000	–	10.00000	–	10.00000	–	10.00000	–	–
	6	3.99496	10.02432	9.11312	10.01314	8.93873	10.00001	5.12215	10.00000	–	10.00000	–	10.00000

Table 4.4: The bound $1 - 1/F(r,d)$ through Chebyshev moment–SOS relaxation of order d for the icositetrachoron.

For $r = 1$, the numerically computed bound seems to converge to 4. For $r \geq 2$, the best possible bound we obtained is assumed at $r = 2$ and $d = 7$, respectively $d = 6$. For r odd, the value is always smaller than for even r.

What is remarkable here is, that, for B_4, we have $F(2,7) \geq F(4,7)$ although 2 divides 4. This is because the monotonous growth in Theorem 4.8 only holds for $d \to \infty$. In the D_4 case, we have the same for $F(2,6) \geq F(4,6)$. We display the optimal coefficients for the corresponding measure below.

	B_4		D_4	
r	$1 - 1/F(r,7)$	c_α	$1 - 1/F(r,6)$	c_α
1	3.99961	$c_{1000} = 0.33303$	3.99496	$c_{1000} = 0.33305$
				$c_{0010} = 0.33348$
		$c_{0001} = 0.66697$		$c_{0001} = 0.33348$
2	10.02434	$c_{0100} = 0.40062$	10.02432	$c_{0100} = 0.40188$
		$c_{1001} = 0.35491$		$c_{1001} = 0.17692$
				$c_{1010} = 0.17692$
		$c_{0010} = 0.17769$		$c_{0011} = 0.17726$
		$c_{0002} = 0.04444$		$c_{0002} = 0.02228$
				$c_{0020} = 0.02228$
		$c_{2000} = 0.02234$		$c_{2000} = 0.02245$

Table 4.5: The optimal coefficients for $F(r,7)$, respectively $F(r,6)$.

Recall that the fundamental weights satisfy $\omega_i^{\mathrm{B}} = \omega_i^{\mathrm{D}}$ for $i = 1,3,4$ and $\omega_3^{\mathrm{B}} = \omega_3^{\mathrm{D}} + \omega_4^{\mathrm{D}}$. In the case of $r = 2$ in Table 4.5, we observe that

1. the centers of facets are weighted with $0.40062 \approx 0.40188$,

2. the centers of faces are not weighted,

3. the centers of edges are weighted with $0.35491 \approx 0.17692 + 0.17692$ and $0.17769 \approx 0.17726$ and

4. the vertices are weighted with $0.02234 \approx 0.02245$ and $0.04444 \approx 0.02228 + 0.02228$.

Further computations are limited by the size of the semi–definite program, see Table 3.1. The chromatic number of $\mathbb{R}^4$ for the icositetrachoron polytope is at least 15 [BBMP19, Theorem 5], proven analytically via a discrete subgraph and its clique density.

3.2 Computing numerical bounds on $\chi(\mathbb{Z}^n, S_r)$

Theorem 4.8 also applies when Ω is replaced by another lattice such as $\mathbb{Z}^n$. We compute $F(r,d)$ for $S_r = \mathbb{B}_r^1 \cap \mathbb{Z}^n$, where S_r is a subset of the weight lattice Ω for root systems of type B_n, C_n and D_n. This gives a lower bound for the chromatic number of the graph $G(\mathbb{Z}^n, S_r)$ and implicitly also for the measurable chromatic number $\chi_m(\mathbb{R}^n, \|\cdot\|_1)$ of $\mathbb{R}^n$. We already know what to expect for $r = 2$ ($\chi(\mathbb{Z}^n, S_2) = 2n$, Theorem 4.16) and for r odd ($\chi(\mathbb{Z}^n, S_r) = 2$, Lemma 4.15). Thus, we will only consider $F(r,d)$ for r even, keeping $F(2,d)$ as a benchmark.

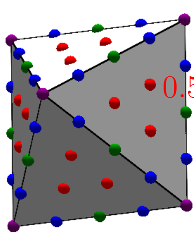
For $n = 2$ and r even, we already know that $\chi(\mathbb{Z}^2, S_r) = 4$ from Corollary 4.17. For $n \geq 3$ and $r \geq 4$ even, [FK04] gives lower and upper bound $2n + 1 \leq \chi(\mathbb{Z}^n, S_r) \leq 3r^{n-2}$.

Example: $n = 3, r \leq 14$

R	$d \backslash r$	2	4	6	8	10	12	14
B_3	3	6.00000	6.28148	6.01551	–	–	–	–
	4	6.00000	6.28148	6.07717	6.28148	–	–	–
	5	6.00000	6.28148	6.29004	6.28183	6.12543	–	–
	6	6.00000	6.28148	6.30244	6.29799	6.27850	6.28234	–
	7	6.00000	6.28148	6.30269	6.30435	6.30031	6.29708	6.27830
	8	6.00000	6.28148	6.30269	6.30463	6.30053	6.30088	6.29604
	9	6.00000	6.28148	6.30269	6.30501	6.30502	6.30227	6.301858
C_3	3	6.00000	6.28148	6.02310	–	–	–	–
	4	6.00000	6.28148	6.29021	6.28198	–	–	–
	5	6.00000	6.28148	6.30182	6.29951	6.29810	–	–
	6	6.00000	6.28148	6.30269	6.30455	6.30048	6.30069	–
	7	6.00000	6.28148	6.30269	6.30494	6.30057	6.30229	6.30156

Table 4.6: The bound $1 - 1/F(r, d)$ through Chebyshev moment–SOS relaxation of order d for $\mathbb{Z}^3$.

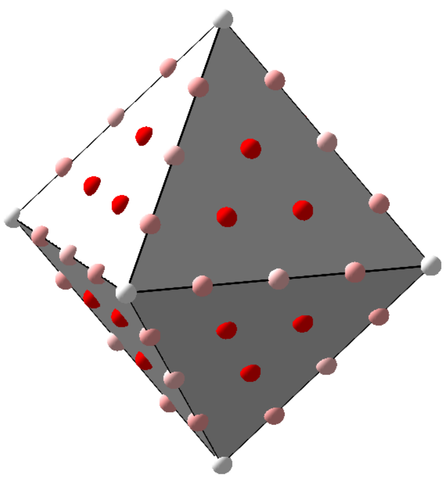
The value $\chi(\mathbb{Z}^3, S_2) = 6$ is obtained immediately with $F(2, 1)$. The highest value is $F(9, 10)$ for B_3, giving our best obtainable bound on $\chi_m(\mathbb{R}^3, \|\cdot\|_1)$ for the moment. Furthermore, $F(4, d)$ seems to be stable in the cases of both root systems. We give the optimal coefficients, which coincide for both B_3 and C_3.



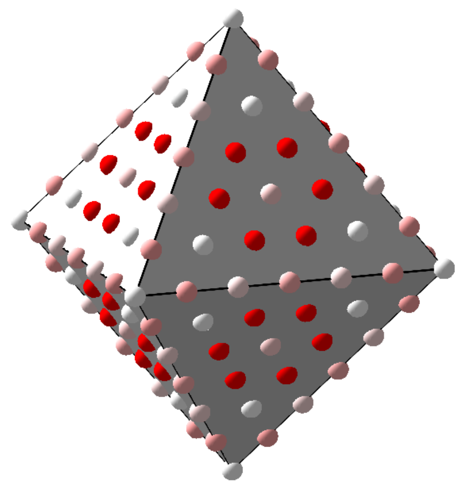
C_3		B_3	
$1 - 1/F(4, 7)$	c_α	$1 - 1/F(4, 9)$	c_α
6.28148	$c_{400} = 0.01752$	6.28148	$c_{400} = 0.01754$
	$c_{210} = 0.22681$		$c_{210} = 0.22680$
	$c_{101} = 0.59380$		$c_{102} = 0.59375$
	$c_{020} = 0.16185$		$c_{020} = 0.16189$

Figure 4.9: The sphere of $\|\cdot\|_1$ with radius $r = 4$ and the optimal coefficients for $F(4, 9)$. Supporting points α in the same Weyl group orbit have the same coefficients, denoted by red, blue, green and purple dots.

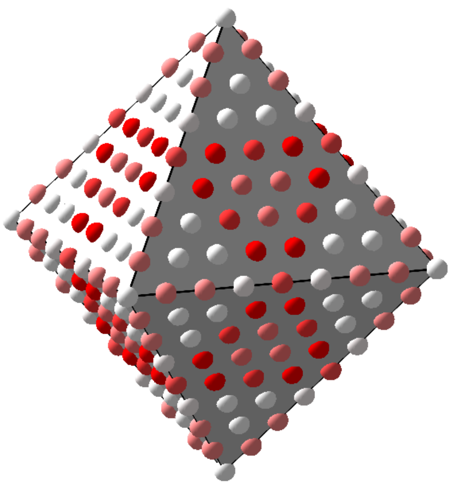
This result confirms the lower bound of 7 from [FK04], although we do not obtain it numerically. This indicates again that there is a gap between the spectral bound and the chromatic number.



