Geometric Packings of Non-Spherical Shapes

Inaugural-Dissertation

zur

Erlangung des Doktorgrades

der Mathematisch-Naturwissenschaftlichen Fakultät

der Universität zu Köln

vorgelegt von

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Köln, 2017

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Tag der mündlichen Prüfung: 29.06.2017

Preface

The last four years were an exciting time for me. I gained so much new experience, I learned a lot, and I met many great people. I would like to take the chance to thank those people who supported me during that time the most.

First of all I would like to thank my supervisor Frank Vallentin for everything he did for me. I am glad that he gave me the chance to do my PhD under his supervision and made this thesis possible. I am very thankful for his guidance during my PhD studies, for the introduction into these interesting topics, for fruitful impulses, as well as for helping me to become an independent researcher. Thank you for all your support and that you always had time for me!

Furthermore, I would like to thank my co-authors Cristóbal Guzmán, Stefan Krupp, Fernando Oliveira, Jan Rolfes, and Frank Vallentin. It was fun to work with you. The work with Cristóbal, Fernando, and Frank forms an essential part of my thesis. I would like to thank you for the fruitful discussions and I hope to continue working with you in the future.

Last year, I co-supervised the master thesis of Alexander Pütz. I am happy that we are still working together. Thank you for the great collaboration.

Furthermore, I would like to thank my colleagues Anna Gundert, Frederik von Heymann, Stefan Krupp, and Jan Rolfes for giving me a great time during the last years. In particular, many thanks for your support in the last weeks and for your awesome surprise after I handed in my thesis. I am thankful that I was part of this great group and I am happy to count you as friends. Moreover, I would like to thank little Ida who made working in this group even more enjoyable.

Thank you to Anna Gundert, David de Laat, Frederik von Heymann, Stefan Krupp, Klaus Müller, Jan Rolfes, and Benjamin Schröter for proof-reading parts of my thesis.

Also many thanks to Timo de Wolff for his support, especially, for taking an interest in my research, as well as for giving me helpful feedback.

Moreover, I would like to thank Heinz Schmitz. He was the supervisor of my master thesis as well as one of my collaborators. During my master studies, I was a research assistant and I had the honor to work with him. He enthused me with complexity theory as well as the study of optimization problems. Without him, I might not have chosen this way.

Many thanks to my family and friends who supported me all the time, especially I would like to thank my parents. Finally, I cannot thank enough Klaus for all his support. He encouraged me and helped me not to worry too much. Thank you for always being there for me and making me happy.

Kurzfassung

Der Fokus dieser Arbeit liegt auf geometrischen Packungen dreidimensionaler Körper, die nicht einer Kugel entsprechen. Es ist schwierig die maximale und somit optimale Packungsdichte zu berechnen, daher werden untere und obere Schranken an die optimale Dichte ermittelt. Hierzu werden zwei Spezialfälle geometrischer Packungen betrachtet: translative Packungen und Gitterpackungen.

Wir bestimmen obere Schranken für *translative Packungen*, also Packungen in denen ausschließlich Verschiebungen der Körper und keine Rotationen erlaubt sind. Von Cohn und Elkies stammt ein lineares Programm zur Berechnung solcher oberer Schranken, das durch unendlich viele Bedingungen definiert ist und in dem über eine unendlich-dimensionale Menge zu optimieren ist. Wir relaxieren das Programm zu einem semidefiniten Programm mit endlich vielen Bedingungen, da diese im Allgemeinen effizient lösbar sind. In unseren Berechnungen betrachten wir dreidimensionale konvexe Körper mit Tetraeder- oder Ikosaedersymmetrie. Zur Vereinfachung des resultierenden Programms nutzen wir die Invariantentheorie endlicher Pseudo-Spiegelungsgruppen. Die Lösungen werden mit Hilfe numerischer Berechnungen bestimmt, daher passen wir sie anschließend gegebenfalls an um zulässige Lösungen für das Cohn-Elkies Programm zu erhalten.

Diese Methoden werden unter anderem auf dreidimensionale Superkugeln angewendet, das heißt auf Einheitskugeln bezüglich der ℓ_3^p-Norm. Für $p \in (1, \infty) \setminus \{2\}$ bestimmen wir neue obere Schranken. Darüber hinaus wird mit diesem Verfahren Zong's kürzlich gefundene obere Schranke für die optimale Dichte von translativen Packungen von Tetraeder von $0.3840\ldots$ auf $0.3683\ldots$ verbessert. Somit ist die neue obere Schranke dicht an $0.3673\ldots$, der besten bekannten unteren Schranke.

Im letzten Teil dieser Arbeit werden *Gitterpackungen* von Superkugeln untersucht. Gitterpackungen sind translative Packungen, in denen die Mittelpunkte der Körper ein Gitter bilden. Insbesondere ist die Dichte jeder Gitterpackung also eine untere Schranke für die optimale Dichte translativer Packungen. Mit Hilfe eines Theorems von Minkowski können lokal optimale Gitterpackungen für Superkugeln berechnet werden. Wir berechnen Gitterpackungen für $p \in [1, 8]$ deren Dichte mindestens so groß ist wie die Dichte der bisher besten Gitterpackungen von Jiao, Stillinger und Torquato. Für $p \in (1, 2) \setminus [\log_2 3, 1.6]$ finden wir sogar dichtere Gitterpackungen. Vor allem die oberen Schranken für $p \in [3, 8]$ und die numerischen Resultate für obere Schranken für $p \in [1, \log_2 3]$ befinden sich sehr nah an den unteren Schranken, die wir mit Hilfe der Gitterpackungen bestimmen.

Abstract

The focus of this thesis lies on geometric packings of non-spherical shapes in three-dimensional Euclidean space. Since computing the optimal packing density is difficult, we investigate lower and upper bounds for the optimal value. For this, we consider two special kinds of geometric packings: translative packings and lattice packings.

We study upper bounds for the optimal packing density of *translative packings*. These are packings in which just translations and no rotations of the solids are allowed. Cohn and Elkies determined a linear program for the computation of such upper bounds that is defined by infinitely many inequalities optimizing over an infinite dimensional set. We relax this problem to a semidefinite problem with finitely many constraints, since this kind of problem is efficiently solvable in general. In our computation we consider three-dimensional convex bodies with tetrahedral or icosahedral symmetry. To obtain a program that is not too large for current solvers, we use invariant theory of finite pseudo-reflection groups to simplify the constraints. Since we solve this program by using numerical computations, the solutions might be slightly infeasible. Therefore, we verify the obtained solutions to ensure that they can be made feasible for the Cohn-Elkies program.

With this approach we find new upper bounds for three-dimensional superballs, which are unit balls for the ℓ_3^p norm, for $p \in (1, \infty) \setminus \{2\}$. Furthermore, using our approach, we improve Zong's recent upper bound for the translative packing density of tetrahedra from $0.3840\ldots$ to $0.3683\ldots$, which is very close to the best known lower bound of $0.3673\ldots$.

The last part of this thesis deals with *lattice packings* of superballs. Lattice packings are translative packings in which the centers of the solids form a lattice. Thus, any lattice packing density is in particular a lower bound for the optimal translative packing density. Using a theorem of Minkowski, we compute locally optimal lattice packings for superballs. We obtain lattice packings for $p \in [1, 8]$ whose density is at least as high as the density of the currently best lattice packings provided by Jiao, Stillinger, and Torquato. For $p \in (1, 2) \setminus [\log_2 3, 1.6]$, we even improve these lattice packings. The upper bounds for $p \in [3, 8]$, as well as the numerical results for the upper bounds for $p \in [1, \log_2, 3]$, are remarkably close to the lower bounds we obtain by these lattice packings.

Contents

Chapter One

Introduction and preliminaries

1.1 Packing problems

1.1.1 Introduction

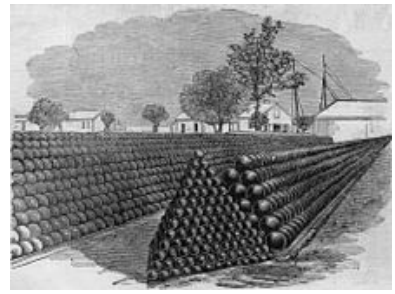


Figure 1.1: Packing of cannonballs [1]

Everyone had probably a situation, where he or she wants to find the best arrangement of some objects. For example, if one wants to put as many cookies on the baking tray as possible. But not just in dimension two there exist packing problems in everyday life. What is the best way to put oranges or table tennis balls into a box? In the 1590th Thomas Hariot had such a problem, too, because Sir Walter Raleigh prompted him to determine a formula for calculating the number of cannonballs in regular stacked piles [43]. Hariot, who was at that time Raleigh's mathematical assistant, investigated also the most efficient way to arrange cannonballs on a ship and was able to find dense configurations. He wrote about this problem to the mathematician and astronomer Johannes Kepler, who asserts in 1611 that the density of any packing of equal-sized spheres into three-dimensional Euclidean space is not greater than $\pi/\sqrt{18} \approx 0.7404\ldots$. This packing density is for example achieved by the packing pictured in Figure 1.3. The problem of finding a densest packing of three-dimensional balls all of the same size is the famous *sphere packing problem*, which is one of the most popular problems in geometric optimization.

Since this problem has infinity many solutions, it is in general hard to find the densest packing or to prove the optimality of a given packing. The examples above show applications for the sphere packing problem in dimension two and three. This problem is not restricted to these two dimensions, since there are also concrete applications for the sphere packing problem in higher dimensions. In dimension one the problem is trivial and for dimension two the problem was solved by the Norwegian mathematician Thue in 1892 [75]. He showed that the *hexagonal packing*, pictured in Figure 1.2, gives a densest packing of

circles. Furthermore, the Hungarian mathematician Fejes Tóth gave a rigorous proof of the optimality in 1940 [33]. Besides the optimality of this packing, he also proved that it is unique up to rotations, uniform scaling, and translations among periodic packings, which we consider in Section 1.1.5. For dimension three, Kepler asserts that there is no packing with a higher density than $\pi/\sqrt{18}$, but it took almost 390 years until this conjecture was proven. Thomas Hales and his PhD student Samuel Ferguson were able to give a computer based proof in 1998 involving more than 5,000 subproblems and using more than 50,000 lines of computer code [43]. Since there are uncountable many optimal solution, proving this conjecture was extremely complicated.

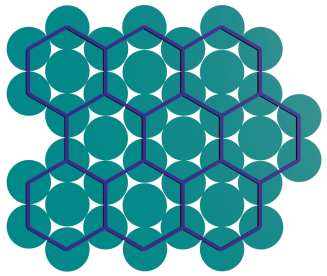


Figure 1.2: Hexagonal packing

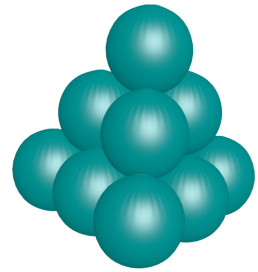


Figure 1.3: Optimal packing of spheres

As mentioned before, there are also applications for the sphere packing problem in higher dimensions. For example the problem of finding an error-correcting code can be formulated as a sphere packing problem in higher dimensions like, for example, in dimension 24 [21]. In 2016, Maryna Viazovska [78] solved the sphere problem in dimension eight and based on this result she was able to solve the sphere packing problem for dimension 24 together with Henry Cohn, Abhinav Kumar, Stephen D. Miller, and Danylo Radchenko [20]. For all other dimensions the sphere packing problem is currently unsolved.

Beside the sphere packing problem, there are also applications for packing problems of non-spherical objects. For example in materials science, it is useful to arrange physical granular material accurately. This problem can be formulated as the packing problem of superballs B_3^p in dimension three. These solids are unit balls for the ℓ_3^p norm, which means $B_3^p = \{x \in \mathbb{R}^3 : \sum_{i=1}^3 |x_i|^p \leq 1\}$. For some values of p the superball is pictured in Figure 1.4.

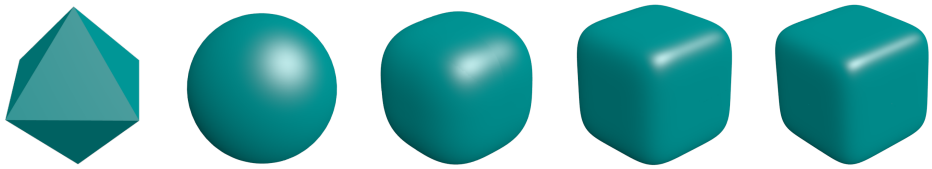


Figure 1.4: Superballs for $p = 1, 2, 3, 5$, and 6

The problem of finding the densest packing of superballs is unsolved for every dimension greater or equal three with $p \notin \{2, \infty\}$. In Chapter 3, upper bounds for the densest packing of superballs in dimension three will be presented. Furthermore, in this thesis we

will also have a look at packing problems of other solids, which are useful, for example, in materials science. In [76], Torquato and Jiao stated:

> Dense packings of hard particles have served as useful models to understand the structure of liquid, glassy and crystal states of matter, granular media, and heterogeneous materials. Understanding the symmetries and other mathematical properties of the densest packings in arbitrary dimensions is a problem of long-standing interest in discrete geometry and number theory.

It is possible to arrange cubes in all dimensions or hexagons in the plane in such a way that the whole space is filled. But, is this also possible for regular tetrahedra in three dimensions? More than 2300 years ago, Aristotle investigated this problem, too, and his answer was: "Among surfaces it is agreed that there are three figures which fill place that contain them - the triangle, the square and the hexagon: among solids only two, the pyramid and the cube" [4, Book III, Chapter VIII, in translation by Guthrie]. Here, by the *pyramid* he refers to the regular tetrahedron, which is one of the five Platonic solids: the tetrahedron, the cube, the octahedron, the dodecahedron, and the icosahedron. Unfortunately, Aristotle was wrong. If we consider a face-to-face arrangement, there is always a gap as pictured in Figure 1.5.

Figure 1.5: Tetrahedra packing

It can also be shown that for other arrangements it is not possible to fill the space with tetrahedra. One of Aristotle's main commentators Simplicius of Cicilia stated that twelve regular tetrahedra fill the space locally around a point [45]. Averroës, who wrote many works on medicine, philosophy and law, commented also on most of the works of Aristotle and gave some arguments to confirm the correctness of Simplicius statement: The sum of the angles between two faces which meet at the same vertex of a cube is $3 \cdot 90° = 270°$. Furthermore, the sum of these angles at a vertex of a tetrahedron is $3 \cdot 60° = 180$. Since $8 \cdot 270 = 12 \cdot 160$ and eight cubes fill space around a point, he concludes that twelve tetrahedra fill space around a point, too.

However, there were still some doubts about this statement and Roger Bacon defended Averroës claim and wrote in [6, Chapter XI, pp. 135-140] that "there is a fool in Paris who says that Averroës was incorrect, twenty pyramids do not fill space around a point. Regiomontanus (Johannes Müller von Königsberg 1436-1476) was the first who disproved the statement of Aristotle's as well as the statement of Averroës. Unfortunately, just the title of his manuscript was published, but there are no doubts that he really disproved these claims in his work. The mathematician and astronomer Francesco Maurolico (1494-1575) corrected Aristotle's statement and showed [57]:

> There exists a tiling of space using regular polyhedra other than the cube: this tiling is a periodic face-to-face tiling using a mixture of regular tetrahedra and regular octahedra having the same side length.

A part of such an arrangement of regular tetrahedra and regular octahedra is pictured in Figure 1.6. Thus, after a long discussion over more than 2000 years it was shown that it is not possible to fill the space just using tetrahedra.

Figure 1.6: Packing of octahedra and tetrahedra

But what is the maximal amount of space which can be filled by tetrahedra? This question was also stated by Hilbert [47] at ICM in 1900 in Paris, where he presented more than twenty open problems. Thus, the new goal was finding the densest packing of tetrahedra. The densest packing, which is known, was found 2010 by Chen, Engel, and Glotzer [17]. They published a construction of a tetrahedra packing with density $4000/4671 = 0.8563\ldots$ Even today, it is not known whether this is the densest packing for tetrahedra. Therefore, it is also interesting to calculate upper bounds. Gravel, Elster, and Kallus proved in 2011 [40] that there is no packing with higher density than $1 - 2.6\ldots \cdot 10^{-25}$.
In 1904, Minkowski states that he found the optimal lattice packing for tetrahedra with density $9/38$. Lattice packings, are packings in which just translations are allowed and the centers of the solids form a lattice. In Section 1.1.2, we give a definition of lattice packings. Minkowski's approach is based on the Minkowski difference $T - T = \{x - y : x, y \in T\}$ of a tetrahedra T. In 1962, Groemer [41] discovered a mistake in Minkowski's work: The Minkowski difference of a tetrahedron with itself is a cuboctahedron, not an octahedron. Furthermore, Groemer gives a construction of a lattice packing for tetrahedra with density $18/49$. In 1970, Hoylman [51] proved that the optimal lattice packing density for tetrahedra is indeed $18/49$. Since lattice packings are in particular translative packings, in which the packing contains just translations of the solid, the obtained optimal lattice packing density gives a lower bound for the optimal translative packing density. For translative packings of tetrahedra Dostert, Guzmán, Oliveira, and Vallentin [30] were able to find an upper bound with $0.3745\ldots$ in 2015 and, thus, they improved the upper bound $0.3840\ldots$ from Zong [80] found in 2014. Moreover in 2017, Pütz [64] determined the best known upper bound with $0.3683\ldots$ based on the approach of Dostert, Guzmán, Oliveira, and Vallentin.
This result leads to the conjecture, that the optimal lattice packing density $18/49 = 0.3673\ldots$ is equal to the optimal translative packing density.

From the new upper bound for the translative packing density of regular tetrahedra, we get directly a new upper bound for the translative packing density of cuboctahedra, too. In

[61], Minkowski showed that

$$\bigcup_{i\in\mathbb{N}} \{x_i + \mathcal{K}\} \text{ is a translative packing of } \mathcal{K}$$

if and only if

$$\bigcup_{i\in\mathbb{N}} \left\{x_i + \frac{1}{2}(\mathcal{K}-\mathcal{K})\right\} \text{ is a translative packing of } \frac{1}{2}(\mathcal{K}-\mathcal{K}),$$

where

$$\mathcal{K}-\mathcal{K} = \{x-y : x, y \in \mathcal{K}\}$$

is the Minkowski difference of $\mathcal{K}$ with itself. The Minkowski difference of a regular tetrahedron with itself is a cuboctahedron whose volume is $2^3 \cdot 5/2$ times larger, thus, we get $0.9208\ldots$ as an upper bound for the translative density of cuboctahedra.