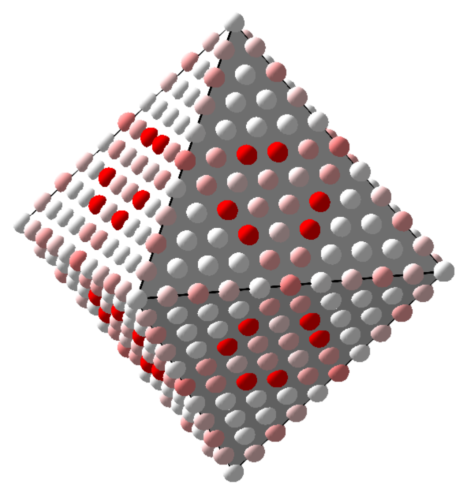
(a) $r = 4$



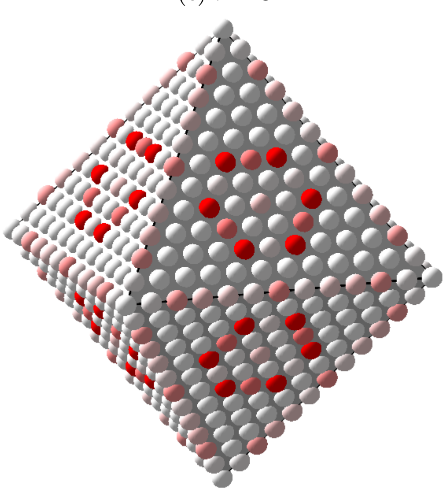
(b) $r = 6$



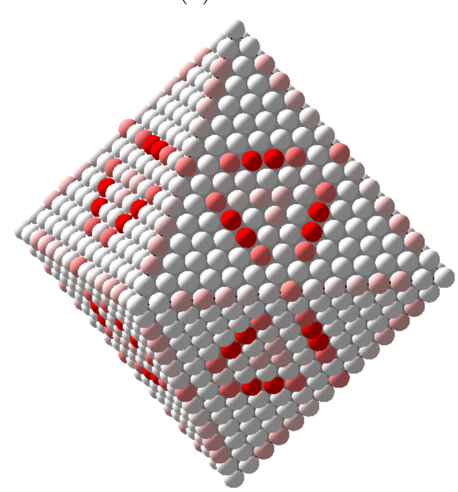
(c) $r = 8$



(d) $r = 10$



(e) $r = 12$



(f) $r = 14$

Figure 4.10: The coefficients c_α for $F(r, 9)$ in the case of B_3, indicated by the intensity of the color as $\mathrm{RGB}(1, 1 - (c_\alpha - c_{\min})/(c_{\max} - c_{\min}), 1 - (c_\alpha - c_{\min})/(c_{\max} - c_{\min}))$.

Example: $n = 4, r \leq 14$

R	$d\backslash r$	2	4	6	8	10	12	14
B_4	4	8.00000	10.33968	9.09234	10.33968	–	–	–
	5	8.00000	10.33969	9.72339	10.33969	9.17503	–	–
	6	8.00000	10.83655	10.18050	10.33969	9.90514	10.33968	–
	7	8.00000	10.86019	10.51696	10.51282	10.16103	10.33968	10.03938
C_4	4	8.00000	10.33993	9.72014	10.33968	–	–	–
	5	8.00000	10.83902	10.07664	10.33968	9.94864	–	–
D_4	4	8.00000	10.34750	9.08887	10.33969	–	–	–
	5	8.00000	10.39184	9.72430	10.34011	9.52887	–	–
	6	8.00000	10.83844	10.34886	10.35578	9.97888	10.33971	–

Table 4.7: The bound $1 - 1/F(r, d)$ through Chebyshev moment–SOS relaxation of order d for $\mathbb{Z}^4$.

The value $\chi(\mathbb{Z}^4, S_2) = 8$ is obtained immediately with $F(2, 1)$. The highest value is $F(4, 7)$ for B_4, giving our best obtainable bound on $\chi_m(\mathbb{R}^4, \|\cdot\|_1)$ for the moment. None of the computed bounds $F(r, d)$ is stable in d and we are limited by the size of the semi–definite program, see Table 3.1. Again, in the case of B_4 for example, we see that $F(4, 9) \geq F(8, 9)$, because we do not take the limit.

This result improves the lower bound 9 given in [FK04] by +2.

3.3 Computational aspects

The numerical results can be reproduced with Python as follows. First, a text file is required, which contains the matrices A_α from Equation (3.14). This file can be obtained via the command CHEBYSHEVSDPDATA from the MAPLE package GENERALIZEDCHEBYSHEV. Since the A_α depend on the dimension n and the relaxation order d, those parameters need to be specified.

If the user wishes to work with a ".sdpa" based solver, the file must be modified to the required format. We indicate here how to conduct the computation in Python. Assume that CHEBYSHEVSDPDATA has produced a file "example.csv" with the following content.

```
A0 =   [ [...] , ... , [...] ]  ;
A  = [ [ [...] , ... , [...] ]  , ... , [ [...] , ... , [...] ] ]  ;
```

This file needs to be renamed to "example.py". Then f^d_{sos} from Equation (3.13) can be solved for known indices S (as a list of integers), coefficients $c0, c$ and a solver "SOLVER" with the following Python code.

```
import cvxpy as cp
import numpy as np
import math

from example import A0,A
n,m = len(A0),len(A)
A0 = np.array(A0)
A = [np.array(A[i]) for i in range(m)]
X = cp.Variable((n, n), PSD=True)
objectiveP = c0 - cp.trace(A0@X)

L=list(set([i for i in range(m)]) - set(S))
constraintsP = [cp.trace(A[i]@X) == 0 for i in L]
for i in S: constraintsP.append(cp.trace(A[i]@X) == c[i])

probP = cp.Problem(cp.Maximize(objectiveP), constraintsP)
vP=probP.solve(solver='SOLVER')
```

Furthermore, for known indices S, but unknown coefficients, f^d_{mix} from Equation (3.18) can be solved by modifying the code to the following.

```
objectiveP = - cp.trace(A0@X)

L=list(set([i for i in range(m)]) - set(S))
constraintsP = [cp.trace(A[i]@X) == 0 for i in L]
for i in S: constraintsP.append(cp.trace(A[i]@X) >= 0)

constraintsP.append(cp.trace((sum([A[i] for i in S]))@X) == 1)
probP = cp.Problem(cp.Maximize(objectiveP), constraintsP)
vP=probP.solve(solver='SOLVER')

c=np.array([np.trace(A[i]@X.value) for i in S])
sum(c)
for i in range(len(S)): c[i]
```

For the presented numerical results, [MOS] has been used as a solver.

Conclusion and future research directions

We have established a systematic approach to the problem of trigonometric optimization. Under the assumption of crystallographic symmetry, a trigonometric polynomial on $\mathbb{R}^n$ can be written as a sum of generalized Chebyshev polynomials on the $\mathbb{T}$–orbit space of the associated nonlinear Weyl group action as

$$f^* = \inf_{u\in\mathbb{R}^n} \sum_{\mu\in\Omega} c_\mu \exp(-2\pi\mathrm{i}\,\langle \mu, u\rangle) = \inf_{z\in\mathcal{T}} \sum_{\alpha\in\mathbb{N}^n} c_\alpha\, T_\alpha(z) = \inf_{z\in\mathcal{T}} \sum_{\alpha\in\mathbb{N}^n} c_\alpha\, T_\alpha(z).$$

We can then solve the optimization problem with tools from polynomial optimization, which reduces the complexity of the semi–definite relaxations.

The first main result of this thesis is the explicit polynomial description for the $\mathbb{T}$–orbit space $\mathcal{T}$ of the nonlinear Weyl group action on the compact torus associated to a root system of type A_{n-1}, C_n, B_n, D_n and G_2. This covers all of the four infinite families of irreducible root systems. With G_2, we have also covered one of the special cases. Ongoing work revolves around finding an explicit formula for the two $\mathrm{E}_{6,7,8}$ and F_4 remaining cases, since a unifying formula for all eight families is desirable. Altogether, this will allow for the characterization of the $\mathbb{T}$–orbit space of any crystallographic group by decomposing the associated root system into its irreducible components.

One application of the $\mathbb{T}$–orbit space description is the characterization of the multiplicative invariants, which assume only positive or non–negative values on the compact torus. Another application is the polynomial description for the region of orthogonality for generalized Chebyshev polynomials of the first and second kind. For the latter, an explicit formula is provided for the orthogonalizing weight function in Appendix B.

Orbit spaces have further applications. To give a concrete one, consider the problem of finding a cubature formula for a linear form with a representing measure. This was studied in [FP05, CH18] with moment methods. For a positive Borel measure η with compact support contained in a basic semi–algebraic set $\mathcal{T}$, a linear form $\mathscr{L}$ is called a **cubature of degree** d, if

$$\mathscr{L}(f) = \int_{\mathcal{T}} f(z)\,\mathrm{d}\eta(z)$$

is true for all $f \in \mathbb{R}[z]_{\leq d}$, the space of multivariate polynomials of degree at most d. Since $\mathbb{R}[z]_{\leq d}$ is finite dimensional, $\mathscr{L}$ can, by the Crathéodory theorem, be assumed to be a finite sum of point evaluations. When $\mathcal{T}$ is the $\mathbb{T}$–orbit space of a Weyl group and moments are replaced by Chebyshev moments, then we are in the setting of Chapter 3. A cubature formula for Steiner's hypocycloid, see Figure 2.1, and more generally, for $\mathbb{T}$–orbit spaces associated to A_{n-1} root systems, was provided in [LX10]. A similar formula exists for G_2 [LSX12]. Advancing this theory could potentially allow for optimality certificates in polynomial optimization, such as flat extension [LM09], but in the basis of generalized Chebyshev polynomials and with the notion of weighted degree.