Since more than 2300 years, mathematicians are searching for the densest packing of three-dimensional Platonic solids. Before we define Platonic solids, we give the definition of a polyhedron: A *polyhedron P* is an intersection of finitely many closed half-spaces, that is $P = \{x \in \mathbb{R}^n : Ax \leq b\}$ with $A \in \mathbb{R}^{m\times n}, b \in \mathbb{R}^m$. Platonic and Archimedean solids are special polyhedra. A polyhedron whose faces are all congruent to each other and whose faces are regular polygons, is called a *regular polyhedron* or a *Platonic solid*. If just the second condition holds, then it is called a *semiregular polyhedron* or an *Archimedean solid*.

In Chapter 3, upper bounds for the density of translative packings of three-dimensional convex bodies having tetrahedral symmetry or icosahedral symmetry will be presented. Besides the superballs for $p \in [1,\infty)$, which are invariant under the tetrahedral symmetry, the considered solids are pictured in Figure 1.7. Three-dimensional superballs with $p < 1.0$ are not convex, therefore these solids are not included. In the calculations, we will not consider the cube and the truncated octahedron, since both bodies are space fillers.

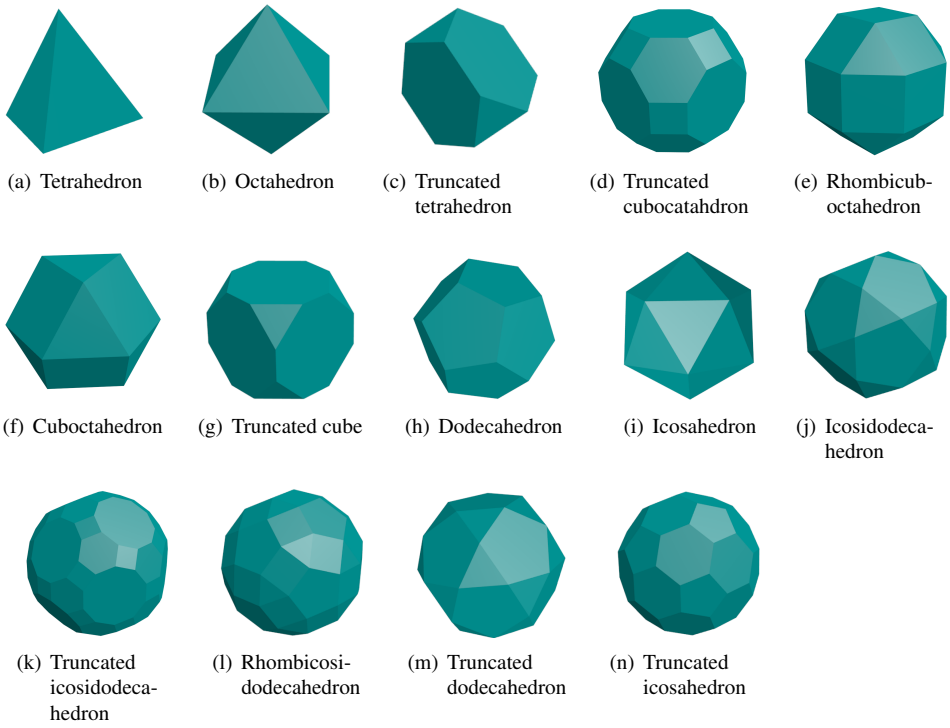
Betke and Henk [9] give a construction for optimal lattice packings for three-dimensional polytopes. Since the corresponding densities are lower bounds for the translative packing density, we compare them to the obtained upper bounds in Chapter 3. For superballs with $p \notin \{1, 2, \infty\}$, which are no polytopes, the optimal lattice packing density in not known. In Chapter 4, we give a construction for lattice packings of superballs and provide new lower bounds for $p \in (1,2) \setminus [\log_2 3, 1.6]$.

1.1.2 Packings and density

For the classical sphere packing problem, we do not have to care about rotations of the spheres, because they are invariant under rotations. For considering packings of non-spherical objects, the difficulty of the problem depends, among others, on the question whether rotations of the objects in the packings are allowed or not. Therefore, it makes sense to distinguish between different kinds of packings.

The most general packing is the *congruent packing*:

$$\mathcal{P} = \bigcup_{i\in\mathbb{N}} (x_i + A_i\mathcal{K}), \quad \text{with } (x_i, A_i) \in \mathbb{R}^n \times \mathrm{SO}(n), i \in \mathbb{N},$$



(a) Tetrahedron (b) Octahedron (c) Truncated tetrahedron (d) Truncated cubocatahdron (e) Rhombicub-octahedron

(f) Cuboctahedron (g) Truncated cube (h) Dodecahedron (i) Icosahedron (j) Icosidodeca-hedron

(k) Truncated icosidodeca-hedron (l) Rhombicosi-dodecahedron (m) Truncated dodecahedron (n) Truncated icosahedron

Figure 1.7: Platonic and Archimedean solids having tetrahedral symmetry (a)-(g) or icosahedral symmetry (h)-(n), except of the cube and the truncated octahedron.

where $x_i + A_i\mathcal{K}^\circ \cap x_j + A_j\mathcal{K}^\circ = \emptyset$ whenever $i \neq j$. With $\mathcal{K}^\circ$ we denote the topological interior and $\mathrm{SO}(n)$ is defined as

$$\mathrm{SO}(n) = \{A \in \mathbb{R}^{n\times n} : AA^\mathsf{T} = I_n,\ \det A = 1\},$$

a subgroup of the *orthogonal group*

$$\mathrm{O}(n) = \{A \in \mathbb{R}^{n\times n} : AA^\mathsf{T} = I_n\}.$$

The intersection above has to be empty to make sure that the objects in the packing will not intersect in their interior. Such packings contain congruent copies of $\mathcal{K}$, that means translations and rotations are allowed. The (upper) *density of a congruent packing* $\mathcal{P}$ is given by

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

where $B(c,r)$ is the Euclidean ball with center $c \in \mathbb{R}^n$ and radius $r \in \mathbb{R}_{>0}$. The *congruent packing density* of a solid $\mathcal{K}$ is the maximal density over all congruent packings.

Because of the freedom of congruent packings, finding a densest one is very difficult and there are no efficient methods known yet. For solving this problem it is therefore

common to consider packings, which are more restrictive and better studied. *Translative packings* are congruent packings, where just translations of the solid are allowed. This means A_i has to be the identity and, thus, translative packings are defined as

$$\mathcal{P} = \bigcup_{i \in \mathbb{N}} (x_i + \mathcal{K}), \quad \text{with } x_i \in \mathbb{R}^n, i \in \mathbb{N},$$

where $x_i + \mathcal{K}^\circ \cap x_j + \mathcal{K}^\circ = \emptyset$ whenever $i \neq j$. If we restrict the set of x_i to form a lattice, which we will define in the next chapter, then this packing is called a *lattice packing*. This kind of packings is very restrictive, but it is well studied and many results are known. Packing problems are in general very difficult to solve, therefore it is interesting to investigate techniques for calculating lower and upper bounds, which, we hope, are close together.

1.1.3 Lower bounds via lattice packings

The density of each translative packing is less or equal to the maximal translative packing density. Therefore, the density of a translative packing is a lower bound of the maximal density. For calculating a lower bound, we could construct a translative packing and calculate its density. If we consider an arbitrary translative packing, the corresponding density might be much smaller than the optimal density. To be able to find a good approximation of the optimal density, we are interested in constructing a packing with a high density. As mentioned before, lattice packings are well studied and there are many results known. Since a lattice packing is a translative packing with further restrictions, the density of a lattice packing is a lower bound of the maximal density of translative packings. For some solids it is known, that the optimal translative packing density is equal to the optimal lattice packing density, for example for spheres in dimension 2, 3, 8, and 24. Let $b_1, \ldots, b_n \in \mathbb{R}^n$ be linearly independent vectors. The corresponding *lattice* L is then defined by

$$L = \left\{ \sum_{i=1}^{n} \alpha_i b_i : \alpha_i \in \mathbb{Z} \right\}.$$

If we translate copies of a given solid $\mathcal{K}$ at each lattice point $p \in L$, this packing is a *lattice packing* for $\mathcal{K}$ if these solids do not intersect in their interior. For dimension two and three examples for lattice packings are pictured in Figure 1.8.

As mentioned before, in dimension eight the sphere packing problem is solved and an optimal packing with density 0.25367 . . . [21] is given by the E_8-*lattice*, defined by

$$\begin{aligned} E_8 &= \left\{ x \in \mathbb{R}^8 : x \in \mathbb{Z}^8 \cup \left(\frac{1}{2} + \mathbb{Z}\right)^8 \text{ and } \sum_{i=1}^{8} x_i \in 2\,\mathbb{Z} \right\} \\ &= \left\{ \sum_{i=1}^{n} a_i b_i : a_i \in \mathbb{Z} \right\}, \end{aligned}$$

with basis vectors b_i which are written in the columns of the following matrix:

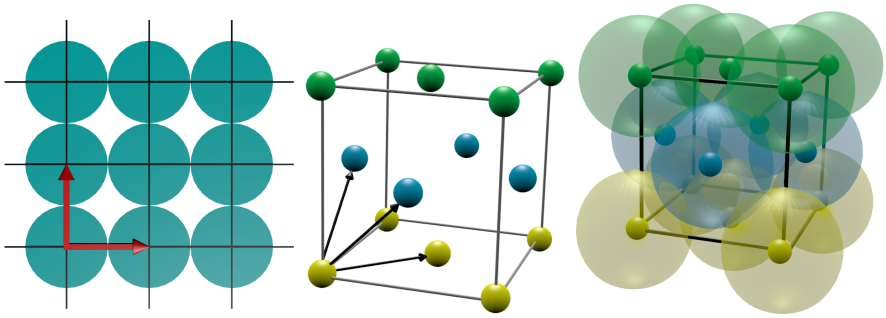


Figure 1.8: Left: Lattice packing in dimension two, Center: Lattice points in dimension three [31], Right: Lattice packing corresponding to lattice in the center [31].

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1/2 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix}.$$

In [61], Minkowski gave a method to calculate an optimal lattice packing for three-dimensional convex bodies. In this approach it is necessary to consider all facets of the given solid $\mathcal{K}$. Betke and Henk calculated optimal lattice packings for three-dimensional convex polytopes by using Minkowski's work. Unfortunately, superballs have infinitely many extreme points for $p \notin \{1, \infty\}$, therefore this algorithm cannot be used for calculating optimal lattice packings for superballs. Minkowski published in [61] also a theorem which characterizes the contacting neighbors in an optimal lattice packing. Based on this, we computed lattice packings for superballs, which will be presented in Chapter 4.

1.1.4 Upper bounds via insphere

For congruent packings of a solid $\mathcal{K}$ in any dimension, Jiao and Torquato published in [76] the following upper bound of the optimal congruent packing density by using the *insphere* of the considered solid $\mathcal{K}$, that is the largest sphere which is entirely contained in $\mathcal{K}$.

Lemma 1.1. *The maximal density of a packing of congruent non-spherical particles $\mathcal{K}$ in dimension d is bounded from above according to the following bound*

$$\delta(P) \leq \min\left[\frac{\operatorname{vol}\mathcal{K}}{\operatorname{vol} S}\alpha, 1\right],$$

where S is the insphere of $\mathcal{K}$, and α is the maximal density of an n-dimensional packing of congruent spheres.

Furthermore, they make this lemma concrete for dimension three, in which the maximal density of the sphere packing, and thus, α is equal to $\pi/\sqrt{18}$. Applying this *insphere method* the obtained upper bound for the congruent packing density of rhombicuboctahedra coincides with the lattice packing density found by Graf, Roij, and Dijkstra [26]. Unfortunately, for the tetrahedron, cube, octahedron, truncated tetrahedron, cuboctahedron, truncated cube, truncated octahedron, and for superballs with $p \leq 1.3$ or $p \geq 2.9628$, the calculated upper bound is equal to one.

1.1.5 Upper bounds via optimization

A powerful technique for computing upper bounds for the maximal density of a packing is given by using linear optimization. For this, we consider a special kind of functions: Let $f : \mathbb{R}^n \to \mathbb{C}$ be a function, such that for all $x \in \mathbb{R}^n$ and for all $\beta \in \mathbb{N}^n$ the derivatives $D^\beta f(x)$ exist, and for all $\alpha, \beta \in \mathbb{N}^n$ the inequality $\sup\{|x^\alpha D^\alpha f(x)| : x \in \mathbb{R}^n\} < \infty$ holds. Such a function is called a *Schwartz function* and the space consisting of Schwartz functions is called the *Schwartz space* and it is denoted by $\mathcal{S}(\mathbb{R}^n)$. Henry Cohn and Noam Elkies published in [19] the following theorem, which can be used to find an upper bound for the packing density.

Theorem 1.2. *Let $\mathcal{K}$ be a convex body in $\mathbb{R}^n$ and let $f \in \mathcal{S}(\mathbb{R}^n)$ be a Schwartz function. Let*

$$\widehat{f}(u) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i u \cdot x}\, dx$$

denote the Fourier transform of f at u. Suppose f satisfies the following conditions

(i) $\widehat{f}(0) \geq \operatorname{vol} \mathcal{K}$,

(ii) f *is of positive type, i.e.* $\widehat{f}(u) \geq 0$ *for every* $u \in \mathbb{R}^n$,

(iii) $f(x) \leq 0$ *whenever* $\mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset$.

Then the density of any packing of translates of $\mathcal{K}$ in $\mathbb{R}^n$ is at most $f(0)$.

A class of more general packings than lattice packings are *periodic packings*. A packing $\mathcal{P}$ is called a periodic packing, if there exists a lattice $L \subseteq \mathbb{R}^n$, which keeps the packing invariant by moving it along the lattice, which means $\mathcal{P} = v + \mathcal{P}$, for all $v \in L$. In other words, the arrangement of the solids in $\mathcal{P}$ repeats at each copy of a fundamental domain as shown in Figure 1.9. In this picture, the basis vectors $v_1, v_2 \in L$ are displayed in red and the centers x_i of the solids contained in one fundamental domain are represented by blue points and labeled in white.

A *translative periodic packing* $\mathcal{P}$ of a solid $\mathcal{K}$ is defined as

$$\mathcal{P} = \bigcup_{v \in L} \bigcup_{i=1}^{m} v + x_i + \mathcal{K}$$

based on a lattice L. Its density is given by

$$\delta(\mathcal{P}) = \frac{m \cdot \operatorname{vol} \mathcal{K}}{\operatorname{vol}(\mathbb{R}^n / L)},$$

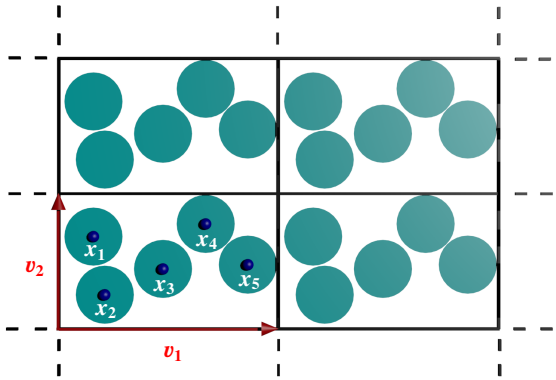


Figure 1.9: Periodic packing

where $\mathrm{vol}(\mathbb{R}^n/L)$ is the volume of a fundamental domain of the lattice $L \subseteq \mathbb{R}^n$. Since the arrangement of the solids in the periodic packing repeats at each fundamental domain, the density of the packing corresponds to the density of the packing in one fundamental domain. In contrast to nonperiodic packings, every periodic packings has a density. Furthermore, the supremum of the upper density of any packing will also be reached by a periodic packing: Let $\delta(\mathcal{P})$ be the upper density of a packing $\mathcal{P}$ and let R be the fundamental domain of any lattice $L \subseteq \mathbb{R}^n$. Moreover, let $\varepsilon > 0$. For a large enough factor r, the total volume of the solids in $\mathcal{P}$ which lie on the boundary of rR is at most $\varepsilon \,\mathrm{vol}\, rR$. Thus, the total volume of solids in $\mathcal{P}$ which lie entirely in rR is at leat $(\delta(\mathcal{P}) - \varepsilon)\,\mathrm{vol}\, rR$. We define a period packing $\mathcal{P}'$ in such a way, that it contains all solids, which lie entirely in rR and all their translations by rL. Then, $\delta(\mathcal{P}') = \delta(\mathcal{P}) - \varepsilon$. Since we can choose ε arbitrary small, the desired property holds. This property is especially useful for the computation of upper bounds for the optimal density of packings, because we can restrict the computation to periodic packings. Furthermore, we use this restriction in the proof of Theorem 1.2.

Proof of Theorem 1.2. Let $\mathcal{K}$ be a convex body in $\mathbb{R}^n$ and let $f \in \mathcal{S}(\mathbb{R}^n)$ be a Schwartz function, which satisfies condition *(i), (ii),* and *(iii)* of Theorem 1.2. We consider the vectors $z = v + x_i - x_j$ with $v \in L$ and $i, j \in [m]$, which are the differences between the centers of two solids in the periodic packing $\mathcal{P}$. The set $\mathcal{K}^\circ \cap (z + \mathcal{K}^\circ)$ is nonempty, whenever $v = 0$ and $x_i = x_j$. Together with condition (*iii*), this implies that the value of $f(z)$ is negative, except in the m cases where $z = 0$. Thus, we get

$$m \,\mathrm{vol}_{\mathcal{K}}\, f(0) \geq \sum_{v \in L} \sum_{i,j=1}^{m} \mathrm{vol}_{\mathcal{K}}\, f(v + x_i - x_j).$$

For the next step, we make use of a result in harmonic analysis. To do so, we introduce the *Poisson summation formula*

$$\sum_{v \in L} f(x + v) = \frac{1}{\mathrm{vol}(\mathbb{R}^n/L)} \sum_{u \in L^*} \hat{f}(u) e^{2\pi i u \cdot x}$$

for all $x \in \mathbb{R}^n$, where the *dual lattice* of L is $L^* = \{u \in \mathbb{R}^n : u \cdot x \in \mathbb{Z} \text{ for all } x \in L\}$. Using the Poisson summation formula the following equation holds

$$\sum_{v \in L} \sum_{i,j=1}^{m} \mathrm{vol}\mathcal{K} f(v + x_i - x_j) = \sum_{u \in L^*} \sum_{i,j=1}^{m} \frac{\mathrm{vol}\mathcal{K}\ \hat{f}(u)\ e^{2\pi i (x_i - x_j)\cdot u}}{\mathrm{vol}(\mathbb{R}^n/L)}.$$

Due to condition *(ii)*, the function $\hat{f}(u)$ is positive for all $u \in \mathbb{R}^n$. Moreover

$$\frac{\mathrm{vol}\mathcal{K}}{\mathrm{vol}(\mathbb{R}^n/L)} \sum_{u \in L^*} \widehat{f}(u) \sum_{i,j=1}^{m} e^{2\pi i (x_i - x_j)\cdot u} = \frac{\mathrm{vol}\mathcal{K}}{\mathrm{vol}(\mathbb{R}^n/L)} \sum_{u \in L^*} \widehat{f}(u) \left| \sum_{i=1}^{m} e^{2\pi i x_i \cdot u} \right|^2,$$

therefore each term of the sum over the dual lattice L^* is nonnegative. Thus, this sum is bounded from below by the term with $u = 0$. Hence, we obtain

$$\frac{\mathrm{vol}\mathcal{K}}{\mathrm{vol}(\mathbb{R}^n/L)} \sum_{u \in L^*} \widehat{f}(u) \sum_{i,j=1}^{m} e^{2\pi i (x_i - x_j)\cdot u} \geq \frac{\mathrm{vol}\mathcal{K}}{\mathrm{vol}(\mathbb{R}^n/L)}\ \hat{f}(0) \left| \sum_{i=1}^{m} e^{0} \right|^2 = \frac{\mathrm{vol}\mathcal{K}}{\mathrm{vol}(\mathbb{R}^n/L)}\ \hat{f}(0)\, m^2.$$

Condition (i), which states $\hat{f}(0) \geq \mathrm{vol}\mathcal{K}$, gives the estimation

$$m^2\ \frac{\mathrm{vol}\mathcal{K}\ \hat{f}(0)}{\mathrm{vol}(\mathbb{R}^n/L)} \geq \frac{(m\ \mathrm{vol}\mathcal{K})^2}{\mathrm{vol}(\mathbb{R}^n/L)},$$

thus, the claim follows

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

□

Due to Theorem 1.2, an upper bound for the translative packing density can be computed by a linear program optimizing over the set of Schwartz functions. In the special case, where the solid $\mathcal{K}$ is a ball, we can use the rotational symmetry of a ball, because $\mathcal{K}$ is invariant under that symmetry. The benefit is that we can restrict the optimization variable f to functions whose values $f(x)$ just depend on the norm $\|x\|$, named *radial functions*, which makes the problem much easier to solve. By using this restriction, Cohn and Elkies were able to calculate upper bounds for the sphere packing problem in dimension 1 to 36 [19]. The sphere packing problem in dimension 8 and in dimension 24 was solved by determining a feasible function f for Theorem 1.2 where $f(0)$ is equal to the lattice packing density of the lattices E_8 and Λ_{24}. The linear program of Theorem 1.2 gives upper bounds for translative packings, but in the case of balls, any congruent packing is a translative packing. Thus, the results are even upper bounds for the maximal density of congruent packings of balls.

For non-spherical objects we cannot restrict f to a radial function, which makes it difficult to solve the program of Cohn and Elkies. In their paper [19] they stated:

> Unfortunately, when [the body we want to pack] is not a sphere, there does not seem to be a good analogue of the reduction to radial functions in Theorem 1.2. That makes these cases somewhat less convenient to deal with.

The first time this theorem is used for calculating upper bounds for non-spherical solids is in the work [30] of Maria Dostert, Cristóbal Guzmán, Fernando Mário de Oliveira Filho, and Frank Vallentin. To make this problem tractable, we formulate the infinite dimensional linear program as a polynomial optimization problem, where we optimize over real polynomials up to a given degree instead of all Schwartz functions. Moreover, we use invariant theory of pseudo-reflection groups in polynomial optimization to obtain a program, which one can solve in practice.

1.2 Outline of the thesis

This thesis is subdivided into four chapters, starting with the introduction. A short description of the other three chapters is given below.

Chapter 2. Techniques.

We give an introduction into convex optimization and especially into semidefinite optimization, which is a special class of convex optimization problems. Semidefinite problems are well studied and in general they can be solved efficiently. A more challenging class of optimization problems are polynomial optimization problems. They are in general NP-hard. Fortunately, there exists techniques to relax these problems to semidefinite problems. We will also have a look at the representation theory of finite groups and how to check whether a polynomial, which is invariant under a finite pseudo-reflection group, is nonnegative.

Chapter 3. New upper bounds for the density of translative packings.

Cohn and Elkies published an infinite dimensional linear program to compute an upper bound for the density of translative packings of convex bodies. As mentioned in Chapter 1, we relax this problem to a polynomial optimization problem. In Chapter 3, we will demonstrate this relaxation in detail and how we further relax the polynomial optimization problem to a solvable semidefinite program. By using this program, we have calculated new upper bounds for the density of translative packings of three-dimensional convex bodies having tetrahedral symmetry or icosahedral symmetry. Since to compute these bounds we applied a numerical semidefinite optimization solver, the results are numerical solutions and, thus, they could be slightly infeasible. Therefore, we will also explain how we can verify the solutions to make sure that these results are rigorous bounds.

Chapter 4. Locally optimal lattice packings of superballs.

We consider the problem of finding an optimal lattice packing for superballs in dimension three. The optimal solution will also be a lower bound for the maximal density of translative packings of superballs. First, we provide a polynomial optimization problem which is based on the work of Minkowski [61]. Unfortunately, we could not solve the polynomial optimization problem using SOS relaxations. In this chapter, we will show how to use the Karush-Kuhn-Tucker-conditions, described in Section 2.1.3, to calculate locally optimal solutions by using Newton's method. Jiao, Stillinger, and Torquato divide the range of

$p \in [1, \infty)$ into four regimes: $[1, \log_2 3], [\log_2 3, 2], [2, 2.3018\ldots], [2.3018\ldots, \infty)$. For each of these regimes, they give a family of lattices [53, 54]. For the first two regimes, we were able to find lattices with a higher packing lattice density. For the other two regimes the best packing lattices we received, are equal to the lattices of Jiao, Stillinger, and Torquato. The density of the lattice packings in the first and last regime are very close to the upper bounds we calculated in Chapter 3. Therefore, we conjecture, that these lattices are optimal.

1.3 New upper bounds for translative packings

We have calculated new upper bounds for three-dimensional convex bodies having tetrahedral or icosahedral symmetry. In the following tables, the best known lower and upper bounds for lattice, translative, and congruent packings of these solids are presented.

Body	Lattice packing	
	lower bound	upper bound
B_3^1	$18/19 = 0.9473\ldots$ [61]	$18/19$ [61]
B_3^2	$\pi/\sqrt{18} = 0.7404\ldots$	$\pi/\sqrt{18}$ [38]
B_3^3	$0.8095\ldots$ [53]	*0.8236...*
B_3^4	$0.8698\ldots$ [53]	*0.8742...*
B_3^5	$0.9080\ldots$ [53]	*0.9224...*
B_3^6	$0.9318\ldots$ [53]	*0.9338...*

Body	Translative packing	
	lower bound	upper bound
B_3^1	$18/19 = 0.9473\ldots$ [61]	*0.9729...*
B_3^2	$\pi/\sqrt{18} = 0.7404\ldots$	$\pi/\sqrt{18}$ [43]
B_3^3	$0.8095\ldots$ [53]	*0.8236...*
B_3^4	$0.8698\ldots$ [53]	*0.8742...*
B_3^5	$0.9080\ldots$ [53]	*0.9224...*
B_3^6	$0.9318\ldots$ [53]	*0.9338...*

Body	Congruent packing	
	lower bound	upper bound
B_3^1	$18/19 = 0.9473\ldots$ [61]	$1 - 1.4\ldots \cdot 10^{-12}$ [40]
B_3^2	$\pi/\sqrt{18} = 0.7404\ldots$	$\pi/\sqrt{18}$ [43]
B_3^3	$0.8095\ldots$ [53]	< 1
B_3^4	$0.8698\ldots$ [53]	< 1
B_3^5	$0.9080\ldots$ [53]	< 1
B_3^6	$0.9318\ldots$ [53]	< 1

Table 1.1: Best known bounds for packings of three-dimensional superballs. Our new bounds are written in italics.

For superballs with $p = 2$, that is round balls, our bound is equal to the bound of Cohn and Elkies. In all other cases, we were able to find a new upper bound. Except for the upper bound for the congruent packing density of superballs with $p \in \{1, 2\}$, there were no upper bounds for translative packing densities known before.

Body	Lattice packing	
	lower bound	upper bound
Tetrahedron	$18/49 = 0.3673\ldots$ [41]	$18/49$ [51]
Truncated tetrahedron	$0.6809\ldots$ [9]	$0.6809\ldots$ [9]
Truncated cuboctahedron	$0.8493\ldots$ [9]	$0.8493\ldots$ [9]
Rhombicuboctahedron	$0.8758\ldots$ [9]	$0.8758\ldots$ [9]
Cuboctahedron	$0.9183\ldots$ [41]	$0.9183\ldots$ [51]
Truncated cube	$0.9737\ldots$ [9]	$0.9737\ldots$ [9]

Body	Translative packing	
	lower bound	upper bound
Tetrahedron	$18/49 = 0.3673\ldots$ [41]	*0.3683...*
Truncated tetrahedron	$0.6809\ldots$ [9]	*0.7170...*
Truncated cuboctahedron	$0.8493\ldots$ [9]	$0.8758\ldots$ [76]
Rhombicuboctahedron	$0.8758\ldots$ [9]	$0.8758\ldots$ [26]
Cuboctahedron	$0.9183\ldots$ [41]	*0.9208...*
Truncated cube	$0.9737\ldots$ [9]	*0.9805...*

Body	Congruent packing	
	lower bound	upper bound
Tetrahedron	$4000/4671 = 0.8563\ldots$ [17]	$1 - 2.6\ldots \cdot 10^{-25}$ [40]
Truncated tetrahedron	$207/208 = 0.9951\ldots$ [55], [23]	< 1
Truncated cuboctahedron	$0.8493\ldots$ [9]	$0.8758\ldots$ [76]
Rhombicuboctahedron	$0.8758\ldots$ [9]	$0.8758\ldots$ [26]
Cuboctahedron	$0.9183\ldots$ [41]	< 1
Truncated cube	$0.9737\ldots$ [9]	< 1

Table 1.2: Best known bounds for packings of three-dimensional Platonic and Archimedean solids with tetrahedral symmetry. The octahedron, the cube, and the truncated octahedron are omitted. Our new bounds are written in italics.

We improved the upper bound of the regular tetrahedron. For the truncated tetrahedron, cuboctahedron, and truncated cube, there were no upper bound for the translative packing density known before.

Body	Lattice packing	
	lower bound	upper bound
Icosahedron	0.8363... [9]	0.8363... [9]
Dodecahedron	0.9045... [9]	0.9045... [9]
Truncated icosahedron	0.7849... [9]	0.7849... [9]
Rhombicosidodecahedron	0.8047... [9]	0.8047... [9]
Truncated icosidodecahedron	0.8272... [9]	0.8272... [9]
Icosidodecahedron	0.8647... [9]	0.8647... [9]
Truncated dodecahedron	0.8977... [9]	0.8977... [9]

Body	Translative packing	
	lower bound	upper bound
Icosahedron	0.8363... [9]	*0.8796...*
Dodecahedron	0.9045... [9]	*0.9183...*
Truncated icosahedron	0.7849... [9]	*0.8345...*
Rhombicosidodecahedron	0.8047... [9]	0.8359... [76]
Truncated icosidodecahedron	0.8272... [9]	*0.8602...*
Icosidodecahedron	0.8647... [9]	*0.8832...*
Truncated dodecahedron	0.8977... [9]	*0.9114...*

Body	Congruent packing	
	lower bound	upper bound
Icosahedron	0.8363... [9]	0.8934... [76]
Dodecahedron	0.9045... [9]	0.9811... [76]
Truncated icosahedron	0.7849... [9]	0.8385... [76]
Rhombicosidodecahedron	0.8047... [9]	0.8359... [76]
Truncated icosidodecahedron	0.8272... [9]	0.8973... [76]
Icosidodecahedron	0.8647... [9]	0.9380... [76]
Truncated dodecahedron	0.8977... [9]	0.9738... [76]

Table 1.3: Best known bounds for packings of three-dimensional Platonic and Archimedean solids with icosahedral symmetry. Our new bounds are written in italics.

Except for the Rhombicosidodecahedron, we were able to improve all upper bounds for the translative packing density. In these cases, the upper bounds for the congruent packing density were the best known upper bounds for the translative packing density before.

1.4 Locally optimal lattice packings for superballs

Our calculation for locally optimal lattice packings for three-dimensional superballs is based on the following theorem of Minkowski [61], which characterizes the contact points in an optimal lattice packing:

Theorem 1.3. *Let $\mathcal{K}$ be a three-dimensional centrally-symmetric convex body. Then there exists an optimal lattice 2Λ with basis $2b_1, 2b_2, 2b_3$, such that exactly one of the following cases holds:*

1. $\mathcal{U}_B^1 \subset \partial\mathcal{K}$ *and* $(-1,1,1)_B, (1,-1,1)_B, (1,1,-1)_B \notin K$,
2. $\mathcal{U}_B^2 \subset \partial\mathcal{K}$ *and* $(1,1,1)_B \notin \mathcal{K}$,
3. $\mathcal{U}_B^3 \subset \partial\mathcal{K}$,

where $\partial\mathcal{K}$ denotes the boundary of $\mathcal{K}$, $x_B = x_1b_1 + x_2b_2 + x_3b_3$ is the vector x in the basis b_1, b_2, b_3, which are the columns of the matrix B, and

$$\mathcal{U}_B^1 = \{(1,0,0)_B, (0,1,0)_B, (0,0,1)_B, (1,-1,0)_B, (0,1,-1)_B, (1,0,-1)_B\},$$

$$\mathcal{U}_B^2 = \{(1,0,0)_B, (0,1,0)_B, (0,0,1)_B, (1,1,0)_B, (0,1,1)_B, (1,0,1)_B\},$$

$$\mathcal{U}_B^3 = \mathcal{U}_B^2 \cup \{(1,1,1)_B\}.$$

Analogously to the lattice packings of superballs found by Jiao, Stillinger, and Torquato, we divide the range of $p \in [1,\infty)$ into four different regimes. For each of these regimes, we calculated locally optimal lattice packings. The best obtained results are given in Table 1.4

value of p	Case 1	Case 2	Case 3
$[1, \log_2 3]$	L_1	L_2	L_3
$(\log_2 3, 2]$	*	X	X
$[2, 2.3018\ldots]$	C_0	X	X
$[2.3018\ldots, \infty)$	C_1	X	X

Table 1.4: Best obtained locally optimal lattice for each case in each regime. The entry X means, that our computations did not find any locally optimal lattice.

For each of these regimes, the best obtained lattice packing densities as well as a picture of the lattice packing is given in Section 4.3.

First regime:

For $p \in \{1, 1.05, \ldots, 1.55\}$ and for $p = \log_2 3$, the best obtained locally optimal lattice packing for Case 1 is given by the lattice

$$L_1 = \mathbb{Z}\, b_1 + \mathbb{Z}\, b_2 + \mathbb{Z}\, b_3$$

with

$$b_1 = \left(2^{1-\frac{1}{p}}, 2^{1-\frac{1}{p}}, 0\right)^{\mathsf{T}},\ b_2 = \left(2x, 2^{1-\frac{1}{p}} - 2x, -2w\right)^{\mathsf{T}},\ b_3 = \left(-2y, 2^{1-\frac{1}{p}} + 2y, -2z\right)^{\mathsf{T}},$$

where $w, x, y, z \in \mathbb{R}_{>0}$ such that

$$\begin{aligned} x^p + w^p + (2^{-1/p} - x)^p &= 1 \\ y^p + z^p + (2^{-1/p} + y)^p &= 1 \\ 2(x+y)^p + (w-z)^p &= 1. \end{aligned}$$

It has density

$$\frac{\operatorname{vol} B_3^p}{2^{3-1/p}\left(2^{-1/p}w - 2^{-1/p}z + 2xz + 2wy\right)},$$

where the volume of a superball is defined by

$$\operatorname{vol} B_3^p = 8\,\Gamma(1+1/p)^3 / \,\Gamma(1+3/p).$$

For Case 2 the lattice L_2 had always the highest density in the first regime, except for the case $p = 1.1$. In this case the best obtained lattice packing is given by the lattice with basis vectors

$$b_1 = 2\,(-0.313, 0.302, 0.486)^{\mathsf{T}},\ b_2 = 2\,(0.296, 0.301, 0.503)^{\mathsf{T}},\ b_3 = 2\,(0.370, -0.475, -0.256)^{\mathsf{T}}.$$

For all other values of p, the best packing for Case 2 is given by

$$L_2 = \mathbb{Z}\,b_1 + \mathbb{Z}\,b_2 + \mathbb{Z}\,b_3$$

with

$$b_1 = (2x, -2x, 2y)^{\mathsf{T}},\ b_2 = (-2y, -2x, -2x)^{\mathsf{T}},\ b_3 = (2x, 2y, -2x)^{\mathsf{T}},$$

where $x, y \in \mathbb{R}_{>0}$ such that

$$\begin{aligned} (1 - 2x^p)^{1/p} &= y \\ 2\left(x - (1-2x^p)^{1/p}\right)^p + (2x)^p &= 1\,. \end{aligned}$$

It has density

$$\frac{\operatorname{vol} B_3^p}{8\,(2x^3 + 3x^2y - y^2)}\,.$$

The best lattice packing over all locally optimal lattice packings we obtained for the first regime satisfying Case 3, is given by

$$L_3 = \mathbb{Z}\,b_1 + \mathbb{Z}\,b_2 + \mathbb{Z}\,b_3$$

with

$$b_1 = (-2x, 2y, 2z)^{\mathsf{T}},\ b_2 = (2z, -2x, 2y)^{\mathsf{T}},\ b_3 = (2y, 2z, -2x)^{\mathsf{T}},$$

where $x, y, z \in \mathbb{R}_{>0}$ with $z \geq x \geq y$ such that

$$\begin{aligned} z &= 3^{-1/p} + x - y \\ x^p + y^p + z^p &= 1 \\ (x-y)^p + (3^{-1/p} + x)^p + (3^{-1/p} - y)^p &= 1. \end{aligned}$$

It has density

$$\frac{\operatorname{vol} B_3^p}{8 \cdot 3^{-1/p} \left(3^{-2/p} + 3\left(3^{-1/p}(x-y) + (x-y)^2 + xy\right)\right)}.$$

Furthermore, this lattice gives the best lattice packing for the first regime over all cases.