The polynomial description of the $\mathbb{T}$–orbit space hardly completes the study of multiplicative invariants for Weyl groups. A known result in the linear setting is the analog version of Theorem 1.30. The Chevalley–Shephard–Todd Theorem (1954) states that a linear group is a finite reflection group if and only if the ring of invariants is a polynomial algebra. Furthermore, this is equivalent to the coordinate ring being a free module over the ring of invariants. This statement can be extended to the ring of all morphisms being a free module [Shc82]. Future work revolves around the study of the Shchvartsman theorem in the context of multiplicative actions and potential applications.

For geometric graphs, several new proofs and experimental results have been presented. In general, spectral bounds for the chromatic number and independence number of distance graphs for tiling polytope norms can be computed with the techniques from Chapter 3, as long as one finds a representation with weights of a crystallographic root system. However, the computed bound does not reach the desired chromatic number 2^n (or other theoretically known values) in several cases. There are two possible reasons for that. Either the number of supporting points is not sufficient, or the spectral bound does not provide a sharp bound when discrete measures are used. The de Bruijn–Erdös theorem states that the chromatic number is the supremum of the chromatic numbers of the finite subgraphs. Thus, when the computed bound stabilizes at some level, one can not conclude that the spectral bound is sharp. Furthermore, it is remarkable that the best numerical bounds are obtained at even weighted degree for the hexagon Table 4.2, the rhombic dodecahedron Table 4.3 and the icositetrachoron Table 4.5. Furthermore, the arising semi–definite programs of the Chebyshev moment and SOS relaxation are always feasible for even weighted degree. A similar behavior is to be noted with the chromatic number of $\mathbb{Z}^n$ for the 1–norm.

To advance these numerical bounds, work on improving the MAPLE package GENERALIZEDCHEBYSHEV is ongoing. Improvements are necessary to eventually handle the cases of the E_8 root lattice or the leech lattice.

Appendix A

Background of Crystallographic Symmetries

Root systems can be used to classify the semi–simple complex Lie algebras. Given a splitting Cartan subalgebra, the weights of the adjoint representation form a root system in the sense of Chapter 1. This allows to decompose the Lie algebra and to understand the Lie bracket. Taking all representations of the Lie algebra, the union of their weights forms the weight lattice of the root system, which leads to Weyl's character formula and the theorem of the highest weight. In particular, the motivation for minuscule weight in Chapter 2 originates from this theory. Finally, we review the role of root systems in multiplicative invariant theory.

1 Semi–simple Lie algebras

Root systems, as they were introduced in Chapter 1, are historically relevant for the classification of simple complex Lie algebras due to Wilhelm Killing and Élie Cartan in 1880. This classification is summarized here, motivating the definitions and giving a background for weight lattices, which play an essential role in this thesis.

1.1 Definitions and Ado's theorem

A **complex Lie algebra** $\mathfrak{g}$ is a $\mathbb{C}$–vector space together with a Lie bracket $[\cdot,\cdot]$, that is, a bilinear, alternating form, which satisfies the Jacobi–identity.

Definition A.1. *Let $\mathfrak{g}$ be a complex Lie algebra and $A, B \subseteq \mathfrak{g}$ be $\mathbb{C}$–vector subspaces. We denote the product of A and B by $[A,B] := \langle [a,b] \,|\, a \in A, b \in B\rangle_{\mathbb{C}}$. For a $\mathbb{C}$–vector space V, the Lie algebra of endomorphisms on V is denoted by $\mathfrak{gl}(V)$.*

1. *The **centralizer** of A in $\mathfrak{g}$ is $C_{\mathfrak{g}}(A) := \{g \in \mathfrak{g} \,|\, [g,A] = 0\}$.*
2. *The **center** of $\mathfrak{g}$ is $Z(\mathfrak{g}) := C_{\mathfrak{g}}(\mathfrak{g})$.*
3. *$\mathfrak{g}$ is called **Abelian**, if $Z(\mathfrak{g}) = \mathfrak{g}$.*
4. *The **normalizer** of A in $\mathfrak{g}$ is $N_{\mathfrak{g}}(A) := \{g \in \mathfrak{g} \,|\, [g,A] \subseteq A\}$.*
5. *A is called an **ideal** in $\mathfrak{g}$, if $N_{\mathfrak{g}}(A) = \mathfrak{g}$.*
6. *$\mathfrak{g}$ is called **simple**, if $\mathfrak{g}$ is not Abelian and $0, \mathfrak{g}$ are the only ideals in $\mathfrak{g}$.*
7. *$\mathfrak{g}$ is called **nilpotent**, if $\mathfrak{g}_{(k)} = 0$ for some $k \in \mathbb{N}$, where $\mathfrak{g}_{(0)} := \mathfrak{g}$ and $\mathfrak{g}_{(k+1)} := [\mathfrak{g}_{(k)}, \mathfrak{g}]$.*
8. *$\mathfrak{g}$ is called **solvable**, if $\mathfrak{g}^{(k)} = 0$ for some $k \in \mathbb{N}$, where $\mathfrak{g}^{(0)} := \mathfrak{g}$ and $\mathfrak{g}^{(k+1)} := [\mathfrak{g}^{(k)}, \mathfrak{g}^{(k)}]$.*
9. *The **radical** of $\mathfrak{g}$ is the unique solvable ideal $\mathrm{rad}(\mathfrak{g}) \neq \mathfrak{g}$, which is maximal with respect to inclusion.*
10. *$\mathfrak{g}$ is called **semi–simple**, if $\mathrm{rad}(\mathfrak{g}) = 0$.*
11. *A **representation** of $\mathfrak{g}$ or a $\mathfrak{g}$–**module** is a $\mathbb{C}$–vector space V, together with a Lie algebra homomorphism $\mathfrak{g} \to \mathfrak{gl}(V)$.*

The following theorem allows us to think of a complex Lie algebra as an algebra of matrices with Lie bracket given by the commutator $[g,h] = gh - hg$ for $g, h \in \mathfrak{g}$. Hence, the notions trace, diagonalizable and triangularizable are defined canonically. When we speak of "subalgebras" and "isomorphisms", we mean Lie subalgebras and Lie algebra isomorphisms.

Theorem A.2. [Ado47] *Every finite–dimensional complex Lie algebra is a subalgebra of $\mathfrak{gl}_n(\mathbb{C})$ up to isomorphism.*

1.2 Cartan decomposition

Let $\mathfrak{g}$ be a finite–dimensional semi–simple complex Lie algebra. We revisit a known theorem by which $\mathfrak{g}$ has a natural decomposition in positive and negative roots.

Example A.3. *Consider the Lie algebra $\mathfrak{g} := \mathfrak{sl}_n(\mathbb{C})$ of the special linear group. A basis of $\mathfrak{g}$ is given by*

$$e_{ij} \quad \textit{for} \quad 1 \le i < j \le n, \quad e_{ji} \quad \textit{for} \quad 1 \le j < i \le n, \quad e_{ii} - e_{nn} \quad \textit{for} \quad 1 \le i \le n-1,$$

where e_{ij} *is the matrix with entry* 1 *at* (i,j) *and* 0 *elsewhere. Define the Abelian subalgebra*

$$\mathfrak{h} := \left\{ \begin{bmatrix} r_1 & & 0 \\ & \ddots & \\ 0 & & r_n \end{bmatrix} \middle| \, r_1,\ldots,r_n \in \mathbb{C}, \sum_{i=1}^{n} r_i = 0 \right\}.$$

With $\mathfrak{g}_{ij} := \langle e_{ij} \rangle_{\mathbb{C}}$ *as a* $\mathbb{C}$*–vector space, there is a decomposition of* $\mathfrak{g}$ *as*

$$\mathfrak{g} = \bigoplus_{i<j} \mathfrak{g}_{ij} \oplus \bigoplus_{i>j} \mathfrak{g}_{ij} \oplus \mathfrak{h}.$$

Since $\mathfrak{h}$ *is Abelian, it suffices to know the* $[h, e_{ij}]$ *and* $[e_{ij}, e_{k\ell}]$ *for* $h \in \mathfrak{h}$*,* $i \neq j$ *and* $k \neq \ell$*, in order to describe the Lie bracket on* $\mathfrak{g}$*, see also* [Bou75, Chapitre VIII, Lemma 2]*.*

We consider the **adjoint representation**

$$\begin{aligned} \mathrm{ad} : \ \mathfrak{g} &\to \mathfrak{gl}(\mathfrak{g}), \\ g &\mapsto \mathrm{ad}_g : \begin{cases} \mathfrak{g} & \to \mathfrak{g}, \\ h & \mapsto [g,h] \end{cases} \end{aligned}$$

of $\mathfrak{g}$. Here, ad_g is called the **adjoint operator** associated to $g \in \mathfrak{g}$. The **Killing form** of $\mathfrak{g}$ is the bilinear form

$$\begin{aligned} \chi_{\mathfrak{g}} : \ \mathfrak{g} \times \mathfrak{g} &\to \mathbb{C}, \\ (g,h) &\mapsto \mathrm{Trace}(\mathrm{ad}_g \, \mathrm{ad}_h). \end{aligned}$$

Cartan's Criterion states that $\mathfrak{g}$ is semi–simple if and only if the Killing form is non–degenerate.