Second regime:

For the values of $p \in \{1.59, 1.6, \ldots, 2\}$ our calculations just found locally optimal lattices for Case 1. Unfortunately, we did not find any pattern in these lattices in order to give a family of lattices depending on p. For the considered values of p, the numerical values of the basis vectors for the best locally optimal lattices we obtained, are given in the appendix.

Third regime:

For $p \in \{2, 2.05, \ldots, 2.3\}$ and for $p = 2.3018$, our calculations did not find any local optimal lattice for Case 2 or 3. For the first case, the best obtained lattice packing is given by the following family of lattices, which is equal to the one found by Jiao, Stillinger, and Torquato [53]

$$C_0 = \mathbb{Z}\, b_1 + \mathbb{Z}\, b_2 + \mathbb{Z}\, b_3$$

with

$$b_1 = \left(2^{1-\frac{1}{p}}, 2^{1-\frac{1}{p}}, 0\right)^{\mathsf{T}},\ b_2 = (0,0,2)^{\mathsf{T}},\ b_3 = \left(-2s, 2\left(s + 2^{-\frac{1}{p}}\right), 1\right)^{\mathsf{T}},$$

where s is the smallest positive root of the equation

$$\left(s + 2^{-\frac{1}{p}}\right)^p + s^p + 2^{-p} - 1 = 0\,.$$

It has density

$$\frac{\operatorname{vol} B_3^p}{2^{3-\frac{1}{p}}\left(2s + 2^{-\frac{1}{p}}\right)}\,.$$

Fourth regime:

Similarly to the second and third regime, our calculations did not find any locally optimal lattice packing satisfying Case 2 or 3 for $p \in \{2.4, 2.5, \ldots, 6\}$ or for $p \in \{2.3018, 2.31, 6.5, 7, 7.5, 8\}$. For Case 1, the best obtained lattice packing corresponds to the family of lattices found by Jiao, Stillinger, and Torquato, too, and is given by

$$C_1 = \mathbb{Z}\, b_1 + \mathbb{Z}\, b_2 + \mathbb{Z}\, b_3$$

with

$$b_1 = \left(2^{1-\frac{1}{p}}, 2^{1-\frac{1}{p}}, 0\right)^{\mathsf{T}}, \; b_2 = \left(2^{1-\frac{1}{p}}, 0, 2^{1-\frac{1}{p}}\right)^{\mathsf{T}}, \; b_3 = \left(2s + 2^{1-\frac{1}{p}}, -2s, -2s\right)^{\mathsf{T}},$$

where s is the smallest positive root of the equation

$$\left(s + 2^{-\frac{1}{p}}\right)^p + 2s^p - 1 = 0 \, .$$

It has density

$$\frac{\operatorname{vol} B_3^p}{2^{3-\frac{2}{p}}\left(3s + 2^{-\frac{1}{p}}\right)} \, .$$

The obtained results for the lower and upper bounds for $p \in [1, 8]$ are pictured in Figure 1.10. For the upper bounds, we applied the rigorous verification to our numerical results for $p \in [6]$, thus, the other upper bounds are numerical results.

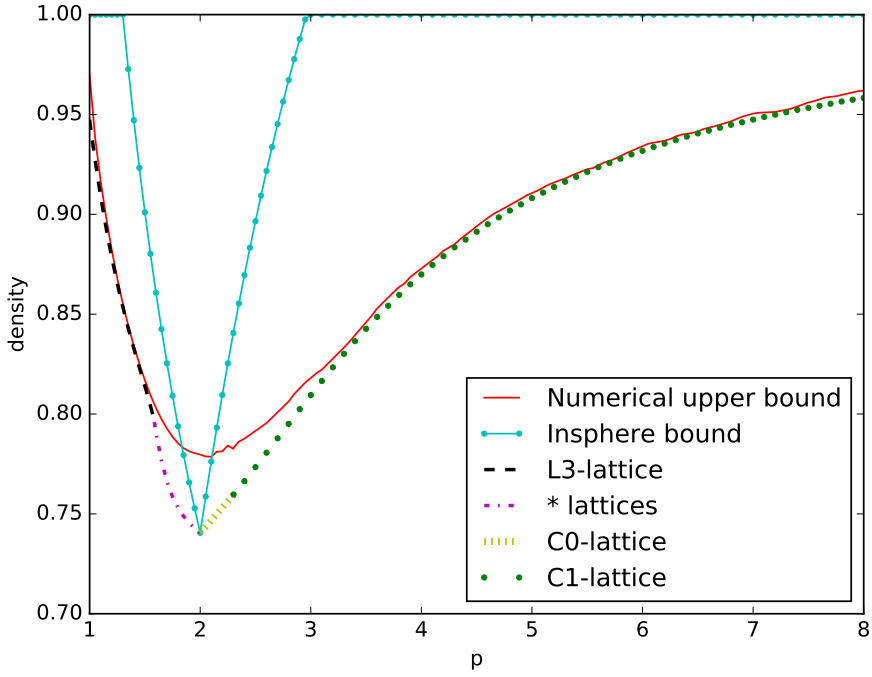


Figure 1.10: Lower bounds given by the locally optimal lattice packings in Section 4.3. Upper bounds obtained by the approach explained in Section 3. For $p \notin [6]$ the upper bounds are given by numerical results. For $p \in [6]$, the upper bounds are rigorous.

Chapter Two

Techniques

In this chapter, we introduce the techniques, which we apply in this thesis. In Section 2.1, we consider convex optimization, and especially semidefinite optimization. Furthermore, we study polynomial optimization and how one can relax these problems to semidefinite problems. In Section 2.2, we give an introduction into the representation theory of finite groups. Furthermore, Section 2.3 deals with polynomials which can be written as sums of Hermitian squares (SOHS). Additionally, we consider the simplification of the SOHS checking for polynomials invariant under finite pseudo-reflection groups. For the SOHS checking we can use semidefinite optimization. Moreover, we consider the SOHS checking for polynomials invariant under the octahedral group or the icosahedral group, explicitly.

2.1 Convex optimization

Traditionally, an *optimization problem* is given in the form:

$$\begin{aligned} &\text{minimize} && f_0(x) \\ &\text{subject to} && x \in \mathbb{R}^n \\ & && f_i(x) \leq b_i \ \ \forall i \in \{1, \ldots, m\}, \end{aligned}$$

where $f_0 : \mathbb{R}^n \to \mathbb{R}$ is the *objective function*, $f_i : \mathbb{R}^n \to \mathbb{R}$ are the *constraint functions*, $b_i \in \mathbb{R}$ are constants, and $x \in \mathbb{R}^n$ is the *optimization variable*. If the objective function and the constraint functions are linear, the given problem is called a *linear problem*, otherwise it is called a *nonlinear problem*. Linear problems are well studied and efficiently solvable, whereas nonlinear problems are very general and, thus, difficult to solve. However, during the last decade, there has been great progress in studying *convex optimization problems*, optimization problems, where the objective and constraints are convex functions, especially in developing methods for solving these kind of problems. For more information about the rich theory of convex optimization problems, see, for example, the book [13] of Boyd and Vandenberghe. A well-studied class of convex optimization problems is, beside linear problems, the class of *semidefinite optimization problems*, a generalization of linear problems, which are generally efficiently solvable [27].

2.1.1 Semidefinite optimization

The problem of optimizing a linear function over a set of *positive semidefinite matrices* $\mathcal{S}^n_{\succeq 0}$ (real symmetric matrices of dimension n with nonnegative eigenvalues), restricted by linear matrix equalities is called a *semidefinite problem (SDP)*. Hence the feasibility set of an SDP is described by a spectrahedron, which is the intersection of the set of positive semidefinite matrices and an affine linear subspace. This problem is a generalization of linear problems, where a linear function has to be optimized over a polyhedron. An SDP is defined by

$$\begin{aligned} p^* = \sup \quad & \langle C, X \rangle && (2.1)\\ \text{subject to} \quad & X \in \mathcal{S}^n_{\succeq 0} && (2.2)\\ & \langle A_i, X \rangle = b_i \ \ \forall i \in \{1, \dots, m\}, && (2.3) \end{aligned}$$

where $C, A_i \in \mathcal{S}^n$ are symmetric matrices and $\mathcal{S}^n_{\succeq 0}$ is the set of positive semidefinite matrices of dimension n. Furthermore, the inner product $\langle X, Y \rangle$ of two matrices $X, Y \in \mathbb{R}^{n \times n}$ is defined by the trace $\mathsf{Tr}(X^\mathsf{T} Y) = \sum_{i,j=1}^n X_{ij} Y_{ij}$. An SDP is typically defined as a maximization problem. However, by using

$$\inf \ \langle C, X \rangle = - \sup \ - \langle C, X \rangle$$

it can also be described as a minimization problem.

If the matrices C and A_i for all $i \in [m]$ are diagonal matrices, the corresponding SDP is equivalent to the following linear problem

$$\begin{aligned} \sup \quad & \langle c, x \rangle \\ \text{subject to} \quad & x \in \mathbb{R}^n \\ & x \geq 0 \\ & \langle a_i, x \rangle = b_i \ \ \forall i \in \{1, \dots, m\}, \end{aligned}$$

where $c, a_i \in \mathbb{R}^n$ contain the diagonal elements of the corresponding matrix.

The definition of an SDP is given by using the supremum instead of the maximum, because the optimal value p^* might not be attained. For example, consider

$$C = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, \ A_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \ m = 1, \ b_1 \in \mathbb{R}_{>0}.$$

The matrix X is positive semidefinite if and only if all its principal minors, which are , in this case, its entries and the determinant $X_{11}X_{22} - X_{12}^2$, are nonnegative. Since there is no restriction to the element X_{22}, the value of X_{11} can be arbitrary close to 0, which means the supremum of this problem is equal to 0. Since b_1 is strictly positive, X_{12} and thus also X_{11} has to be strictly positive, and therefore the supremum cannot be attained by a feasible X.

We give an important theorem about real symmetric matrices.

Theorem 2.1 (**Spectral decomposition theorem [49]**). *Any real symmetric matrix $X \in \mathcal{S}^n$ can be decomposed as*

$$X = \sum_{i=1}^n \lambda_i u_i u_i^\mathsf{T},$$

where $u_1, \ldots u_n$ are eigenvectors of X, which form an orthonormal basis of $\mathbb{R}^n$, with eigenvalues $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$. Alternatively, this decomposition can be given in matrix form, where $X = PDP^\mathsf{T}$, D is the diagonal matrix consisting of the eigenvalues λ_i, and P is the orthogonal matrix with columns u_i.

From Theorem 2.1, the following properties of positive semidefinite matrices can be deduced.

Lemma 2.2. *Let $X \in \mathcal{S}^n$ be a symmetric matrix. The following properties are equivalent:*

(1) $X \in \mathcal{S}^n_{\succeq 0}$.

(2) $x^\mathsf{T} X x \geq 0$ for all $x \in \mathbb{R}^n$.

(3) There exists a matrix $L \in \mathbb{R}^{n \times l}$ such that $X = LL^\mathsf{T}$. This is called a Cholesky decomposition of X .

(4) There exists vectors $x_1, \ldots x_n \in \mathbb{R}^l$ such that $X_{ij} = x_i^\mathsf{T} x_j$ for all $i, j \in [n]$. This is called a Gram representation of X .

(5) All eigenvalues of X are nonnegative .

A proof of Theorem 2.1 and Lemma 2.2, and more information about positive semidefinite matrices are given in the book *Matrix Analysis* of Horn and Johnson [49].

Instead of $A \in \mathcal{S}^n_{\succeq 0}$, we also write $A \succeq 0$. We can check whether a given matrix is positive semidefinite by using efficient methods, like, for example, by calculating the Cholesky decomposition or by determining the eigenvalues. Another property which is useful for checking positive semidefiniteness, in more theoretical contexts, is the *Schur complement*: Let

$$X = \begin{pmatrix} A & B \\ B^\mathsf{T} & C \end{pmatrix}$$

be a symmetric matrix in block form and A be nonsingular, then

$$X \succeq 0 \iff A \succeq 0 \text{ and } C - B^\mathsf{T} A^{-1} B \succeq 0.$$

An upper bound of the optimal value of the SDP, is given by any feasible solution for the corresponding dual program. The dual problem of the SDP (2.1) – (2.3) is defined by:

$$\begin{aligned} d^* = \inf \quad & b^\mathsf{T} y \\ \text{subject to} \quad & y \in \mathbb{R}^m \\ & \sum_{i=1}^m y_i A_i - C \succeq 0. \end{aligned}$$

An overview of semidefinite optimization, and in particular, of its duality theory, is given by Blekherman, Parrilo, and Thomas in [10], by Ben-Tal and Nemirovski in [8], and by Laurent and Vallentin in [60].

2.1.2 Polynomial optimization and sums of squares

Many difficult optimization problems can be described as *polynomial optimization problems*

$$p_{min} = \inf_{x \in \mathcal{K}} p(x) \,, \tag{2.4}$$

where

$$\mathcal{K} = \{x \in \mathbb{R}^n : g_i(x) \geq 0 \ \forall i \in [m] \} \tag{2.5}$$

is a subset of $\mathbb{R}^n$ defined by polynomial nonnegativity conditions and real polynomials $p, g_1, \ldots, g_m \in \mathbb{R}[x]$. This problem can also be formulated as

$$p_{min} = \sup \{\lambda : p - \lambda \in \mathcal{P}(\mathcal{K}) \} \,,$$

where

$$\mathcal{P}(\mathcal{K}) = \{g \in \mathbb{R}[x] : g(x) \geq 0 \ \ \forall x \in \mathcal{K} \} \,,$$

is the set of nonnegative polynomials on $\mathcal{K}$. In general, checking whether a polynomial with degree at least four is nonnegative everywhere is computationally difficult, because this is an NP-hard problem [10]. A way to make this condition tractable is to relax it to a sufficient condition which is easier to check. A multivariate real polynomial $p(x) \in \mathbb{R}[x_1, \ldots, x_n]_{\leq 2d}$ (or short $\mathbb{R}[x]_{\leq 2d}$) of degree at most $2d$, can be written as a *sum of squares* if there exists polynomials $q_1, \ldots, q_m \in \mathbb{R}[x]_{\leq d}$, such that $p(x) = \sum_{i=1}^m q_i^2(x)$. In this case, we say that p is *SOS*. If a polynomial is SOS, then it has to be globally nonnegative, therefore this condition gives a certificate for the nonnegativity. The other direction is not true as for example the Motzkin-polynomial $p(x) = x_1^2 x_2^2 (x_1^2 + x_2^2 - 3) + 1$ is nonnegative, but it is not SOS. Hilbert published 1888 in [46] the following theorem.

Theorem 2.3. *Every nonnegative n-variate polynomial of even degree d is a sum of squares if and only if $n = 1$, or $d = 2$, or $(n, d) = (2, 4)$.*

Apart from these few special cases, the SOS condition is a strict relaxation of the nonnegativity condition. More information about the theory of SOS polynomials in the field of polynomial optimization and real algebraic geometry, is given by Blekherman, Parrilo, and Thomas in [10]. Fortunately, we can check the SOS condition by using semidefinite optimization.

Theorem 2.4. *A polynomial $p \in \mathbb{R}[x_1, \cdots, x_n]_{\leq 2d}$ of degree at most $2d$ can be written as sums of squares, if and only if, there is a positive semidefinite matrix $A \in \mathbb{R}^{N \times N}$ such that*

$$p(x_1, \cdots, x_n) = b(x_1, \cdots, x_n)^\mathsf{T} \, A \, b(x_1, \cdots, x_n),$$

where $N = \binom{n+d}{d}$ and $b(x_1, \cdots, x_n) \in \mathbb{R}[x]^N$ contains a basis of the space of polynomials of degree at most d.

Proof. Let $p(x) \in \mathbb{R}[x_1, \cdots, x_n]_{\leq 2d}$ be a polynomial of degree at most $2d$. If p is SOS, then there exist polynomials $q_1, \ldots, q_m \in \mathbb{R}[x]_{\leq d}$ such that $p(x) = \sum_{i=1}^m q_i^2(x)$ holds. We can

construct a real matrix V, such that

$$\begin{bmatrix} q_1(x) \\ \vdots \\ q_m(x) \end{bmatrix} = V \cdot b(x).$$

Define the matrix $A = V^\mathsf{T} V$, then $V^\mathsf{T} V$ is a Cholesky decomposition of A. Hence we get:

$$p(x) = \sum_{i=0}^{m} q_i^2(x) = (V \cdot b(x))^\mathsf{T}(V \cdot b(x)) = b(x)^\mathsf{T}(V^\mathsf{T} V)b(x) = b(x)^\mathsf{T} A b(x).$$

Due to the Cholesky decomposition, the N-dimensional matrix A is positive semidefinite. Conversely, by applying the Cholesky decomposition to a positive semidefinite matrix A with $p(x) = b(x)^\mathsf{T} A b(x)$, we obtain an SOS decomposition of $p(x)$. □

For solving a general polynomial optimization problem we have to check whether a given polynomial p is contained in the set $\mathcal{P}(\mathcal{K})$. Since, this problem is in general hard to solve, we relax it. The idea is to find a sequence of convex cones $C_1 \subseteq C_2 \subseteq \ldots \subseteq \mathcal{P}(\mathcal{K})$, for which, the problem $\sup\{\lambda : p - \lambda \in C_i\}$ is easier to solve. Let p_i be the supremum of $p - \lambda \in C_i$, then $p_1 \leq p_2 \leq \ldots \leq p_{\min}$, because each C_i is a subset of C_{i+1}. Furthermore, the cones C_i and C_{i+1} are defined in such a way that the calculation of p_i is easier than the calculation of p_{i+1}. By this approach, we get a lower bound on the optimal value $p_{\min}$. To do so, we can define the sets C_i by restricting the maximal degree of the contained polynomials.

Let $\Sigma_{n,2d}$ denote the set of n-variate SOS polynomials of degree at most $2d$. Then, we define an SOS relaxation of $p_{\min}$ by

$$p_{sos,d} = \sup\left\{\lambda : p - \lambda \in \Sigma_{n,2d} + \sum_{i=1}^{m} g_i \Sigma_{n,2d}\right\},$$

and thus,

$$p_{sos,1} \leq p_{sos,2} \leq \ldots \leq p_{\min}.$$

In general, an SOS relaxation of the problem p_{min} is given by

$$p_{sos} = \{\lambda : p - \lambda \in \Sigma + g_1\Sigma + \ldots + g_m\Sigma\},$$

where Σ consists of all SOS polynomials. The benefit of this relaxation is that it is describable as an SDP and thus efficiently solvable. More details about nonnegative polynomials and sums of squares are given by Lasserre in [58] and by Laurent in [59].

2.1.3 Karush-Kuhn-Tucker conditions

A feasible solution x of a minimization problem with an objective function f_0 is called a *locally optimal solution* if there exists $\varepsilon \in \mathbb{R}_{>0}$ such that for all feasible solutions y with $\|x - y\| \leq \varepsilon$ the inequality $f_0(x) \leq f_0(y)$ holds. For convex optimization problems, locally optimal solutions are also globally optimal. Theorem 2.6 states necessary conditions for

local optimality in nonlinear optimization problems. The *gradient* of a function $f : \mathbb{R}^n \to \mathbb{R}$ is

$$\nabla_x f(x_1, \ldots, x_n) = \left(\frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_n} \right)^\mathsf{T}$$

and the *Hessian matrix* is defined componentwise by

$$\left(\nabla_x^2 f(x) \right)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \, \partial x_j}$$

for $i, j \in [n]$. For the necessary conditions, we have to introduce the *first order constraint qualification*, which is given in the following lemma.

Lemma 2.5. *Let x^0 be a feasible solution of the problem:*

$$\begin{aligned} p_{inf} = \min \quad & f(x) && (2.6)\\ \text{subject to} \quad & h_i(x) = 0 \quad \textit{for all } i \in \{1, \ldots, m\} && (2.7)\\ & g_j(x) \leq 0 \quad \textit{for all } j \in \{1, \ldots n\}. && (2.8) \end{aligned}$$

Assume that the functions h_i for $i \in [m]$ and g_i for $i \in [n]$ are once-differentiable. Then the first order constraint qualification holds at x^0 if for any nonzero vector z, such that $z^\mathsf{T} \nabla_x \, g_i(x^0) \geq 0$ for all $i \in B_0 = \{i : g_i(x^0) = 0\}$ and $z^\mathsf{T} \nabla_x h_j(x^0)$, $j = 1, \ldots, m$, z is tangent to a once-differentiable arc, the arc emanating from x^0 and contained in the constraint region.

By using Lemma 2.5 we can formulate a necessary condition for local optimality.

Theorem 2.6. *If x^* is a locally optimal solution of the following problem:*

$$\begin{aligned} p_{inf} = \min \quad & f(x) && (2.9)\\ \text{subject to} \quad & h_i(x) = 0 \quad \textit{for all } i \in \{1, \ldots, m\} && (2.10)\\ & g_j(x) \leq 0 \quad \textit{for all } j \in \{1, \ldots n\}, && (2.11) \end{aligned}$$

where f, g_j for $j \in [n]$, and h_i for $i \in [m]$ are differentiable at x^*, and if the first order constraint qualification holds at x^*, then there exist Lagrange multipliers $\mu^* = \{\mu_1^*, \ldots, \mu_m^*\}$ and $\nu = \{\nu_1^*, \ldots, \nu_n^*\}$ such that

$$\begin{aligned} \nabla_x \mathcal{L}(x^*, \mu^*, \nu^*) = 0 && && (2.12)\\ g_j(x^*) \leq 0 && \textit{for all } j \in \{1, \ldots, n\} && (2.13)\\ h_i(x^*) = 0 && \textit{for all } i \in \{1, \ldots, m\} && (2.14)\\ \nu_j^* \geq 0 && \textit{for all } j \in \{1, \ldots, n\} && (2.15)\\ \nu_j^* g_j(x^*) = 0 && \textit{for all } j \in \{1, \ldots, n\} && (2.16) \end{aligned}$$

where the Lagrange function is defined by

$$\mathcal{L}(x, \mu, \nu) = f(x) + \sum_{i=1}^{m} \mu_i h_i(x) + \sum_{j=1}^{n} \nu_j g_j(x). \tag{2.17}$$

Conditions (2.12) to (2.16) are called *Karush-Kuhn-Tucker conditions* (KKT conditions) or *first order condition*. A proof of Lemma 2.5 and of Theorem 2.6 is given by Fiacco and McCormick in [34, Chapter 2]. Moreover, there exists a sufficient condition for local optimality in nonlinear optimization problems called *second order condition*, which is defined in Theorem 2.7. A proof of this theorem is given in [34, Chapter 2], too.

Theorem 2.7. *Let x^* be a feasible solution of the previous problem (2.9) – (2.11), where f, g_j for $j \in [n]$, and h_i for $i \in [m]$ are twice-differentiable functions, and let μ^* and ν^* be Lagrange multipliers such that (x^*, μ^*, ν^*) satisfies the KKT conditions (2.12) – (2.16). If furthermore for all $y \neq 0$ satisfying the following conditions:*

$$y^\mathsf{T} g_j(x^*) = 0 \text{ for all } j \text{ where } \nu_j^* > 0 \tag{2.18}$$

$$y^\mathsf{T} \nabla g_j(x^*) \geq 0 \text{ for all } j \text{ where } g_j(x^*) = 0,\ \nu_j^* = 0 \tag{2.19}$$

$$y^\mathsf{T} \nabla h_i(x^*) = 0 \text{ for all } i \in \{1, \ldots, m\} \tag{2.20}$$

the inequality

$$y^\mathsf{T} \left(\nabla_x^2 \mathcal{L}(x^*, \mu^*, \nu^*) \right) y > 0 \tag{2.21}$$

holds, then x^* is a local minimizer of the corresponding problem (2.9) – (2.11).

2.2 Representation theory

Let V be an n-dimensional vector space over the field $\mathbb{C}$. The set

$$\mathrm{GL}(V) = \{T : V \to V : T \text{ is linear and invertible }\}$$

is the group of invertible linear transformations. Furthermore, we define

$$\mathrm{GL}_n(\mathbb{C}) = \{M \in \mathbb{C}^{n \times n} : M \text{ is invertible }\}$$

to be the group of invertible square matrices of dimension n. Since the dimension of V is n, each transformation in $\mathrm{GL}(V)$ can be identified with a matrix in $\mathrm{GL}_n(\mathbb{C})$. To do so, we define

$$\psi : V \to \mathbb{C}^n, \text{ with } b_i \mapsto e_i,$$

where e_i denotes the ith unit vector in $\mathbb{C}^n$ and $\{b_1, \ldots, b_n\}$ is a basis of V. For each transformation $\rho(g) \in \mathrm{GL}(V)$, we can calculate the corresponding matrix $\tilde{\rho} \in \mathrm{GL}_n(\mathbb{C})$ by

$$(\tilde{\rho}(g))_{ij} = \left(\psi \left(\rho(g)\, b_j \right) \right)_i .$$

Furthermore, the unitary set is

$$\mathrm{U}_n(\mathbb{C}) = \{M \in \mathrm{GL}_n(\mathbb{C}) : MM^* = I\},$$

where $T^* = \overline{T^\mathsf{T}}$ is the conjugate transpose of T and I is the identity matrix. We also write $\mathrm{U}(n)$ instead of $\mathrm{U}_n(\mathbb{C})$. The group elements can be represented as matrices, so that the group operations are expressible by matrix multiplications. Let G be a group. The function

$\rho : G \to \mathrm{GL}(V)$ is a *representation* of G if and only if it is a *group homomorphism*. This is the case if each element $s \in G$ is assigned to an element $\rho(s) \in \mathrm{GL}(V)$ such that

$$\rho(st) = \rho(s)\rho(t) \text{ for all } s, t \in G.$$

Note that the identity of G is 1 and therefore $\rho(1) = I$. Moreover, the definition implies that $\rho(s^{-1}) = \rho(s)^{-1}$ for all $s \in G$. A representation ρ of G is said to be unitary if $\rho : G \to \mathrm{U}(n)$. Let $\mathbb{C}[x_1, \ldots, x_n]$, or short $\mathbb{C}[x]$, be the set of complex polynomials with n variables. A representation $\pi : G \to \mathrm{GL}(\mathbb{C}^n)$ gives a representation on $\mathbb{C}[x]$ by the equation

$$(\pi(g)p)(x_1, \cdots, x_n) = p\left(\pi\left(g^{-1}\right)(x_1, \cdots, x_n)\right).$$

For simplicity, we write gp instead of $\pi(g)p$ and $g^{-1}x$ instead of $\pi(g)^{-1}x$. A polynomial p is said to be invariant under G, or short *G-invariant*, if and only if $gp = p$ for all elements g in G. The set of polynomials $p \in \mathbb{C}[x]$ that are G-invariant is denoted by $\mathbb{C}[x]^G$. This set is also called the *invariant ring* of G and formally it is defined as

$$\mathbb{C}[x]^G = \{p \in \mathbb{C}[x] : gp = g \text{ for all } g \in G\}.$$

There exists a linear transformation called *Reynolds operator* of the polynomials in $\mathbb{C}[x]$ onto the set of G-invariant polynomials by taking the group average, which is for finite groups defined as

$$Mf(x) = \frac{1}{|G|} \sum_{g \in G} gp(x), \tag{2.22}$$

where $|G|$ is the order of the group G. By considering the representations of G in matrix form, we can define a set $S \subset \mathbb{C}^n$ to be G-invariant, if and only if, for all $g \in G$, the equation

$$gS = S \text{ with } gS = \{gs : s \in S\}$$

holds. Two representations $\alpha : G \to \mathrm{GL}(V)$ and $\beta : G \to \mathrm{GL}(V')$ of G are *equivalent* (or *isomorphic*) if and only if there exists a linear isomorphism $\tau : V \to V'$ that transforms α into β. Hence τ has to satisfy the following equation:

$$\tau \circ \alpha(g) = \beta(g) \circ \tau \text{ for all } g \in G.$$

Furthermore, two representations $\alpha, \beta \in \mathrm{GL}_n(\mathbb{C})$ in matrix form are equivalent if and only if there exists a matrix $T \in \mathrm{GL}_n(\mathbb{C})$, such that

$$T\alpha(g)T^{-1} = \beta(g) \text{ for all } g \in G.$$

Lemma 2.8. *[71, Proposition 3.2.4] Every representation of a finite group is equivalent to a unitary representation.*

A linear representation $\pi : G \to \mathrm{GL}_n(\mathbb{C})$ can be transformed into an equivalent unitary representation $\pi_u : G \to \mathrm{U}(n)$ using the Gram-Schmidt orthonormalization with respect to the G-invariant inner product defined as

$$\langle u, v \rangle_G = \frac{1}{|G|} \sum_{g \in G} (\pi(g)u)^* (\pi(g)v) \text{ for all } u, v \in V.$$

This is equal to the following formulation

$$\langle u, v\rangle_G = u^* \left(\frac{1}{|G|} \sum_{g\in G} \pi(g)^* \pi(g) \right) v \text{ for all } u, v \in V. \tag{2.23}$$

The Gram matrix of the G-invariant inner product is

$$\frac{1}{|G|} \sum_{g\in G} \pi(g)^* \, \pi(g) \, .$$

Note that $\langle v, v\rangle_G = \frac{1}{|G|} \sum_{g\in G} \|\pi(g)v\|^2 \geq 0$ and $\langle v, v\rangle = 0$ if and only if $v = 0$, thus, the inner product is positive definite.

Let $\pi : G \to \mathrm{GL}(V)$ be a representation of G and let $W \subseteq V$. If $gW \subseteq W$ for all $g \in G$, the representation $\rho(g) = \pi(g)|_W$ is said to be a *subrepresentation* of π. If the subrepresentations of π are only π itself and 0, then the representation π is called an *irreducible representation*. The set of all irreducible unitary representations of G up to equivalence is denoted by $\widehat{G}$. Let $\rho : G \to \mathrm{GL}(V_1)$ be a representation on V_1 and let $\sigma : G \to \mathrm{GL}(V_2)$ be a representation on V_2. The *direct sum* of two representations is defined by

$$\rho(g) \oplus \sigma(g) = \alpha\left(\rho(g), \sigma(g)\right) \text{ for all } g \in G,$$

where $\alpha : \mathrm{GL}(V_1) \times \mathrm{GL}(V_2) \to \mathrm{GL}(V_1 \oplus V_2)$. Then, the obtained representation maps group elements to linear transformations in $\mathrm{GL}(V_1 \oplus V_2)$. If the representations are in matrix form, that is $\rho : G \to \mathrm{GL}_n(\mathbb{C})$ and $\sigma : G \to \mathrm{GL}_m(\mathbb{C})$, then the direct sum is defined as

$$\rho(g) \oplus \sigma(g) = \begin{pmatrix} \rho(g) & 0 \\ 0 & \sigma(g) \end{pmatrix} \quad \text{for all } g \in G.$$

Thus, $\rho \oplus \sigma : G \to \mathrm{GL}_{m+n}(\mathbb{C})$.

Lemma 2.9. *[67, Chapter 1.3, Theorem 1] Let $\pi : G \to GL(V)$ be a representation of G on V. If π is not irreducible, then there exist two subrepresentations $\rho : G \to GL(V_1)$ and $\sigma : G \to GL(V_2)$ with V_1, V_2 subspaces of V, such that π is equivalent to $(\rho \oplus \sigma) : G \to GL(V_1 \oplus V_2)$.*

If a subrepresentation is not irreducible, one can decompose it again into further subrepresentations. Consequently, the decomposition can be continued until all subrepresentations are irreducible.

Corollary 2.10. *[67, Chapter 1.4, Theorem 2] A representation of a finite group is equivalent to a direct sum of irreducible representations.*

Let π be an irreducible subrepresentation of $\rho : G \to \mathrm{GL}(V)$ and let $\pi_1, \ldots, \pi_{m_\pi}$ be the irreducible subrepresentations of ρ, which are equivalent to π. Then

$$\rho = \bigoplus_{\pi\in\widehat{G}} m_\pi \pi = \bigoplus_{\pi\in\widehat{G}} \bigoplus_{i=1}^{m_\pi} \pi_i, \tag{2.24}$$

where $\widehat{G}$ is the set of non-equivalent irreducible unitary representations of G and $\pi_i : G \to \mathrm{GL}(V^{\pi_i})$ is a representation on V^{π_i}. For each $\pi \in \widehat{G}$, we define $V^\pi = V^{\pi_1} \oplus \ldots \oplus V^{\pi_{m_\pi}}$. Thus, we obtain V^π by collecting all subspaces with equivalent representation together. Since each subspace V^π can be decomposed into isomorphic subspaces, V^π is called an *isotypic component* and the decomposition $V = \bigoplus_{\pi\in\widehat{G}} V^\pi$ is called the *isotypic decomposition* of V.

Let $\pi_i : G \to \mathrm{GL}(V^{\pi_i})$ with $\pi \in \widehat{G}$ and $i \in [m_\pi]$ be irreducible representations of $\rho : G \to \mathrm{GL}(V)$, then we get a following decomposition of the vector spaces

$$V = \bigoplus_{\pi\in\widehat{G}} V^\pi, \text{ with } V^\pi = \bigoplus_{i=1}^{m_\pi} V^{\pi_i}. \tag{2.25}$$

Here we are interested in special representations, called regular representations, for which we calculate these decompositions. First let us define regular representations. Let $\rho : G \to \mathrm{GL}(V)$ be a representation of G. If the dimension of the vector space V with a basis $\{e_t : t \in G\}$ is equal to the order of G and $\rho(g) : e_t \to e_{gt}$ holds for all $g, t \in G$, then ρ is called a *regular representation*. A nice property of such a representation is that the multiplicity m_π of every irreducible unitary representation π is equal to its dimension.

Theorem 2.11. *[67, Chapter 2.4] Let V be a complex vector space such that the dimension of V is equal to the order of G, and let $d_\pi = \dim \pi$ for $\pi \in \widehat{G}$. Then there exist vector subspaces V^{π_i} of V such that*

$$V = \bigoplus_{\pi\in\widehat{G}} V^\pi \text{ and } V^\pi = \bigoplus_{i=1}^{d_\pi} V^{\pi_i}, \tag{2.26}$$

with $\pi_i : G \to U(d_\pi)$, where $\pi_1, \ldots, \pi_{d_\pi}$ are irreducible unitary representations, which are equivalent to π. Hence $\sum_{\pi\in\widehat{G}} d_\pi^2 = |G|$.

Since Theorem 2.11 is important for the sum of Hermitian squares decomposition in Section 2.3, we give a proof after introducing the characters of a group. For this, we first define the *trace* $\mathrm{Tr}(\rho(g))$ of a linear transformation $\rho(g) \in \mathrm{GL}(V)$. We already saw how to transform ρ into a representation $\tilde{\rho} : G \to \mathrm{GL}_n(\mathbb{C})$ in matrix form with $n = \dim V$. The trace of $\rho(g)$ is equal to the trace of the matrix $\tilde{\rho}(g)$ given by

$$\mathrm{Tr}(\tilde{\rho}(g)) = \sum_{i,j=1}^{n} (\tilde{\rho}(g))_{ij} \ .$$

Note that the trace of $\rho(g)$ is independent of the basis of V, which we use to obtain the representation in matrix from. The function

$$\chi_\rho : G \to \mathbb{C} \quad \text{with} \quad \chi_\rho(g) = \mathrm{Tr}\,(\rho(g))\,,$$

is called the *character* of the representation ρ. A character is irreducible if and only if its corresponding representation is irreducible. Furthermore, $\chi_\rho(1)$ is equal to the dimension of ρ.