Definition A.4. *A subalgebra* $\mathfrak{h}$ *of* $\mathfrak{g}$ *is called a* ***Cartan subalgebra*** *in* $\mathfrak{g}$*, if* $\mathfrak{h}$ *is nilpotent and* $N_{\mathfrak{g}}(\mathfrak{h}) = \mathfrak{h}$*.*

One can show that every Cartan subalgebra $\mathfrak{h}$ is splitting, that is, for all $h \in \mathfrak{h}$, ad_h is diagonalizable in the sense of Ado's theorem. This is not true when $\mathbb{C}$ is replaced with a field, which is not algebraically closed [Bou75, Chapitre 8, §2, Remarques 1 et 2].

From now on, we fix a Cartan subalgebra $\mathfrak{h}$ of $\mathfrak{g}$. For a linear form $\rho \in \mathfrak{h}^*$, we define the $\mathbb{C}$–vector subspace

$$\mathfrak{g}_\rho := \{ g \in \mathfrak{g} \,|\, \forall\, h \in \mathfrak{h} : \, [h,g] = \rho(h)\, g \}.$$

We denote by R the set of all $0 \neq \rho \in \mathfrak{h}^*$, such that $\mathfrak{g}_\rho \neq 0$. The elements of R are the **roots** of $\mathfrak{g}$.

Theorem A.5. [Cartan decomposition] R *is finite and*

$$\mathfrak{g} = \mathfrak{h} \oplus \bigoplus_{\rho \in \mathrm{R}} \mathfrak{g}_\rho.$$

For $\rho \in \mathrm{R}$, we define the $\mathbb{C}$–vector subspace $\mathfrak{h}_\rho := [\mathfrak{g}_\rho, \mathfrak{g}_{-\rho}]$.

Proposition A.6. [Bou75, Chapitre VIII, §2, Théorème 1 et Proposition 2] *Let* $\rho, \rho' \in \mathrm{R}$*. The following statements hold.*

1. $\mathfrak{g}_\rho$ *and* $\mathfrak{h}_\rho$ *both have dimension* 1*.*
2. $\mathfrak{h}_\rho$ *contains a unique* $\rho^\vee$*, such that* $\rho(\rho^\vee) = 2$*.*
3. *We have* $\chi_{\mathfrak{g}}(\rho^\vee, (\rho')^\vee) \in \mathbb{Z}$*.*

With the previous statement, one can show that the Cartan decomposition admits a root system. Thanks to Cartan's criterion, $\chi_{\mathfrak{g}}$ yields an inner product on $\mathfrak{h}^*$.

Theorem A.7. [Bou75, Chapitre VIII, §2, Théorème 2] *In the sense of Definition 1.1,* R *is a root system in the* $\mathbb{R}$*–vector space* $\langle \mathrm{R}\rangle_{\mathbb{R}} \subseteq \mathfrak{h}^*$ *with respect to the inner product defined by* $\chi_{\mathfrak{g}}$*.*

When $\mathfrak{h}$ as a finite–dimensional space is identified with its dual, the coroots are precisely the $\rho^\vee$. A Lie algebra $\mathfrak{g}$ is simple if and only if its root system R is irreducible.

Example A.8. *Some simple Lie algebras are the following.*

1. *The Lie algebra* $\mathfrak{sl}_n(\mathbb{C})$ *of the special linear group admits a root system of type* A_{n-1}*.*
2. *The Lie algebra* $\mathfrak{sp}_{2n}(\mathbb{C})$ *of the symplectic group admits a root system of type* C_n*.*
3. *The Lie algebra* $\mathfrak{so}_{2n+1}(\mathbb{C})$ *of the special orthogonal group admits a root system of type* B_n*.*
4. *The Lie algebra* $\mathfrak{so}_{2n}(\mathbb{C})$ *of the special orthogonal group admits a root system of type* D_n*.*

The Cartan decomposition of $\mathfrak{sl}_n(\mathbb{C})$ *from Example A.3 motivates the notion of positive roots* ($i > j$) *and negative roots* ($i < j$) *for the base of* A_{n-1} *given in Equation (1.3).*

1.3 Weights

Let $\mathfrak{g}$ be a semi–simple complex Lie algebra and $\mathfrak{h}$ a Cartan subalgebra. For a linear form $\mu \in \mathfrak{h}^*$ and a representation V of $\mathfrak{g}$, define the $\mathbb{C}$–vector subspace

$$V_\mu := \{u \in V \,|\, \forall\, h \in \mathfrak{h} :\, \mu(h)\, u = h\, u\},$$

where $h\,u$ is the module operation of $\mathfrak{g}$ on V. We assume all representations of $\mathfrak{g}$ to be finite–dimensional.

Definition A.9. *Let* V *be a representation of* $\mathfrak{g}$ *and* $\mu \in \mathfrak{h}^*$*. We call* μ *a* ***weight*** *of* V*, if* $V_\mu \neq 0$*. In this case, the* ***multiplicity*** n_μ *of* μ *is the* $\mathbb{C}$*–vector space dimension of* V_μ*.*

Remark A.10. [Bou75, Chapitre VIII, §7, Proposition 1] *Let* R *be the root system associated to* $\mathfrak{g}$*. Then the weights of* R *are those elements of* $\mathfrak{h}^*$*, which are the weight of any representation. By the adjoint representation, every root is a weight. The weights, which are simultaneously contained in the lattice spanned by the roots, are the radical weights.*

From now on, let $\mathfrak{g}$ be simple, R be the root system associated to $\mathfrak{g}$ with Weyl group $\mathcal{W}$ and V be an irreducible representation of $\mathfrak{g}$, that is, the only representations of $\mathfrak{g}$ contained in V are 0 and V itself. Recall that the choice of a base for a root system defines a partial ordering $\succeq$ in terms of positive roots.

Theorem A.11. [Bou75, Chapitre VIII, §6, Lemma 2, Proposition 3 et Théorème 1] *Denote by* Ω_V *the weights of* V*. Then*

$$V = \bigoplus_{\mu \in \Omega_V} V_\mu.$$

For a fixed base B *of* R*, there exists a unique dominant weight* $\mu = \mu(V) \in \Omega_V$*, such that, for every* $\mu' \in \Omega_V$*,* $\mu(V) \succeq \mu'$*. If* V' *is an irreducible representation of* $\mathfrak{g}$ *isomorphic to* V*, then* $\mu(V') = \mu(V)$*.*

A dominant weight $\mu = \mu(V)$, which satisfies Theorem A.11, is called the **highest weight** of V with respect to B. An irreducible representation V of $\mathfrak{g}$ is finite–dimensional if and only if its highest weight is dominant [Bou75, Chapitre VIII, §7, Théorème 1].

We define an important class of weights, which are invariant under the Weyl group of the root system associated to $\mathfrak{g}$.

Definition A.12. *Let $S \subseteq \Omega$ be a set of weights.*

1. *S is called* R*–**saturated**, if, for all $\mu \in S$ and $\rho \in \mathrm{R}$, one of the following statements holds.*
   - *$\mu(\rho^\vee) \geq 0$ and, for $0 \leq \ell \leq \mu(\rho^\vee)$, we have $\mu - \ell\,\rho \in S$.*
   - *$\mu(\rho^\vee) < 0$ and, for $\mu(\rho^\vee) \leq \ell \leq 0$, we have $\mu - \ell\,\rho \in S$.*
2. *$\mu \in S$ is called* R*–**extremal** in S, if, for all $\rho \in \mathrm{R}$, we have either $\mu + \rho \notin S$ or $\mu - \rho \notin S$.*

Proposition A.13. [Bou75, Chapitre VIII, §7, Proposition 5] *Denote by Ω_V the weights of V and by μ its highest weight. The following statements hold.*

1. *Ω_V is, with respect to inclusion, the minimal* R*–saturated subset of Ω containing μ.*
2. *The orbit $\mathcal{W}\mu$ is the set of* R*–extremal elements in Ω_V.*

Theorem A.14. [Bou75, Chapitre VIII, §7, Proposition 6, 7 et 8] *Let $\mu \in \Omega$ be dominant and $\mathrm{B} = \{\rho_1, \ldots, \rho_n\}$ be a base for* R*, such that $\tilde{\rho} = \alpha_1\,\rho_1 + \ldots + \alpha_n\,\rho_n$ is the highest root of $\mathrm{R}^\vee$ for some $\alpha \in \mathbb{N}^n$. The following statements are equivalent.*

1. *$\Omega_V = \mathcal{W}\mu$.*
2. *For every $\rho \in \mathrm{R}$, $\mu(\rho^\vee) \in \{0, \pm 1\}$.*
3. *$\mu(\tilde{\rho}) = 1$.*
4. *There exists $1 \leq i \leq n$, such that $\alpha_i = 1$ and μ is the i–th fundamental weight of* R*.*

A weight μ, which satisfies the equivalent statements of Theorem A.14, is called a **minuscule weight** of $\mathfrak{g}$. Bourbaki uses the term "minuscule", whereas Humphreys calls such weights "minimal" [Hum72].

2 Multiplicative invariant theory

A general introduction to multiplicative invariant theory is given in [Lor05]. We recall how this theory is related to root systems and crystallographic symmetries.

2.1 Group lattices

Let $\mathcal{W}$ be a finite group with a representation over $\mathbb{R}^n$ and $\Omega \cong \mathbb{Z}^n$ a free $\mathbb{Z}$–module. We say that Ω is a $\mathcal{W}$**–lattice**, if there exists a homomorphism

$$\mathcal{W} \to \mathrm{GL}(\Omega).$$

Denote by I_n, respectively 0, the neutral element of $\mathcal{W}$, respectively Ω.

Definition A.15. *Let Ω be a $\mathcal{W}$–lattice.*

1. *Ω is called **faithful**, if $\{A \in \mathcal{W} \,|\, \forall\, \mu \in \Omega :\; A\mu = \mu\} = \{I_n\}$.*
2. *Ω is called **trivial**, if $\{A \in \mathcal{W} \,|\, \forall\, \mu \in \Omega :\; A\mu = \mu\} = \mathcal{W}$.*
3. *Ω is called **effective**, if $\{\mu \in \Omega \,|\, \forall\, A \in \mathcal{W} :\; A\mu = \mu\} = \{0\}$.*

The weight lattice of a root system is a faithful, effective lattice of the Weyl group.

2.2 Defining root systems via reflections

Let V be an n–dimensional $\mathbb{R}$–vector space, such that $\Omega \subseteq V$. We think of $\mathcal{W}$ as a subgroup of $\mathrm{GL}(V) \cong \mathrm{GL}_n(\mathbb{R})$. An element $A \in \mathcal{W}$ is called a **reflection**, if

$$\mathrm{Rank}(A - I_n) \leq 1.$$

Remark A.16. *In* $\mathrm{GL}_n(\mathbb{R})$*, a reflection* $A \neq I_n$ *is conjugate to* $\mathrm{diag}(1, \ldots, 1, -1)$*. Thus, the* $\mathbb{Z}$*–module*

$$\ker_\Omega(A + I_n) = \{\mu \in \Omega \,|\, A\mu + \mu = 0\}$$

has exactly two generators denoted by $\pm\rho_A$*.*

We can now establish the connection to root systems.

Theorem A.17. [Lor05, Proposition 1.9.1] *Let* Ω *be a faithful* $\mathcal{W}$*–lattice. Denote by* R *the set of all* $\pm\rho_A$ *with* $A \neq I_n$ *a reflection in* $\mathcal{W}$ *and by* $\mathcal{W}(\mathrm{R})$ *the group of all reflections in* $\mathcal{W}$*. Then* R *is a root system in* $\ker(\varphi)$*, where*

$$\begin{array}{rccl} \varphi: & V & \to & V, \\ & u & \mapsto & \frac{1}{|\mathcal{W}(\mathrm{R})|} \sum\limits_{A \in \mathcal{W}(\mathrm{R})} A\, u. \end{array}$$

The Weyl group of R *is* $\mathcal{W}(\mathrm{R})$ *and the weight lattice is*

$$\Omega(\mathrm{R}) = \{u - \varphi(u) \,|\, u \in V, \forall\, A \in \mathcal{W}(\mathrm{R}):\ (A - I_n)\, u \in \Omega\}.$$

Appendix B

Fourier analysis in terms of Chebyshev polynomials

We study multiplicative invariants, Chebyshev polynomials and $\mathbb{T}$–orbit spaces from a Fourier analytical point of view. First we introduce a notion of derivation on Laurent polynomials. This allows us to conjecture a characterization of the $\mathbb{T}$–orbit space, which is compared with that in Chapter 2. We then give a self–contained proof of the known fact that the $\mathbb{T}$–orbit space is the region of orthogonality for the generalized Chebyshev polynomials of both the first and second kind. The orthogonalizing measure is given explicitly.

1 Orthogonality of Chebyshev polynomials

Classical Fourier analysis studies the approximation of functions with trigonometric polynomials, going back to the work of Jean–Baptiste Fourier (1768–1830). In the discrete univariate case, this means to consider maps $u \mapsto \exp(-2\pi \mathrm{i}\, \ell\, u)$ with $u \in \mathbb{R}$ and $\ell \in \mathbb{Z}$, arising for example as eigenfunctions of the Laplace operator. Generalizations of such functions are of relevance in signal processing and sampling theory on compact domains, see for example [Mar91]. Multivariate Fourier analysis on compact domains was investigated in several works. Koornwinder showed for dimension 2 in [Koo74] the orthogonality of a family of polynomials, which fits in the context of generalized Chebyshev polynomials. The periodicity domain is a hexagon, which is transformed into the orthogonality region of the Koornwinder polynomials. Furthermore, the hexagonal domain has been studied in [Pin85, LSX08]. Generalizing these cases, discrete Fourier analysis on the periodicity domain of the A_{n-1} lattice was conducted in [LX10], giving a cubature formula on the associated $\mathbb{T}$–orbit space, see Figure 2.1.

Multivariate generalizations of cosine and sine functions, as well as related orthogonal polynomials, are known in Fourier analysis since the works of Nicholson [Nic71], Koornwinder [Koo74] and Winograd [Win76].

In a more general context, [MKNR12] introduces Fourier analysis on the periodicity regions of Abelian groups. This fits in our framework of coroot lattices Λ, which form a semi–direct product with Weyl groups $\mathcal{W}$ of crystallographic root systems. We have introduced this product as the affine Weyl group. In this chapter, we give a detailed proof of [MKNR12, Equation 1.40], which states that the $\mathbb{T}$–orbit space is the region of orthogonality for the generalized Chebyshev polynomials. The proof is independent from that given in [HW88, Theorem 5.1] and comes naturally with a study of the $\mathbb{T}$–orbit space, for which we conjecture a characterization closer to that in [PS85].

1.1 Euler derivations

In this section, we consider the general case of a finite group $\mathcal{G}$ with an integer representation $\mathcal{G}$. This fits in the context of our theory established in the first section of Chapter 2. $\mathcal{G}$ has a nonlinear action on the algebraic torus, which induces a linear action on the ring of Laurent polynomials, see Equation (1.15) and Equation (1.16). Assume that the ring of invariants is $\mathbb{R}[x^\pm]^\mathcal{G} = \mathbb{R}[\theta_1, \ldots, \theta_m]$ for some $m \in \mathbb{N}$. We do not require the θ_i to be algebraically independent.

Definition B.1. *On $\mathbb{R}[x^\pm]$, define the **Euler derivation** $x_i\, \partial/\partial x_i$ with $x_i\, \partial/\partial x_i(x_i) = x_i$ and $x_i\, \partial/\partial x_i(x_j) = 0$ for $1 \leq i \neq j \leq n$ as well as the associated gradient $\tilde{\nabla} := [x_1\, \partial/\partial x_1, \ldots, x_n\, \partial/\partial x_n]^t$.*

We fix a symmetric positive definite matrix $S \in \mathbb{R}^{n\times n}$ with $B^t\, S\, B = S$ for all $B \in \mathcal{G}$. For example, $S = 1/|\mathcal{G}| \sum_{B\in\mathcal{G}} B^t\, B$ has the desired property. We write $\langle\cdot,\cdot\rangle_S$ for the S–induced $\mathcal{G}$–invariant inner product.

Proposition B.2. *Let $f, f' \in \mathbb{R}[x^\pm]^\mathcal{G}$.*

1. *For all $B \in \mathcal{G}$, $B(\tilde{\nabla}\, f)(x^B) = \tilde{\nabla}\, f(x)$.*
2. *We have $\langle \tilde{\nabla}\, f, \tilde{\nabla}\, f'\rangle_S = (\tilde{\nabla}\, f)^t\, S\, (\tilde{\nabla}\, f') \in \mathbb{R}[x^\pm]^\mathcal{G}$.*

Proof. We obtain the first statement from

$$\tilde{\nabla}\, f(x) = \tilde{\nabla}\,(B\cdot f)(x) = B\left(x^{B_{\cdot 1}}\frac{\partial f}{\partial x_1}(x^B), \ldots, x^{B_{\cdot n}}\frac{\partial f}{\partial x_n}(x^B)\right) = B(\tilde{\nabla}\, f)(x^B),$$

where we applied the $\mathcal{G}$–invariance of f and then the chain rule. Therefore,

$$\begin{aligned}(B\cdot((\tilde{\nabla}\, f)^t\, S\,(\tilde{\nabla}\, f')))(x) &= ((\tilde{\nabla}\, f)(x^B))^t\, S\,((\tilde{\nabla}\, f')(x^B))\\ &= (B^{-1}\,\tilde{\nabla}\, f(x))^t\, S\,(B^{-1}\,\tilde{\nabla}\, f'(x))\\ &= (\tilde{\nabla}\, f(x))^t\,(B^{-1})^t\, S\, B^{-1}\,(\tilde{\nabla}\, f'(x))\\ &= ((\tilde{\nabla}\, f)^t\, S\,(\tilde{\nabla}\, f'))(x)\end{aligned}$$

proves the second statement. □

For $f \in \mathbb{R}[x^{\pm}]$, define $\widehat{f} \in \mathbb{R}[x^{\pm}]$ by $\widehat{f}(x) = f(x^{-I_n})$.