We calculate the character of a regular representation: Let $r : G \to \mathrm{GL}(V)$ be a regular representation and let $B = \{b_t : t \in G\}$ be a basis of V. Furthermore, let $\tilde{r} : V \to \mathbb{C}^{|G|}$ be

the regular representation in matrix form with respect to the basis B indexed by the group elements. Then

$$(\tilde{r}(g))_{st} = \begin{cases} 1 & \text{if } b_t = r(g)b_s, \\ 0 & \text{otherwise.} \end{cases}$$

Since r is a regular representation $r(g)b_s = b_{gs}$ for all $g, s \in G$. Thus $b_t = r(g)b_s$ if and only if $g = ts^{-1}$. In particular,

$$(\tilde{r}(g))_{tt} = \begin{cases} 1 & \text{if } g = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Hence, the character χ_r of the regular representation r is

$$\chi_r(g) = \begin{cases} |G|, & \text{if } g = 1, \\ 0, & \text{otherwise.} \end{cases}$$

Since ρ can be decomposed as the direct sum $\rho = \bigoplus_{\pi \in \widehat{G}} m_\pi \pi$, the character of ρ can be decomposed as

$$\chi_\rho = \sum_{\pi \in \widehat{G}} m_\pi \chi_\pi \, .$$

The inner product of two characters χ_1 and χ_2 is defined by

$$\langle \chi_1, \chi_2 \rangle = \frac{1}{|G|} \sum_{g \in G} \chi_1(g^{-1}) \, \chi_2(g) \, .$$

Then, we can compute the multiplicity, since $m_\pi = \langle \chi_\rho, \chi_\pi \rangle$ [67, Chapter 2.3].

Proof of Theorem 2.11. Let V be a $|G|$-dimensional vector space and let $\rho : G \to \mathrm{GL}(V)$ be a regular representation on V. Due to Corollary 2.10 this representation can be decomposed into irreducible representations. Furthermore, by Lemma 2.8, the obtained irreducible representations are equivalent to irreducible unitary representations. We can decompose the vector space V as in (2.25)

$$V = \bigoplus_{\pi \in \widehat{G}} V^\pi, \text{ with } V^\pi = \bigoplus_{i=1}^{m_\pi} V^{\pi_i}. \tag{2.27}$$

Let d_π be the dimension of π. The multiplicity m_π can be calculated by

$$m_\pi = \langle \chi_\rho, \chi_\pi \rangle = \frac{1}{|G|} \sum_{g \in G} \chi_\rho \left(g^{-1} \right) \chi_\pi(g) = \frac{1}{|G|} \cdot |G| \cdot \chi_\pi(1) = \chi_\pi(1) = d_\pi \, .$$

□

Instead of decomposing the finite-dimensional representation directly into its irreducible representations, we first decompose V into its isotypic components V^π, which is a unique decomposition. In [67, Chapter 2.6, Theorem 8], Serre gives the projection p^π of V onto V^π by the formula

$$p^\pi : V \to V \, ,$$

with

$$f \mapsto \frac{d_\pi}{|G|} \sum_{g \in G} \chi^\pi \left(g^{-1}\right) \rho(g) f \,, \tag{2.28}$$

where $\rho : G \to \mathrm{GL}(V)$ and $\chi^\pi : G \to \mathbb{C}$ is the character of $\pi \in \widehat{G}$. After the first decomposition, each isotypic component V^π contains a collection of isomorphic irreducible subspaces V^{π_i}.

Contrary to the first decomposition, there are many ways to decompose the isotypic components into its isomorphic irreducible subspaces. For an irreducible representation π, the vector subspace V^π contains m_π many vector subspaces V^{π_i}. In [67, Chapter 2.7, Proposition 8], Serre gives a projection from V^π into its vector subspaces V^{π_i} explicitly:

Theorem 2.12. *Let $\rho : G \to GL(V)$ be a representation of G. Furthermore, let π be an irreducible representation given as a $d_\pi \times d_\pi$ matrix. For each pair of integers $i, j \in \{1, \ldots, d_\pi\}$ define a linear map $p^\pi_{ij} : V^\pi \to V^\pi$ by*

$$f \mapsto \frac{d_\pi}{|G|} \sum_{g \in G} \pi_{ji} \left(g^{-1}\right) \rho(g) f \,. \tag{2.29}$$

Then the following holds:

(a) The map p^π_{ii} is a projection; its image $p^\pi_{ii}(V^\pi)$ is contained in V^{π_i} and $p^\pi = \sum_{i=1}^{d_\pi} p^\pi_{ii}$.

(b) The linear map p^π_{ij} is an isomorphism from V^{π_j} onto V^{π_i}.

(c) Let x^π_1 be a nonzero element of V^{π_1} and let $x^\pi_i = p^\pi_{i1}(x^\pi_1) \in V^{\pi_i}$. The elements x^π_i are linearly independent and generate a vector space $V(x^\pi_1)$, which is isomorphic to V^π. For each $g \in G$, we have

$$\rho(g)(x^\pi_i) = \sum_{j=1}^{d_\pi} \pi_{ji}(g) x^\pi_j \,.$$

(d) If $(x^\pi_1, \ldots, x^\pi_{d_\pi})$ is a basis of V^{π_1}, then

$$V^\pi = V(x^\pi_1) \oplus \cdots \oplus V(x^\pi_{d_\pi}) \,,$$

with $V(x^\pi_i)$ defined in (c).

Taking a basis of V^{π_1}, we can, thus, calculate a decomposition of $V^\pi = \bigoplus_{i=1}^{d_\pi} V^{\pi_i}$ explicitly.

2.3 Invariant sum of Hermitian squares

2.3.1 Sum of Hermitian squares (SOHS)

There are several methods for solving semidefinite programs in polynomial time, for example, the interior point method [2, 62]. For polynomials with many variables or a high degree

the dimension of the positive semidefinite matrix A of Theorem 2.4, which is needed for checking the SOS condition, will become large. For example, if the polynomial has three variables and degree 30, the matrix A has dimension 816. Unfortunately, such matrices are too large for current high-precision SDP solvers. Therefore, we are interested in simplifying the SOS calculation for polynomials that are invariant under a finite pseudo-reflection group.

Let $v \in \mathbb{R}^n$ be a nonzero vector and H_v be the hyperplane which is orthogonal to v. A *reflection* on the hyperplane H_v is an orthogonal transformation $\rho_v : \mathbb{R}^n \to \mathbb{R}^n$ defined as

$$\rho_v(x) = x - \frac{2\langle x, v\rangle}{\|v\|^2} v.$$

Note that $\rho_v(v) = -v$ and $\rho_v(x) = x$ if and only if $\langle x, v\rangle = 0$. A finite group, generated by reflections ρ_v is called a *finite reflection group* . It is a subgroup of the orthogonal group $\mathrm{O}(n)$. A group generated by a finite number of *pseudo-reflections*, that are invertible linear transformations on $\mathbb{C}^n$ with exactly one eigenvalue not equal to 1, is called a *finite pseudo-reflection group*. Since a reflection $\rho_v(v)$ is in particular a pseudo-reflection, any finite reflection group is also a finite pseudo-reflection group.

Example 2.13. The *octahedral group* $\mathsf{B}_3 = \mathsf{S}_4 \times \mathsf{C}_2$ is a finite reflection group, where S_4 is the symmetric group on 4 elements and C_2 is the cyclic group on 2 elements. The order of the group is 48 and it is generated by the reflecting hyperplanes $x_i = 0$ for $1 \le i \le 3$ and $x_i \pm x_j = 0$ for $1 \le i < j \le 3$. A generating set of reflecting hyperplanes of B_3 is pictured in Figure 2.1.

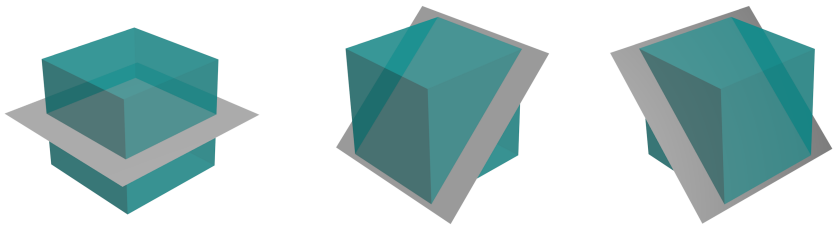


Figure 2.1: Generating set of reflecting hyperplanes of B_3.

Thus, the group can be generated by the matrices

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

These reflections generate all reflections and rotations, which will keep the regular cube $[-1, +1]^3$ unchanged. Therefore, B_3 coincides with the group of symmetries of the regular cube. Furthermore, it is also equal to the symmetry group of the regular octahedron.

Let G be a finite pseudo-reflection group and $p(x) \in \mathbb{R}[x]^G_{\le 2d}$ be a G-invariant SOS polynomial with degree at most $2d$. Using the standard monomial basis, there exists a

positive semidefinite matrix $A \in \mathcal{S}^N_{\geq 0}$ with $N = \binom{n+d}{d}$, such that

$$p = b^\mathsf{T} A b, \tag{2.30}$$

where b is a vector containing all monomials of $V = \mathbb{R}[x]_{\leq d}$ up to degree d. Let $\rho : G \to \mathrm{GL}_N(\mathbb{R})$ be a matrix representation of G with respect to the monomial basis of V. Because of the G-invariance of $p(x)$, the following equations hold for all group elements $g \in G$:

$$b^\mathsf{T} A\, b = p(x) = gp\,(x) = (\rho(g)\, b)^\mathsf{T}\, A\, (\rho(g)\, b) = b^\mathsf{T} \rho(g)^\mathsf{T} A\, \rho(g)\, b.$$

If ρ is an *orthogonal representation*, which means $\rho(g)\, \rho(g)^\mathsf{T} = \rho(g)^\mathsf{T} \rho(g) = I$ for all $g \in G$, then we get

$$A\, \rho(g) = \rho(g)\, A \quad \text{for all } g \in G. \tag{2.31}$$

Let $\mathcal{A} \subseteq \mathbb{R}^{N \times N}$ be the set of matrices satisfying equation (2.31), which is a subspace of the set of symmetric matrices $\mathcal{S}^N$. The set $\mathcal{A}$ is invariant under summation, scalar, matrix multiplication, and taking the adjoint, therefore it defines a *matrix *-algebra*. Wedderburn showed in [79] that each matrix *-algebra is decomposable into basic algebras and a zero algebra. By Lemma 2.8 and Corollary 2.10, we can assume that the representation ρ of (2.31) is unitary and equivalent to a direct sum of irreducible unitary representations $\pi \in \widehat{G}$. Moreover, since ρ is a transformation on $\mathbb{R}^N$, the conjugate transpose $\rho(g)^*$ is equal to the transpose $\rho(g)^\mathsf{T}$, which implies that the unitary representation ρ is orthogonal.

Observe that, since ρ is orthogonal, we can find an orthogonal matrix T, such that

$$\rho(g) = T \left(\bigoplus_{\pi \in \widehat{G}} \pi(g) \right) T^\mathsf{T},$$

for all $g \in G$. Moreover, for all matrices $A \in \mathcal{A}$, we get

$$T^\mathsf{T} A T = \mathrm{Diag}\,(A^\pi)_{\pi \in \widehat{G}} = \begin{pmatrix} A^1 & & 0 \\ & \ddots & \\ 0 & & A^{|\widehat{G}|} \end{pmatrix}, \tag{2.32}$$

with $A^\pi \in \mathcal{S}^{m_\pi \cdot d_\pi}$. Furthermore, each irreducible representation π has m_π equivalent representations in the decomposition. Therefore, each matrix A^π is block diagonalized. These blocks are all equal because of the G-invariance of the polynomial p. Thus,

$$A^\pi = \mathrm{Diag}(\underbrace{Q^\pi \ldots Q^\pi}_{m_\pi}) = \begin{pmatrix} Q^\pi & & 0 \\ & \ddots & \\ 0 & & Q^\pi \end{pmatrix}, \tag{2.33}$$

with $Q^\pi \in \mathcal{S}^{d_\pi}$. For the SOS calculation it is sufficient to calculate just the entries in the blocks, instead of the whole matrix A. Therefore, the block diagonalization makes the SOS calculation tractable. However, to use this technique, we have to calculate the transformation matrix T. Furthermore, we obtain the equations

$$p(x) = b^\mathsf{T} A b = b^\mathsf{T} T T^\mathsf{T} A T T^\mathsf{T} b = \left(T^\mathsf{T} b\right)^\mathsf{T} T^\mathsf{T} A T \left(T^\mathsf{T} b\right).$$

The matrix T decomposes the basis vector b in a similar way as the matrix A. Thus,

$$Tb = (b^{\pi})_{\pi\in\widehat{G}} = \begin{pmatrix} b^1 \\ \vdots \\ b^{|\widehat{G}|} \end{pmatrix}, \text{ with } b^{\pi} = \begin{pmatrix} b_1^{\pi} \\ \vdots \\ b_{m_\pi}^{\pi} \end{pmatrix} \text{ for each } \pi \in \widehat{G} \tag{2.34}$$

and the dimension of b_i^{π} is equal to d_π for $i \in [m_\pi]$. Hence, each b^{π} contains the basis vectors of the vector subspace V^{π}. To calculate b^{π} from b we will use the formula in (2.28), which provides the projection of the vector space V onto the vector subspace V^{π} for each irreducible representation π.

Due to the equations (2.30), (2.32), (2.33) and (2.34), an SOS polynomial p can be written in the form

$$p = \sum_{\pi\in\widehat{G}} \sum_{i=1}^{m_\pi} \left(b_i^{\pi}\right)^{\mathsf{T}} Q^{\pi} b_i^{\pi}, \tag{2.35}$$

with positive semidefinite matrices Q^{π}.

Gatermann and Parrilo give in [37] a method for simplifying the SOS calculation for polynomials invariant under a finite group. For this, they use the *Hironaka-decomposition* of the invariant polynomial ring, which is given by

$$\mathbb{R}[x]^G = \bigoplus_{j=1}^{t} \eta_j(x)\, \mathbb{R}\left[\theta_1(x), \ldots, \theta_n(x)\right], \tag{2.36}$$

with *primary invariants* $\theta_i(x) \in \mathbb{R}[x]$ and *secondary invariants* $\eta_i(x) \in \mathbb{R}[x]$. Primary invariants are also called *basic invariants*. A matrix $A \in \mathbb{R}[x]^{n\times n}$ is named an *SOS matrix* if and only if there exists a matrix $L \in \mathbb{R}[x]^{n\times l}$ such that $A = LL^{\mathsf{T}}$. The results of Gatermann and Parrilo in [37] are stated in the following theorem.

Theorem 2.14. *Let $p(x)$ be an SOS polynomial that is invariant under the action of a finite group G, and let θ_i, η_i be primary and secondary invariants of the corresponding invariant ring. Furthermore, let $\pi_1, \ldots, \pi_h$ be the orthogonal irreducible representations of G. Then there exists r_{π_i} for all $i \in [h]$, such that $p(x)$ has a representation of the form:*

$$p = \sum_{i=1}^{h} \langle Q^{\pi_i}, P^{\pi_i} \rangle \ ,$$

where $Q^{\pi_i} \in \mathbb{R}[\theta, \eta]^{r_{\pi_i}\times r_{\pi_i}}$ depends only on the group action, and $P^{\pi_i} \in \mathbb{R}[\theta]^{r_{\pi_i}\times r_{\pi_i}}$ is an SOS matrix for each $i \in [h]$.

In [37], Gatermann and Parrilo explain how to obtain the dimensions r_{π_i}. Using this theorem for the SOS calculation instead of finding one large matrix P with $p = \left\langle P, b(x)\, b(x)^{\mathsf{T}} \right\rangle$, makes the calculation easier, since less values have to be calculated for the desired matrix. That is, instead of computing one large positive semidefinite matrix, one has to compute h many smaller positive semidefinite matrices. In [5], Bachoc, Gijwijt, Schrijver, and Vallentin give more information about invariant semidefinite programs, and in particular, about invariant SOS polynomials.

Since our goal is to simplify the SOS calculation for polynomials invariant under a finite pseudo-reflection group, we make the abstract theorem of Gaterman and Parrilo concrete by considering finite pseudo-reflection groups. To do so, we use the Peter-Weyl theorem to transform the regular representations into irreducible unitary representations. For this it is more natural to consider Hermitian symmetric polynomials contrary to the work of Gaterman and Parrilo, in which the polynomials are over the field of real numbers.

A polynomial $p \in \mathbb{C}[z_1, \ldots, z_n, \overline{w}_1, \ldots, \overline{w}_n] = \mathbb{C}[z, \overline{w}]$ is called a *Hermitian symmetric polynomial* if the following three equivalent conditions hold (see D'Angelo [25]):

i) Equality $p(z, \overline{w}) = \overline{p(w, \overline{z})}$ holds for all $z, w \in \mathbb{C}^n$.

ii) The function $z \mapsto p(z, \overline{z})$, with $z \in \mathbb{C}^n$, is real-valued.

iii) There is a *Hermitian matrix* $Q = (q_{\alpha\beta})$, such that one can represent p as $p(z, \overline{w}) = \sum_{\alpha\beta} q_{\alpha\beta}\, z^\alpha\, \overline{w}^{\,\beta}$.

Let $p \in \mathbb{C}[z, \overline{w}]$ be a Hermitian symmetric polynomial, then p is said to be a *sum of Hermitian squares* if and only if there are complex polynomials $q_1(x), \ldots, q_m(x) \in \mathbb{C}[x]$ such that

$$p(z, \overline{w}) = \sum_{i=1}^{m} q_i(z)\, \overline{q_i(w)} \tag{2.37}$$

holds. In this case, we also say p is *SOHS*. Since $z \mapsto p(z, \overline{z})$ is real-valued and $p(z, \overline{z}) = \sum_{i=1}^m q_i(z)\, \overline{q_i(z)}$ holds, the sum of Hermitian squares determines a real-valued nonnegative function $z \mapsto \sum_{i=1}^m q_i(z)\, \overline{q_i(z)}$. D'Angelo considered eight different positivity classes of Hermitian symmetric polynomials, whereas being SOHS is the strongest condition among them [24].

The SOHS condition can also be verified by the Gram matrix method. For this, we need Hermitian matrices with nonnegative eigenvalues called *Hermitian positive semidefinite matrices*. Analogously to equation (2.30), we transform equation (2.37) to

$$p(z, \overline{w}) = b(z)^{\mathsf{T}} A\, \overline{b(w)},$$

where A is a Hermitian positive semidefinite matrix of dimension $N = \binom{n+d}{d}$ and where the vector $b(x) \in \mathbb{C}[x]^N$ contains a basis of the space of complex polynomials up to degree d.

Since we are dealing with polynomials invariant under a finite pseudo-reflection group, we have a look at the invariant theory of finite pseudo-reflection groups. Due to Theorem 2.15, well known as the *Shephard-Todd-Chevalley theorem* [72], the invariant ring of finite pseudo-reflection groups, can be described by basic invariants only.