Proposition B.3. *Let $f \in \mathbb{R}[x^{\pm}]$. The following statements hold.*

1. *We have $\tilde{\nabla}\,\widehat{f}(x) = -\widehat{(\tilde{\nabla} f)}(x)$.*
2. *If $f \in \mathbb{R}[x^{\pm}]^{\mathcal{G}}$, then $\widehat{f} \in \mathbb{R}[x^{\pm}]^{\mathcal{G}}$.*

Proof. By the chain rule, we have

$$\tilde{\nabla}\,\widehat{f}(x) = -\left(x^{(-I_n)_{\cdot 1}} \frac{\partial f}{\partial x_1}(x^{-I_n}), \ldots, x^{(-I_n)_{\cdot n}} \frac{\partial f}{\partial x_n}(x^{-I_n}) \right) = -(\tilde{\nabla} f)(x^{-I_n}) = -\widehat{(\tilde{\nabla}\, f)}(x).$$

Furthermore for all $B \in \mathcal{G}$, $(B \cdot \widehat{f})(x) = \widehat{f}(x^B) = f(x^{-B}) = f(x^{-I_n}) = \widehat{f}(x)$. □

Proposition B.4. *For $f \in \mathbb{R}[x^{\pm}]^{\mathcal{G}}$ and $x \in \mathbb{T}^n$, $\langle \tilde{\nabla}\, f, \tilde{\nabla}\, \widehat{f} \rangle_S(x) \leq 0$.*

Proof. By Proposition B.3, we have

$$\langle \tilde{\nabla}\, f, \tilde{\nabla}\, \widehat{f} \rangle_S(x) = -(\tilde{\nabla}\, f(x))^t\, S\, (\widehat{(\tilde{\nabla}\, f)}(x)) = -(\tilde{\nabla}\, f(x))^t\, S\, ((\tilde{\nabla}\, f)(x^{-I_n})).$$

Since $x \in \mathbb{T}^n$, $\overline{x} = (\overline{x}_1, \ldots, \overline{x}_n) = (x_1^{-1}, \ldots, x_n^{-1}) = x^{-I_n}$ and thus,

$$\langle \tilde{\nabla}\, f, \tilde{\nabla}\, \widehat{f} \rangle_S(x) = -(\tilde{\nabla}\, f(x))^t\, S\, ((\tilde{\nabla}\, f)(\overline{x})) = -(\tilde{\nabla}\, f(x))^t\, S\, (\overline{\tilde{\nabla}\, f(x)}) \leq 0$$

completes the proof. □

We can now state a necessary condition for points in $\mathbb{C}^n$ to be contained in the $\mathbb{T}$–orbit space of $\mathcal{G}$ given by the image of $\mathbb{T}^n$ under ϑ.

Proposition B.5. *Define the matrix $\tilde{M} \in (\mathbb{R}[x^{\pm}]^{\mathcal{G}})^{m \times m}$ with entries $\tilde{M}_{ij} = \langle \tilde{\nabla}\, \theta_i, \tilde{\nabla}\, \widehat{\theta}_j \rangle_S$. For $x \in \mathbb{T}^n$, $\tilde{M}(x)$ is Hermitian negative semi–definite.*

Proof. Let $J := [\tilde{\nabla}\, \theta_1 \mid \ldots \mid \tilde{\nabla}\, \theta_m]$ be the Jacobian transpose of ϑ with respect to the Euler derivations and assume that $S = C^t\, C$ is the Cholesky decomposition of S for an upper triangular matrix $C \in \mathbb{R}^{n \times n}$. We write $\tilde{M}(x) = J(x)^t\, S\, \widehat{J}(x)$. Since $x \in \mathbb{T}^n$, $\overline{x} = x^{-I_n}$ and consequently $\widehat{J}(x) = -\overline{J(x)}$. Then

$$\tilde{M}(x) = J(x)^t\, C^t\, C\, J(x) = -(C\, J(x)^t\, (\overline{C\, J(x)})$$

is Hermitian negative semi–definite. □

The following characterization is similar to the one in [PS85] with the invariant inner product made explicit for nonlinear actions.

Conjecture B.6. *Let $M \in (\mathbb{R}[z_1, \ldots, z_m])^{m \times m}$, such that $\tilde{M}(x) = M(\theta_1(x), \ldots, \theta_m(x))$. Furthermore, let $\mathcal{I} \subseteq \mathbb{R}[z]$ be the ideal of relations among the $\theta_1, \ldots, \theta_m$ and denote by $\mathcal{V} \subseteq \mathbb{C}^m$ the variety of $\mathcal{I}$.*

If $z \in \mathcal{V}(\mathcal{I})$ is such that $M(z)$ is Hermitian negative semi–definite, then $z \in \mathcal{T}$.

1.2 Proof of orthogonality

Assume that $\mathcal{W}$ is the Weyl group of a root system R in $\mathbb{R}^n$, reduced and crystallographic as in Definition 1.1, but not necessarily irreducible. $\mathbb{R}^n$ is equipped with the Euclidean scalar product $\langle\cdot,\cdot\rangle$ and $\mathcal{W}$ is the subgroup of the orthogonal matrix group $\mathrm{O}_n(\mathbb{R})$, which is generated by orthogonal reflections s_ρ for $\rho \in \mathrm{R}$. The integer representation of $\mathcal{W}$ is denoted by $\mathcal{G}$ as in Equation (1.14).

Recall the definition of the $\mathcal{G}$–invariant and anti–invariant orbit polynomials Θ_α from Definition 1.24 and Υ_α from Definition 1.26.

Lemma B.7. *Let $\delta := [1,\ldots,1]^t \in \mathbb{N}^n$. For $x \in \mathbb{T}^n$, we have $(\Upsilon_\delta(x))^2 \in \mathbb{R}$.*

Proof. Recall from Proposition 2.6 that there exist $A \in \mathcal{W}$ and a permutation $\sigma \in \mathfrak{S}_n$, such that, for all $1 \leq i \leq n$, we have $A\omega_i = -\omega_{\sigma(i)}$. Then

$$-W\delta = -\omega_0 = -\sum_{i=1}^{n}\omega_i = \sum_{i=1}^{n} -\omega_{\sigma(i)} = A\sum_{i=1}^{n}\omega_i = A\omega_0 = A\,W\delta$$

and thus $\Upsilon_{-\delta}(x) = \mathrm{Det}(A)\,\Upsilon_\delta(x)$. Especially, for $x \in \mathbb{T}^n$, $\Upsilon_\delta(x)$ is either real or imaginary and so its square is real. □

We shall now prove that $\mathcal{T}$ is the domain of orthogonality of the generalized Chebyshev polynomials of the first and second kind and show that the weight function can be given in terms of Υ_δ.

Proposition B.8. *Let $J := [\tilde{\nabla}\,\theta_1|\ldots|\tilde{\nabla}\,\theta_n] \in (\mathbb{R}[x^\pm])^{n\times n}$. Then $\mathrm{Det}(J) \in \mathbb{R}[x^\pm]$ is anti–invariant with*

$$|\mathcal{G}|^n\,\mathrm{Det}(J) = \prod_{i=1}^{n}|\mathrm{Stab}_{\mathcal{G}}(e_i)|\,\Upsilon_\delta.$$

Proof. By Proposition B.2, we have $J(x^B) = B\,J(x)$ for any $B \in \mathcal{G}$. Hence, $\mathrm{Det}(J)$ is anti–invariant in $\mathbb{R}[x^\pm]$ and thus there exists a unique $f \in \mathbb{R}[x^\pm]^{\mathcal{G}}$, such that $\mathrm{Det}(J) = f\,\Upsilon_\delta$. We show that x^δ is the highest monomial of $\mathrm{Det}(J)$ in the partial ordering given by positive roots. We have

$$J_{ij} = (\tilde{\nabla}\,\theta_1|\ldots|\tilde{\nabla}\,\theta_n)_{ij} = x_i\,\partial/\partial x_i\,\theta_j = \frac{|\mathrm{Stab}_{\mathcal{G}}(e_j)|}{|\mathcal{G}|}\,x_i\,\frac{\partial}{\partial\,x_i}\sum_{\alpha\in\mathcal{G}\,e_j} x^\alpha = \frac{|\mathrm{Stab}_{\mathcal{G}}(e_j)|}{|\mathcal{G}|}\,x_i\,\frac{\partial}{\partial\,x_i}\left(x_j + \sum_{\alpha\prec e_j} c_\alpha\,x^\alpha\right),$$

where $c_\alpha \in \{0,1\}$ and $\alpha \prec e_j$ if and only if $0 \neq W(e_i-\alpha)$ is a sum of positive roots. The diagonal elements of the matrix J have highest monomial x_i, while the non–diagonal entries have highest monomial x^α for some $\alpha \prec e_j$. It follows that there exist coefficients $c_\alpha \in \mathbb{N}$, such that

$$f\,\Upsilon_\delta = \mathrm{Det}(J) = \frac{\prod\limits_{i=1}^{n}|\mathrm{Stab}_{\mathcal{G}}(e_i)|}{|\mathcal{G}|^n}\left(x_1\ldots x_n + \sum_{\alpha\prec\delta} c_\alpha\,x^\alpha\right) = \frac{\prod\limits_{i=1}^{n}|\mathrm{Stab}_{\mathcal{G}}(e_i)|}{|\mathcal{G}|^n}\left(x^\delta + \sum_{\alpha\prec\delta} c_\alpha\,x^\alpha\right)$$

and f is the coefficient of x^δ in the determinant. □

On the set of square integrable functions on $\mathcal{W}\triangle$ with basis $\{\mathfrak{e}^\mu\,|\,\mu \in \Omega\}$, we define the gradient $\nabla := (\partial/\partial u_1,\ldots,\partial/\partial u_n)$. The relation to the gradient of Euler derivations $\tilde{\nabla}$ is the following statement.