Theorem 2.15. *The invariant ring $\mathbb{C}[x]^G$ of a finite matrix group $G \subset GL_n(\mathbb{C})$ is generated by n algebraically independent homogeneous invariants if and only if G is a finite pseudo-reflection group.*

Hence, the invariant ring $\mathbb{C}[x]^G$ is generated by n basic invariants:

$$\mathbb{C}[x_1, \ldots x_n]^G = \mathbb{C}[\theta_1, \ldots, \theta_n]\,. \tag{2.38}$$

Since basic invariants are homogeneous, algebraically independent polynomials, the invariant ring is a free algebra. The basic invariants are not uniquely determined by the group, but their degrees are. In [72], Sturmfels gives more information about the invariant theory. Furthermore, Stanley published a survey [68] about the invariant theory of finite groups, in which he also describes the theory of Shephard and Todd, and Chevalley.

Any action of the group keeps the grading of the polynomials invariant. Therefore we can decompose the invariant ring into homogeneous subspaces, which are invariant under the action of G. The set of *homogeneous polynomials* of degree k is defined by

$$\mathrm{Hom}_k = \left\{ p \in \mathbb{C}[x] : p(\alpha x) = \alpha^k p(x) \text{ for all } \alpha \in \mathbb{C}, \deg p = k \right\}. \tag{2.39}$$

The intersection of the homogeneous polynomials with the invariant ring contains the *homogeneous invariant polynomials*:

$$\mathrm{Hom}_k^G = \mathbb{C}[x]^G \cap \mathrm{Hom}_k \,. \tag{2.40}$$

The dimension of each homogeneous invariant subspace can be determined by using the *Molien's series*

$$\sum_{k=0}^{\infty} \dim \mathrm{Hom}_k^G t^k = \left(\prod_{i=1}^{n} \left(1 - t^{d_i}\right) \right)^{-1} , \tag{2.41}$$

where d_i are the degrees of the basic invariants θ_i. For the groups A_n, B_n, D_n, E_6, E_7, E_8, F_4, G_2, H_3, H_4, and $I_2(m)$ Humphrey published in [52] a table showing these degrees. Alternatively, one can compute basic invariants by a computer program like Magma [12] to obtain the desired degrees. Furthermore, Sturmfels describes in [72] an algorithm for computing basic invariants.

Due to Theorem 2.11, we know that a $|G|$-dimensional vector space can be decomposed in $|\widehat{G}|$ many subspaces, which can be further decomposed into d_π many subspaces. We use this decomposition in the SOHS calculation to decompose the desired Hermitian positive semidefinite matrix into smaller matrices. To do so, we consider the *coinvariant algebra*, which is defined as the following quotient space

$$\mathbb{C}[x]_G = \mathbb{C}[x]/I \,, \tag{2.42}$$

where $I = (\theta_1, \ldots, \theta_n)$ is the ideal generated by basic invariants. The coinvariant algebra is a graded algebra of finite dimension $|G|$. Like the invariant ring, we can decompose it into homogeneous subspaces of degree k:

$$\mathbb{C}[x]_G = \bigoplus_{k \in \mathbb{Z}_{\geq 0}} (\mathbb{C}[x]_G \cap \mathrm{Hom}_k) \,. \tag{2.43}$$

The dimension and the degree of these homogeneous subspaces are given by the *Poincaré series*, which is defined as

$$P_G(t) = \sum_{i=0}^{m} \dim V_i \, t^{k_i},$$

where $V_i = \mathbb{C}[x]_G \cap \mathrm{Hom}_{k_i}$ is the subspace of $\mathbb{C}[x]_G$ consisting of the homogeneous polynomials of degree k_i, and $m \in \mathbb{N}$ is the maximal degree. For more details on this, see the work of Chevalley [18]. In [48, p. 83], Hiller give the following formula to compute the Poincaré series.

Lemma 2.16. *Let G be a finite group. Its Poincaré series $P_G(t)$ can be computed as*

$$P_G(t) = (1-t)^{-n} \prod_{i=1}^{n} \left(1 - t^{d_i}\right), \tag{2.44}$$

where d_i are the degrees of the basic invariants θ_i.

An alternative formula to calculate the Poincaré series $P_G(t)$ is given in Lemma 2.17.

Lemma 2.17. *Let G be a finite group. Its Poincaré series $P_G(t)$ can be computed as*

$$P_G(t) = (1-t)^{-n}|G| \left(\sum_{[g]\in\overline{G}} \frac{\|[g]\|}{\det(I_n - tg)} \right)^{-1},$$

where I_n denotes the $n \times n$ identity matrix, $\overline{G}$ is the set of conjugacy classes of G and $g \in [g]$ is a representative of the conjugacy class $[g] \in \overline{G}$.

Lemma 2.17 can be deduced by combining the following results of Hiller [48, (2.1 b), (2.5)]:

$$P_G(t) = \frac{P(t)}{P^G(t)},$$

with

$$P(t) = (1-t)^{-n} \quad \text{and} \quad P^G(t) = \frac{1}{|G|} \sum_{g\in G} \frac{1}{\det(I_n - tg)},$$

where $P(t)$ is the Poincaré series of $\mathbb{C}[x]$ and $P^G(t)$ denotes the Poincaré series of $\mathbb{C}[x]^G$. Analogously to $P_G(t)$, the Poincaré series $P(t)$ and $P^G(t)$ are counting the dimension of the homogeneous subspaces of $\mathbb{C}[x]$ and $\mathbb{C}[x]^G$. We use the following theorem of Chevalley to express the set of complex polynomials.

Theorem 2.18. *Let G be a finite pseudo-reflection group. Then the following equation holds:*

$$\mathbb{C}[x] = \mathbb{C}[x]_G \otimes \mathbb{C}[x]^G.$$

More information about Theorem 2.18 are, for example, given in [72]. For checking whether a polynomial $p(z, \overline{w}) \in \mathbb{C}[z, \overline{w}]$ is SOHS, we can use a basis $b(x)$ of $\mathbb{C}[x]$, for example the standard monomial basis, and try to find a positive semidefinite matrix A satisfying $\mathrm{p}(z, \overline{w}) = \langle A, B\rangle$, with $B = \overline{b(w)}\, b(z)^{\mathsf{T}}$. To simplify the SOHS calculation, we want to decompose the polynomial $p = \langle P, Q\rangle$, such that P contains elements of $\mathbb{C}[x]^G$ and Q contains a basis of $\mathbb{C}[x]_G$. The benefit is that we know how to decompose these subspaces into smaller subspaces. To calculate this decomposition, we have a look at the basis of the coinvariant algebra. Due to the following theorem of Chevalley [52], we know that there exists a regular representation $\rho : G \to \mathrm{GL}(\mathbb{C}[x]_G)$, which we use to calculate the decomposition of $\mathbb{C}[x]_G$.

Theorem 2.19. *Viewed as a $\mathbb{C}[\theta_1, \ldots, \theta_n]$-module, $\mathbb{C}[x_1, \ldots, x_n]$ is free of rank $|G|$. Moreover, the action of G on $\mathbb{C}[x_1, \ldots, x_n]/(\theta_1, \ldots, \theta_n)$ is isomorphic to the regular representation of G.*

This regular representation can be transformed into a unitary representation, which is decomposable into irreducible unitary representations. Furthermore, we can apply the Peter-Weyl theorem [74, Chapter 15]: There exist homogeneous polynomials

$$\varphi_{ij}^{\pi} \text{ with } \pi \in \widehat{G}, \tag{2.45}$$

which form a basis of the coinvariant algebra $\mathbb{C}[x]_G$, such that

$$g\varphi_{ij}^{\pi} = \left(\pi(g)_j\right)^{\mathsf{T}} \begin{pmatrix} \varphi_{i1}^{\pi} \\ \vdots \\ \varphi_{id_\pi}^{\pi} \end{pmatrix}, \quad i = 1, \ldots, d_\pi, \tag{2.46}$$

where d_π is the dimension of π, holds for all $g \in G$. Here, $\pi(g)_j$ denotes the j-th column of the unitary matrix $\pi(g) \in \mathrm{U}(d_\pi)$.

We want to work with Hermitian symmetric polynomials, therefore we have to extend the action of the group G from the complex polynomials $\mathbb{C}[x]$ to the Hermitian symmetric polynomials $\mathbb{C}[z, \overline{w}]$ by

$$(gp)(z, \overline{w}) = p(g^{-1}z, \overline{g^{-1}w}).$$

Analogously, we have to define the *ring of G-invariant Hermitian symmetric polynomials* by

$$\mathbb{C}[z, \overline{w}]^G = \{p \in \mathbb{C}[z, \overline{w}] : gp = p \text{ for all } g \in G\}.$$

As mentioned before, we want to express a polynomial p by using a matrix P, which contains elements of the invariant ring $\mathbb{C}[x]^G$ and a matrix Q, whose elements build a basis of the coinvariant algebra $\mathbb{C}[x]_G$. The coinvariant algebra $\mathbb{C}[x]_G$ can be decomposed into subspaces, such that for each irreducible representation $\pi \in \widehat{G}$, there exists one corresponding subspace. The vectors φ_{ij}^{π} from (2.45) correspond to the basis vectors of the subspace V^{π} of $V = \mathbb{C}[x]_G$. This decomposition implies that the matrix Q is a block matrix. Therefore, the trace inner product $\langle P, Q \rangle$ can be written as $\sum_{\pi \in \widehat{G}} \langle P^{\pi}, Q^{\pi} \rangle$. In the following theorem, we use this decomposition for Hermitian symmetric polynomials to simplify the SOHS checking.

Theorem 2.20. *Let $G \subseteq \mathrm{GL}_n(\mathbb{C})$ be a finite group generated by pseudo-reflections. The convex cone of G-invariant Hermitian symmetric polynomials which can be written as sums of Hermitian squares equals*

$$\Big\{p \in \mathbb{C}[z, \overline{w}]^G : p(z, \overline{w}) = \sum_{\pi \in \widehat{G}} \langle P^{\pi}(z, \overline{w}), Q^{\pi}(z, \overline{w}) \rangle \ , \\ P^{\pi}(z, \overline{w}) \text{ is a Hermitian SOS matrix polynomial in } \theta_i\Big\}.$$

Here $\langle A, B \rangle = \mathrm{Tr}(B^* A)$ denotes the trace inner product, the matrix $P^{\pi}(z, \overline{w})$ is a Hermitian SOS matrix polynomial in the variables $\theta_1, \ldots, \theta_n$, i.e. there is a matrix $L^{\pi}(z)$ with entries in $\mathbb{C}[z]^G = \mathbb{C}[\theta_1, \ldots, \theta_n]$ such that

$$P^{\pi}(z, \overline{w}) = L^{\pi}(z) \, \overline{L^{\pi}(w)}^{\mathsf{T}}$$

holds, and $Q^\pi(z,\overline{w}) \in (\mathbb{C}[z,\overline{w}]^G)^{d_\pi \times d_\pi}$ *is defined componentwise by*

$$[Q^\pi]_{kl}(z,\overline{w}) = \sum_{i=1}^{d_\pi} \varphi_{ki}^\pi(z)\,\overline{\varphi_{li}^\pi(w)}\,.$$

Proof. Let $p(z,\overline{w})$ be a G-invariant SOHS polynomial in $\mathbb{C}[z,\overline{w}]^G$ of degree at most $2d$, thus there exists a Hermitian positive semidefinite matrix A of dimension $N = \binom{n+d}{d}$ such that

$$p(z,\overline{w}) = b(z)^\mathsf{T} A\,\overline{b(w)}\,,$$

where $b(z) \in \mathbb{C}[x]^N$ is a vector that contains a basis of the space of complex polynomials up to degree d. The SOHS polynomial can be decomposed in a similar way as the SOS polynomial in (2.35). Thus, we can decompose the vector space $\mathbb{C}[z,\overline{w}]^N$ into vector subspaces for each irreducible representation $\pi \in \widehat{G}$ and there exists a unitary base change matrix T expressing the corresponding projection. Hence, we get

$$p(z,\overline{w}) = \sum_{\pi\in\widehat{G}} b^\pi(z)^\mathsf{T} S^\pi\,\overline{b^\pi(w)}\,,$$

where

$$Tb(x) = \begin{pmatrix} b^{\pi_1}(x) \\ \vdots \\ b^{\pi_{|\widehat{G}|}}(x) \end{pmatrix} \text{ with } b^\pi \in \mathbb{C}[x]^{m_\pi \cdot d_\pi} \tag{2.47}$$

and S^π is a Hermitian positive semidefinite matrix of dimension $m_\pi \cdot d_\pi$. Furthermore, we define

$$Z^\pi(z,\overline{w}) = \begin{pmatrix} Z_1^\pi(z,\overline{w}) & & 0 \\ & \ddots & \\ 0 & & Z_{m_\pi}^\pi(z,\overline{w}) \end{pmatrix}$$

with

$$Z_i^\pi(z,\overline{w}) = b_i^\pi(z)\,\overline{b_i^\pi(w)}^T \in \mathbb{C}[z,\overline{w}]^{d_\pi \times d_\pi}.$$

Due to Theorem 2.18, the set of complex polynomials is equal to the tensor product of the coinvariant algebra and the invariant ring

$$\mathbb{C}[x] = \mathbb{C}[x]_G \otimes \mathbb{C}[x]^G.$$

Thus, each $q(x) \in \mathbb{C}[x]$ can be computed as a sum of products of a coinvariant monomial and invariant monomials in the basic invariants. Formally, $q(x)$ is equal to a sum over elements

$$\varphi_{jk}^\pi \prod_{i\in[n]} \theta_i(x)^{l_i}, \tag{2.48}$$

with powers $l \in \mathbb{Z}_{\geq 0}^n$, and where φ_{jk}^π for $j,k \in [d_\pi]$ form a basis of $\mathbb{C}[x]_G$. This parameterization of the elements in $\mathbb{C}[x]$ is not unique.

Since the entries of the basis elements $b_i^\pi(x)$ are elements in $\mathbb{C}[x]$, they can be described by the basis elements $\varphi_{ij}^\pi(x)$ of the coinvariant algebra and the basic invariants θ_i as in (2.48). Furthermore, there exists generators of $\mathbb{C}[x]_{\leq d}$ of the form (2.48). The matrix Q^π is defined as in Theorem 2.20:

$$[Q^\pi]_{kl}(z,\overline{w}) = \sum_{i=1}^{d_\pi} \varphi_{ki}^\pi(z)\,\overline{\varphi_{li}^\pi(w)}.$$

Then, we can express the elements in $Z^\pi(z,\overline{w})$ in the form (2.48) by applying a basis change matrix to $Z^\pi(z,\overline{w})$ in such a way that the new matrix is

$$\widetilde{Z}^\pi(z,\overline{w}) = \begin{pmatrix} \widetilde{Z}_{11}^\pi(z,\overline{w}) & \cdots & \widetilde{Z}_{1t_\pi}^\pi(z,\overline{w}) \\ \vdots & \ddots & \vdots \\ \widetilde{Z}_{t_\pi 1}^\pi(z,\overline{w}) & \cdots & \widetilde{Z}_{t_\pi t_\pi}^\pi(z,\overline{w}) \end{pmatrix}$$

with

$$\widetilde{Z}_{ij}^\pi(z,\overline{w}) = v^\pi(z)_i\ \overline{v^\pi(w)}_j^{\mathsf{T}}\ Q^\pi(z,\overline{w}) \quad \text{for all } i,j \in [t_\pi],$$

where $v^\pi(x)$ be a vector that contains all monomials in the basic invariants up to degree $d - \min\{\deg \varphi_{ii}^\pi(x) : i \in [d_\pi]\}$. The value of t_π depends on π as well as on the degree of the basic invariants and on the degree of the elements in the coinvariant algebra. By restricting the degrees, we obtain a unique parameterization. Using this parameterization, the following equation holds

$$\widetilde{Z}^\pi(z,\overline{w}) = \left(v^\pi(z)\,\overline{v^\pi(w)}^{\mathsf{T}}\right) \otimes Q^\pi(z,\overline{w}).$$

According to the previous transformation of $Z^\pi(z,\overline{w})$ to $\widetilde{Z}^\pi(z,\overline{w})$, we can apply a basis change matrix to the Hermitian positive semidefinite matrix S^π to obtain a Hermitian positive semidefinite matrix $\widetilde{S}^\pi$, such that

$$p(z,\overline{w}) = \sum_{\pi\in\widehat{G}} \left\langle \widetilde{S}^\pi, \widetilde{Z}^\pi \right\rangle. \tag{2.49}$$

We first have to compute the basis change matrix for the transformation of $Z^\pi(z,\overline{w})$ and then, we determine a basis change matrix for S^π, such that $\langle S^\pi, Z^\pi\rangle = \langle \widetilde{S}^\pi, \widetilde{Z}^\pi\rangle$ and thus the equation in (2.49) holds. Using the new parameterizations, we get

$$p(z,\overline{w}) = \sum_{\pi\in\widehat{G}} \left\langle \widetilde{S}^\pi, \left(v^\pi(z)\,\overline{v^\pi(w)}^{\mathsf{T}}\right) \otimes Q^\pi(z,\overline{w}) \right\rangle.$$

We want to exchange the factors of the Kronecker product, thus we need to permute the entries of the matrix $\widetilde{S}^\pi$; We denote the new matrix by $\check{S}^\pi$:

$$p(z,\overline{w}) = \sum_{\pi\in\widehat{G}} \left\langle \check{S}^\pi, Q^\pi(z,\overline{w}) \otimes \left(v^\pi(z)\,\overline{v^\pi(w)}^{\mathsf{T}}\right) \right\rangle.$$

Next, we use a property of the Kronecker product which states $(A \otimes B)(C \otimes D) = (AC \otimes BD)$. Since $Q^\pi = I_{d_\pi} Q^\pi I_{d_\pi}$ and $v^\pi(w)\,\overline{v^\pi(w)}^{\mathsf{T}} = v^\pi(w) 1\,\overline{v^\pi(w)}^{\mathsf{T}}$, we obtain

$$p\,(z, \overline{w}) = \sum_{\pi \in \widehat{G}} \left\langle \check{S}^\pi, \left(I_{d_\pi} \otimes v^\pi(z)\right) \left(Q^\pi(z, \overline{w}) \otimes 1\right) \left(I_{d_\pi} \otimes \overline{v^\pi(w)}\right)^{\mathsf{T}} \right\rangle .$$

As the trace is invariant under permutations, we can use $\langle A, BCD\rangle = \langle DAB, C\rangle$ and thus

$$p(z, \overline{w}) = \sum_{\pi \in \widehat{G}} \left\langle \left(I_{d_\pi} \otimes \overline{v^\pi(w)}\right)^{\mathsf{T}} \check{S}^\pi \left(I_{d_\pi} \otimes v^\pi(z)\right), Q^\pi(z, \overline{w}) \right\rangle .$$

For each irreducible representation $\pi \in \widehat{G}$, we define a matrix $P^\pi(z, \overline{w})$ by

$$P^\pi(z, \overline{w}) = \left(I_{d_\pi} \otimes \overline{v^\pi(w)}\right)^{\mathsf{T}} \check{S}^\pi \left(I_{d_\pi} \otimes v^\pi(z)\right) .$$

Thus, the following equation holds

$$p(z, \overline{w}) = \sum_{\pi \in \widehat{G}} \langle P^\pi(z, \overline{w}), Q^\pi(z, \overline{w}) \rangle .$$

Since $\widetilde{S}^\pi$ is positive semidefinite, $\check{S}^\pi$ is as well. Hence, for each matrix $P^\pi(z, \overline{w})$ there exists a matrix $L^\pi(x)$, such that

$$P^\pi(z, \overline{w}) = L^\pi(z)\,\overline{L^\pi(w)}^{\mathsf{T}}.$$

Since all entries of the matrices $P^\pi(z, \overline{w})$ are elements of the invariant ring, the entries of $L^\pi(x)$ have to be elements of $\mathbb{C}[x]^G$. □

The basis elements φ^π_{ij} are independent of the degree of the polynomial p. Due to Theorem 2.20, we can check whether a given polynomial that is invariant under a finite pseudo-reflection group G is SOHS by calculating many smaller Hermitian positive semidefinite matrices instead of one large Hermitian matrix. This makes the calculation much easier, since we calculate less matrix entries.