Proposition B.9. *Let $J = [\tilde{\nabla}\,\theta_1|\ldots|\tilde{\nabla}\,\theta_n] \in \mathbb{R}[x^\pm]^{n\times n}$. Then*

$$[\nabla\,\mathfrak{c}_{\omega_1}|\ldots|\nabla\,\mathfrak{c}_{\omega_n}](u) = 2\pi\mathrm{i}\,W\,J(\mathfrak{e}^{\omega_1}(u),\ldots,\mathfrak{e}^{\omega_n}(u)).$$

Proof. A straightforward computation from the definition shows

$$\begin{aligned}[\nabla\,\mathfrak{c}_{\omega_1}|\dots|\nabla\,\mathfrak{c}_{\omega_n}]_{ij}(u) &= \frac{\partial \mathfrak{c}_{\omega_j}}{\partial u_i}(u) = 2\pi\mathrm{i}\sum_{k=1}^{n}(\omega_k)_i\,x_k\,\frac{\partial\,\theta_j}{\partial x_k}(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u))\\ &= 2\pi\mathrm{i}\sum_{k=1}^{n}W_{ik}\,J_{kj}(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u)) = 2\pi\mathrm{i}(W\,J(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u)))_{ij}.\end{aligned}$$

□

The generalized Chebyshev polynomials satisfy the following orthogonality property.

Theorem B.10. *For $\alpha,\beta\in\mathbb{N}^n$,*

$$\begin{aligned}\int_{\mathcal{T}} T_\alpha(z)\,\overline{T_\beta(z)}\,|\phi(z)|^{-1/2}\,\mathrm{d}z &= \begin{cases}2\pi\,|\mathrm{Det}(W)|\,\prod\limits_{i=1}^{n}|\mathcal{G}\,e_i|\,\dfrac{\mathrm{Vol}(\triangle)\,|\mathrm{Stab}_{\mathcal{G}}(\alpha)|}{|\mathcal{G}|}, & \textit{if } \alpha=\beta\\ 0, & \textit{otherwise}\end{cases}\\ \textit{and}\quad \int_{\mathcal{T}} U_\alpha(z)\,\overline{U_\beta(z)}\,|\phi(z)|^{1/2}\,\mathrm{d}z &= \begin{cases}2\pi\,|\mathrm{Det}(W)|\,\dfrac{\mathrm{Vol}(\triangle)}{|\mathcal{G}|}, & \textit{if } \alpha=\beta\\ 0, & \textit{otherwise}\end{cases},\end{aligned}$$

where the weight function is defined via

$$\phi(\theta_1,\dots,\theta_n) = (\Upsilon_\delta)^2 \in \mathbb{R}[x^{\pm}]^{\mathcal{G}}$$

with $\delta=[1,\dots,1]^t\in\mathbb{Z}^n$.

Proof. Set $\mu := W\alpha$ and $\nu := W\beta =\in \Omega$. By Lemma 3.4 and the definition of generalized Chebyshev polynomials of the first kind, we can conduct the transformation

$$\begin{aligned}\int_{\mathcal{T}} T_\alpha(z)\,\overline{T_\beta(z)}\,|\phi(z)|^{-1/2}\,\mathrm{d}z &= \int_{\triangle}\mathfrak{c}_\mu(u)\,\overline{\mathfrak{c}_\nu}(u)\,\frac{|\mathrm{Det}([\nabla\,\mathfrak{c}_{\omega_1}|\dots|\nabla\,\mathfrak{c}_{\omega_n}]\,(u))|}{|\Upsilon_\delta(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u))|}\,\mathrm{d}u\\ &= \int_{\triangle}\mathfrak{c}_\mu(u)\,\overline{\mathfrak{c}_\nu}(u)\,\frac{|\mathcal{G}|^n}{\prod\limits_{i=1}^{n}|\mathrm{Stab}_{\mathcal{G}}(e_i)|}\,\frac{|2\pi\mathrm{i}\,\mathrm{Det}(W)\,\mathrm{Det}(J)|}{|\mathrm{Det}(J)|}(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u))\,\mathrm{d}u\\ &= \prod_{i=1}^{n}|\mathcal{G}\,e_i|\,|2\pi\mathrm{i}\,\mathrm{Det}(W)|\,\int_{\triangle}\mathfrak{c}_\mu(u)\,\overline{\mathfrak{c}_\nu}(u)\,\mathrm{d}u.\end{aligned}$$

According to Remark 3.6,

$$\int_{\mathcal{T}} T_\alpha(z)\,\overline{T_\beta(z)}\,(\phi(z))^{-1/2}\mathrm{d}z = 2\pi\,|\mathrm{Det}(W)|\,\prod_{i=1}^{n}|\mathcal{G}\,e_i|\,\mathrm{Vol}(\triangle)\,\frac{|\mathrm{Stab}_{\mathcal{G}}(\alpha)|}{|\mathcal{G}|}$$

if $\mu\in\mathcal{W}\,\nu$ and 0 otherwise.

The result on generalized Chebyshev polynomials of the second kind is analogous with

$$U_\alpha(\mathfrak{c}(u))\,\overline{U_\beta(\mathfrak{c}(u))} = \frac{\mathfrak{s}_{\mu+\omega_0}}{\mathfrak{s}_{\omega_0}}(u)\,\frac{\overline{\mathfrak{s}_{\nu+\omega_0}}}{\overline{\mathfrak{s}_{\omega_0}}}(u) = \frac{\mathfrak{s}_{\mu+\omega_0}(u)\,\overline{\mathfrak{s}_{\nu+\omega_0}(u)}}{|\Upsilon_\delta(\mathfrak{e}^{\omega_1}(u),\dots,\mathfrak{e}^{\omega_n}(u))|^2}$$

and then applying Remark 3.6. □

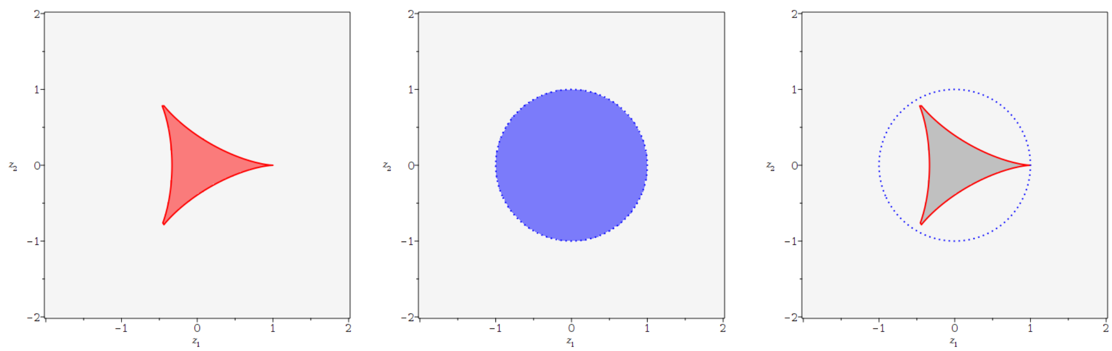
2 Examples

We compare the Hermite matrix polynomial P from Chapter 2 with the matrix M from Conjecture B.6.

2.1 P versus M

For A_2, let $z = (z_1 + \mathrm{i}\, z_2, z_1 - \mathrm{i}\, z_2) \in \mathbb{C}^2$. Then

$$M(z) = \frac{2}{3}\begin{bmatrix} z_1^2 + z_2^2 - 1 & 2\,(z_1 + \mathrm{i}\, z_2)^2 - 2\,(z_1 - \mathrm{i}\, z_2) \\ 2\,(z_1 - \mathrm{i}\, z_2)^2 - 2\,(z_1 + \mathrm{i}\, z_2) & z_1^2 + z_2^2 - 1 \end{bmatrix}.$$



(a) $\mathrm{Det}(-M(z)) \geq 0$ (b) $\mathrm{Trace}(-M(z)) \geq 0$ (c) $M(z) \preceq 0$

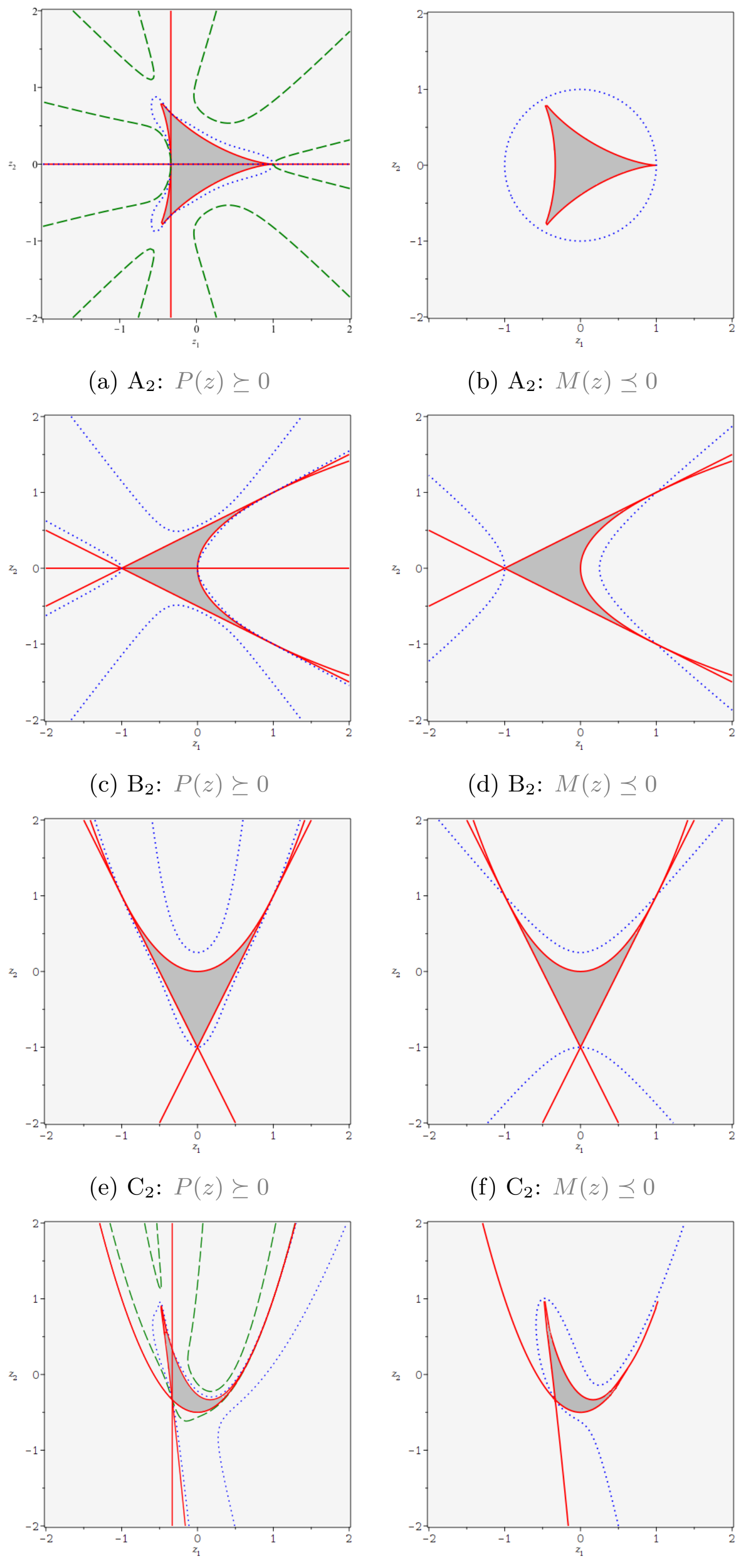
Figure B.1: Vanishing points and positivity regions for determinant and trace of $M(z)$ in the case A_2.

With $g_1(z) := z_1^2 + z_2^2$ and $g_2(z) := z_1\,(z_1^2 - 3\,z_2^2)$ as in the case of P, we observe a $\mathfrak{D}_3$–invariance

$$\begin{aligned} \mathrm{Det}(-M(z)) &= 1/9\,(-12\,z_1^4 - 24\,z_1^2\,z_2^2 - 12\,z_2^4 + 32\,z_1^3 - 96\,z_1\,z_2^2 - 24\,z_1^2 - 24\,z_2^2 + 4) && \text{(solid)} \\ &= 4/9\,(-3\,g_1(z)^2 - 6\,g_1(z) + 8\,g_2(z) + 1), \\ \mathrm{Trace}(-M(z)) &= 4/3\,(-z_1^2 - z_2^2 + 1) = 4/3\,(-g_1(z) + 1). && \text{(dots)} \end{aligned}$$

In further examples, the determinant of $-M$ divides that of P. Indeed, there exists a constant $c = c(\mathrm{R}) > 0$ with

$$\mathrm{Det}(P(z)) = c\,\mathrm{Det}(-M(z)) \begin{cases} (3\,z_1+1)^2\,z_2^4, & \text{if} \quad \mathrm{R} = \mathrm{A}_2 \\ z_2^2, & \text{if} \quad \mathrm{R} = \mathrm{B}_2 \\ 1, & \text{if} \quad \mathrm{R} = \mathrm{C}_2 \\ (-3\,z_1^2 + 2\,z_2 + 1)\,(3\,z_1+1)^2, & \text{if} \quad \mathrm{R} = \mathrm{G}_2 \\ (4\,z_1 + 1 + 3\,z_2)^2\,(4\,z_1 - 1 - 3\,z_2)^2\,z_3^4, & \text{if} \quad \mathrm{R} = \mathrm{A}_3 \\ z_3^2, & \text{if} \quad \mathrm{R} = \mathrm{B}_3 \\ 1, & \text{if} \quad \mathrm{R} = \mathrm{C}_3 \\ z_4^2 & \text{if} \quad \mathrm{R} = \mathrm{B}_4 \\ 1, & \text{if} \quad \mathrm{R} = \mathrm{C}_4 \\ (z_3 - z_4)^2\,(z_3 + z_4)^2 & \text{if} \quad \mathrm{R} = \mathrm{D}_4 \end{cases}.$$



(a) A_2: $P(z) \succeq 0$ (b) A_2: $M(z) \preceq 0$

(c) B_2: $P(z) \succeq 0$ (d) B_2: $M(z) \preceq 0$

(e) C_2: $P(z) \succeq 0$ (f) C_2: $M(z) \preceq 0$

(g) G_2: $P(z) \succeq 0$ (h) G_2: $M(z) \preceq 0$

Figure B.2: The regions "$P(z) \succeq 0$" and "$M(z) \preceq 0$".

2.2 Weight function

We study the weight function from Theorem B.10. In Conjecture B.6, we define $\tilde{M} = J^t\, S\, \widehat{J} \in (\mathbb{R}[x^{\pm}]^{\mathcal{G}})^{m\times m}$ to give the equations of the $\mathbb{T}$–orbit space. According to Proposition 2.6 in the present case of Weyl groups, the fundamental invariants $\theta_1,\ldots,\theta_n$ are such that there exists a permutation $\sigma \in \mathfrak{S}_n$ with $\widehat{\theta_i} = \theta_{\sigma(i)}$. Hence, $\mathrm{Det}(\widehat{J}) = \mathrm{sgn}(\sigma)\,\mathrm{Det}(J)$ and thus the determinant of the matrix M from Conjecture B.6 is a scalar multiple of the weight function from Theorem B.10 in $\mathbb{R}[z]$.

1. In the univariate case A_1, we have $\mathcal{T} = [-1,1]$ and the Weyl denominator is $\Upsilon_\delta = x - x^{-1}$. Therefore,

$$(\Upsilon_\delta)^2 = x^2 - 2 + x^{-2} = 2\,T_2\left(\frac{x+x^{-1}}{2}\right) - 2\,T_0\left(\frac{x+x^{-1}}{2}\right) = 4\,T_1\left(\frac{x+x^{-1}}{2}\right)^2 - 4\,T_0\left(\frac{x+x^{-1}}{2}\right)$$

and $\phi(z) = 4\,(z^2-1)$.

2. For A_2, $\mathcal{T}$ is the compact basic semi–algebraic set in Figure 2.3 and

$$\begin{array}{rcl}(\Upsilon_\delta)^2 & = & \left(-x_1\,x_2 - x_1/x_2^2 - x_2/x_1^2 + 1/(x_1\ x_2) + x_1^2/x_2 + x_2^2/x_1\right)^2 \\ & = & 6\,\Theta_{22} - 6\,\Theta_{30} - 6\,\Theta_{03} + 12\,\Theta_{11} - 6.\end{array}$$

We have $\phi(z) = 81\,z_1^2\,z_2^2 - 108\,z_1^3 - 108\,z_2^3 + 162\,z_1\,z_2 - 27 = 243/3\,\mathrm{Det}(M)$.

3. For B_2, $\mathcal{T}$ is the compact basic semi–algebraic set in Figure 2.7 and

$$\begin{array}{rcl}(\Upsilon_\delta)^2 & = & \left(-x_1/x_2^3 - x_2/x_1^2 + 1/(x_1\,x_2) + x_1^2/x_2^3 + x_2^3/x_1^2 - x_1^2/x_2 - x_2^3/x_1 + x_1\,x_2\right)^2 \\ & = & -8\,\Theta_{04} - 8\,\Theta_{30} + 8\,\Theta_{22} + 16\,\Theta_{12} - 8\,\Theta_{02} - 8\,\Theta_{10} + 8.\end{array}$$

We have $\phi(z) = 256\,z_1^2\,z_2^2 - 1024\,z_2^4 - 256\,z_1^3 + 1536\,z_1\,z_2^2 - 512\,z_1^2 + 256\,z_2^2 - 256\,z_1 = 1024/9\,\mathrm{Det}(M)$.

4. For C_2, $\mathcal{T}$ is the compact basic semi–algebraic set in Figure 2.5 and

$$\begin{array}{rcl}(\Upsilon_\delta)^2 & = & \left(-x_1/x_2^2 - x_2/x_1^3 + 1/(x_1\,x_2) + x_1^3/x_2^2 + x_2^2/x_1^3 - x_1^3/x_2 - x_2^2/x_1 + x_1\,x_2\right)^2 \\ & = & -8\,\Theta_{40} + 8\,\Theta_{22} + 16\,\Theta_{21} - 8\,\Theta_{03} - 8\,\Theta_{20} - 8\,\Theta_{01} + 8.\end{array}$$

We have $\phi(z) = -1024\,z_1^4 + 256\,z_1^2\,z_2^2 + 1536\,z_1^2\,z_2 - 256\,z_2^3 + 256\,z_1^2 - 512\,z_2^2 - 256\,z_2 = 256\,\mathrm{Det}(M)$.

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