If all unitary representations are orthogonal, the G-invariant polynomials have to be real. In this case, we can reformulate Theorem 2.20 as follows

Theorem 2.21. *Let $G \subseteq \mathrm{GL}_n(\mathbb{R})$ be a finite group generated by pseudo-reflections so that all unitary irreducible representation $\pi \in \widehat{G}$ of G are orthogonal. The convex cone of G-invariant real polynomials which can be written as sums of squares equals*

$$\Big\{ p \in \mathbb{C}[x]^G \cap \mathbb{R}[x] : p(x) = \sum_{\pi \in \widehat{G}} \langle P^\pi(x), Q^\pi(x) \rangle \ , \\ P^\pi(x) \text{ is an SOS matrix polynomial in } \theta_i \Big\} .$$

Here the matrix $P^\pi(x)$ is an SOS matrix polynomial in the variables $\theta_1, \ldots, \theta_n$, i.e. there is a matrix $L^\pi(x)$ with entries in $\mathbb{R}[x]^G = \mathbb{R}[\theta_1, \ldots, \theta_n]$ such that

$$P^\pi(x) = L^\pi(x)\, L^\pi(x)^{\mathsf{T}}$$

holds, and $Q^\pi(x) \in (\mathbb{R}[x]^G)^{d_\pi \times d_\pi}$ *is defined componentwise by*

$$[Q^\pi]_{kl}(x) = \sum_{i=1}^{d_\pi} \varphi_{ki}^\pi(x)\, \varphi_{li}^\pi(x) \,.$$

Proof. For a G-invariant real polynomial $p(x) \in \mathbb{C}[x]^G \cap \mathbb{R}[x] =: \mathbb{R}[x]^G$ there exists a positive semidefinite matrix S^π for all $\pi \in \widehat{G}$ such that

$$p(x) = \sum_{\pi \in \widehat{G}} \sum_{i=1}^{m_\pi} \left\langle S_i^\pi, b_i^\pi(x)\, b_i^\pi(x)^\mathsf{T} \right\rangle \,.$$

Since $G \subseteq \mathrm{GL}_n(\mathbb{R})$, the coefficients of the monomials in the basic invariants $\theta_1, \ldots, \theta_n$ are real and, furthermore, for the invariant ring $\mathbb{R}[x]^G = \mathbb{R}[\theta_1, \ldots, \theta_n]$ holds. Moreover, from $G \subseteq \mathrm{GL}_n(\mathbb{R})$ it follows that the unitary matrices $\pi(g)$ are real-valued and thus the projection of Serre maps polynomials in $\mathbb{R}[x]$ to polynomials in $\mathbb{R}[x]$. The polynomials stay real under the Gram-Schmidt orthonormalization method, since the G-invariant norm $\|\cdot\|_G$ is real-valued. Thus, the basis elements $\varphi_{jk}^\pi(x)$ are real polynomials. By using the decomposition $\mathbb{R}[x] = \mathbb{R}[x]^G \otimes \mathbb{R}[x]_G$ the proof of Theorem 2.21 is analogously to the proof of Theorem 2.20. □

To apply Theorem 2.20 or Theorem 2.21, we have to calculate the matrix Q^π, which consists of the basis elements $\varphi_{jk}^\pi(x)$ of the coinvariant algebra $\mathbb{C}[x]_G$ or $\mathbb{R}[x]_G$. We will now just consider the complex case, because for real polynomials the calculation is similar. Since the group action respects the grading on $\mathbb{C}[x]$, the following equation holds

$$p^\pi(\mathbb{C}[x]) = \bigoplus_{k \in \mathbb{Z}_{\geq 0}} p^\pi(\mathrm{Hom}_k) \,,$$

where p^π is the projection given in (2.28). Combining the decomposition in Theorem 2.11 with formula (2.43), the coinvariant algebra can be decomposed as

$$\mathbb{C}[x]_G = \bigoplus_{\pi \in \widehat{G}} \bigoplus_{k=0}^{k_m} V_k^\pi \,, \tag{2.50}$$

where

$$V_k^\pi = p^\pi(\mathbb{C}[x]_G \cap \mathrm{Hom}_k)$$

and k_m is the maximal degree, which is equal to the degree of the Poincaré series.

To avoid zero summands in the decomposition, we are just interested in the values for k which appear in the subset V^π for $\pi \in \widehat{G}$. The Poincaré series $P_G(t)$ can be decomposed into a sum of $P_{G,\pi}(t)$ over the set of irreducible representations $\pi \in \widehat{G}$ to get these information. We define for each $\pi \in \widehat{G}$,

$$P_{G,\pi}(t) = \sum_{i=1}^{d_\pi} d_\pi t^{k_i^\pi},$$

where $d_\pi = \dim \pi$. In [68, p. 489], Stanley gives the following lemma.

Lemma 2.22. *Let G be a finite pseudo-reflection group and $\pi \in \widehat{G}$. The Poincaré series $P_{G,\pi}(t)$ of the isotypic component belonging to π is given by*

$$P_{G,\pi}(t) = \frac{1}{|G|} \prod_{i=1}^{n} \left(1 - t^{d_i}\right) \sum_{g \in G} \frac{\chi^{\pi}(g)}{\det\ (I_n - tg)} \,,$$

where I_n denotes the $n \times n$ identity matrix and the d_i's are the degrees of the basic invariants.

A proof of Lemma 2.22 is given in [16, Proposition 11.1.1]. Instead of summing over all elements of the group G, we can alternatively use the following equation,

$$P_{G,\pi}(t) = \frac{1}{|G|} \prod_{i=1}^{n} \left(1 - t^{d_i}\right) \sum_{[g] \in \overline{G}} \frac{|[g]|\, \chi^{\pi}(g)}{\det\ (I_n - tg)} \,,$$

in which we just have to sum over the conjugacy classes $[g] \in \overline{G}$ of G. Let n_π be the number of non-zero monomials in $P_{G,\pi}(t)$ and $l_1^\pi, \ldots, l_{n_\pi}^\pi$ be the powers of t occurring in $P_{G,\pi}(t)$. We can describe the decomposition in (2.50) by

$$\mathbb{C}[x]_G = \bigoplus_{\pi \in \widehat{G}} \bigoplus_{i=1}^{n_\pi} \tilde{V}_i^\pi \tag{2.51}$$

and

$$\tilde{V}_i^\pi = p^\pi(\mathbb{C}[x]_G \cap \mathrm{Hom}_{l_i^\pi}) \,.$$

Since multiple powers k_j^π can be equal to l_i^π in $P_{G,\pi}(t)$, we can deduce that the dimension of $\tilde{V}_i^\pi$ is a multiple of d_π, which is the dimension of each subspace V_i^π. This multiple factor is denoted by $m(l_i^\pi)$.

Example 2.23. We consider the group H_3: Its Poincaré series is

$$\begin{aligned} P_{\mathsf{H}_3}(t) &= (1-t)^{-3}(1-t^2)(1-t^6)(1-t^{10}) \\ &= 1 + 3t + 5t^2 + 7t^3 + 9t^4 + 11t^5 + 12t^6 + 12t^7 + 12t^8 \\ &\quad + 12t^9 + 11t^{10} + 9t^{11} + 7t^{12} + 5^{13} + 3t^{14} + t^{15} \end{aligned}$$

If we use the decomposition in (2.50), then we would decompose $\mathbb{C}[x]_G$ into subspaces V_k^π for $\pi \in \widehat{G}$ and $k \in [0, \ldots, k_m]$. Since the group H_3 has ten irreducible non-equivalent unitary representations and $k_m = \deg P_{\mathsf{H}_3}(t) = 15$, we would obtain 160 subspaces.

Alternatively, we consider $P_{\mathsf{H}_3,\pi}(t)$, the Poincaré series for each irreducible representation π of H_3, given in Table 2.1. If we decompose $\mathbb{C}[x]_G$ like in (2.51), we obtain the subspaces $\tilde{V}_i^\pi$ for $\pi \in \widehat{G}$ and $i = [n_\pi]$. Since n_π is the number of powers which occur in $P_{\mathsf{H}_3,\pi}(t)$, the number of subspaces $P_{\mathsf{H}_3,\pi}(t)$ is equal to 32. For example for $\pi = T_{2g}$, we get $l_1^\pi = 6$, $l_2^\pi = 10$, $l_3^\pi = 14$, and $n_\pi = 3$.

To apply the projection p^π given in (2.28) on Hom_k, we consider the representation

$$\rho_k : G \to \mathsf{GL}(\mathrm{Hom}_k) \quad \text{with} \quad \rho_k(g)(p) \mapsto gp$$

$A_g : t^0$	$A_u : t^{15}$
$T_{1g} : 3(t^8 + t^{10} + t^{12})$	$T_{1u} : 3(t^3 + t^5, t^7)$
$T_{2g} : 3(t^6 + t^{10} + t^{14})$	$T_{2u} : 3(t^1 + t^5 + t^9)$
$G_g : 4(t^4 + t^6 + t^8 + t^{12})$	$G_u : 4(t^3 + t^7 + t^9 + t^{11})$
$H_g : 5(t^2 + t^4 + t^6 + t^8 + t^{10})$	$H_u : 5(t^5 + t^7 + t^9 + t^{11} + t^{13})$

Table 2.1: Poincaré series $P_{\mathsf{H}_3,\pi}(t)$ for each irreducible representation π of H_3.

and transform this into a representation $\tilde{\rho}_k : G \to \mathrm{GL}_N(\mathbb{C})$ in matrix form, with $N = \dim \mathrm{Hom}_k$: To do so, we define

$$\psi_k : \mathrm{Hom}_k \to \mathbb{C}^N \quad \text{with} \quad m_i \mapsto e_i \,,$$

where $\{m_1, \ldots, m_N\}$ are homogeneous monomials which form a basis of Hom_k. Then, the desired matrix $\tilde{\rho_k}$ is given by

$$(\tilde{\rho_k}(g))_{ij} = \left(\psi_k\left(\rho_k(g)\, m_j\right)\right)_i \,.$$

By using this matrix representation, we can apply p^π of (2.28) on Hom_k: The projection p_k^π with image V_k^π is defined as

$$\begin{aligned} p_k^\pi : \mathrm{Hom}_k \to \mathrm{Hom}_k, \quad p_k^\pi(f) &= \frac{d_\pi}{|G|} \sum_{g\in G} \chi^\pi\left(g^{-1}\right)\, \psi_k^{-1}\left(\tilde{\rho_k}(g)\, \psi_k(f)\right) \\ &= \psi_k^{-1}\left(\left(\frac{d_\pi}{|G|} \sum_{g\in G} \chi^\pi\left(g^{-1}\right)\tilde{\rho_k}(g)\right)\, \psi_k(f)\right) \,. \end{aligned}$$

Since for $p \in \mathrm{Hom}_k$, $\rho(g)$ and $\tilde{\rho_k}(g)$ maps p to gp, we get the identity $p^\pi(\mathrm{Hom}_k) = p_k^\pi(\mathrm{Hom}_k)$.

To calculate a basis φ_{ij}^π for $i, j \in [d_\pi]$ of the coinvariant algebra, which is suitable for Theorem 2.20, the basis elements have to satisfy the equation (2.41). Since due to Peter-Weyl theorem, there exists such a basis for unitary irreducible representations of G, we first transform each irreducible representation $\pi \in \widehat{G}$ into a unitary representation. To do so, we determine a basis of each subspace V_1^π with minimal degree k_1^π and apply the Gram-Schmidt orthonormalization to obtain an orthonormal basis:

Without loss of generality, we assume that $k_1^\pi \leq \ldots \leq k_{d_\pi}^\pi$ and $l_1^\pi < \ldots < l_{n_\pi}^\pi$. By definition $k_1^\pi = l_1^\pi$ and $V_1^\pi \subseteq \tilde{V}_1^\pi$. Furthermore,

$$\tilde{V}_1^\pi = \bigoplus_{j=1}^{m(l_i^\pi)} V_j^\pi \,.$$

In general

$$V_j^\pi \subseteq p^\pi\left(\mathrm{Hom}_{k_j^\pi} \cap \mathbb{C}[x]_G\right) \subseteq p^\pi\left(\mathrm{Hom}_{k_j^\pi}\right).$$

For the icosahedral group H_3 and the octahedral group B_3, we get

$$V_1^\pi = p^\pi\left(\mathrm{Hom}_{k_1^\pi} \cap \mathbb{C}[x]_G\right) = p^\pi\left(\mathrm{Hom}_{k_1^\pi}\right).$$

In that case, we take a basis $\left\{b_1^\pi, \ldots, b_{d_\pi}^\pi\right\}$ of $p^\pi(\mathrm{Hom}_{k_1^\pi})$. To obtain an orthonormal basis $\left\{\varphi_{11}^\pi, \ldots, \varphi_{1d_\pi}^\pi\right\}$ of V_1^π, we apply the Gram-Schmidt orthonormalization method by using the G-invariant inner product defined in (2.23). To do so, we first have to compute a matrix representation $\rho_1^\pi : G \to \mathrm{GL}_{d_\pi}(\mathbb{C})$:

$$\left(\rho_1^\pi(g)\right)_{ij} = \left(\psi_1^\pi\left(g\, b_j^\pi\right)\right)_i,$$

where $\psi_1^\pi : V_1^\pi \to \mathbb{C}^{d_\pi}$ with $b_i^\pi \mapsto e_i$. Using the obtained matrix representation, we can apply the Gram-Schmidt orthonormalization:

$$\begin{aligned}\langle\cdot,\cdot\rangle_G : & V_1^\pi \times V_1^\pi \to \mathbb{C} \\ & (u,v) \to \langle u, v\rangle_G = \overline{\psi_1^\pi(u)}^{\mathsf{T}}\left(\frac{1}{|G|}\sum_{g\in G}\overline{\rho_1^\pi(g)}^{\mathsf{T}}\rho_1^\pi(g)\right)\psi_1^\pi(v)\,,\end{aligned}$$

and the corresponding G-invariant norm

$$\|\cdot\|_G = \sqrt{\langle\cdot,\cdot\rangle_G}\,.$$

The orthonormal basis $\left\{\varphi_{11}^\pi, \ldots, \varphi_{1d_\pi}^\pi\right\}$ for V_1^π can be computed as

$$\begin{aligned}\varphi_{11}^\pi &= \frac{b_1^\pi}{\|b_1^\pi\|_G}, \\ \varphi_{1j}^\pi &= \frac{\tilde{b}_j^\pi}{\|\tilde{b}_j^\pi\|_G}, \text{ with } \tilde{b}_j^\pi = b_j^\pi - \sum_{i=1}^{j-1}\varphi_{1i}^\pi\left\langle\varphi_{1i}^\pi, b_j^\pi\right\rangle_G, \text{ for } j \in \{2,\ldots,d_\pi\}.\end{aligned}$$

Since we have now an orthonormal basis of the vector subspaces V_1^π for each $\pi \in \widehat{G}$, we can apply Weyl's trick to obtain the unitary irreducible representations: Let T be the basis change matrix, which transforms the basis $\left\{b_1^\pi, \ldots, b_{d_\pi}^\pi\right\}$ to the orthonormal basis $\left\{\varphi_{11}^\pi, \ldots, \varphi_{1d_\pi}^\pi\right\}$, that is

$$T_{ij} = \psi_1^\pi\left(\varphi_{1j}^\pi\right)_i\,.$$

As this matrix is orthogonal, the representation

$$\pi(g) = T^{-1}\,\rho_1^\pi(g)\,T$$

is a unitary representation.

The goal is to compute a suitable basis φ_{ij}^π of the coinvariant algebra which we can use to apply Theorem 2.20. For this, we can use Theorem 2.12 and obtain the linear map

$$p_{k,ij}^\pi : \mathrm{Hom}_k \to \mathrm{Hom}_k \quad \text{by} \quad p_{k,ij}^\pi = \frac{d_\pi}{|G|}\sum_{g\in G}\pi_{ji}\left(g^{-1}\right)\tilde{\rho_k}(g). \tag{2.52}$$

We define $V_{k,i}^{\pi} = p_{k,ii}^{\pi}(V_k^{\pi})$ for $i \in \{1, \ldots, d_\pi\}$. Then $p_{k,ij}^{\pi}$ is an isomorphism from $V_{k,i}^{\pi}$ to $V_{k,j}^{\pi}$ and we have the decomposition

$$V_k^{\pi} = V_{k,1}^{\pi} \oplus \ldots \oplus V_{k,d_\pi}^{\pi}.$$

We consider a non-zero element $\varphi_{k,1}^{\pi} \in V_{k,1}^{\pi}$ and obtain the basis elements $\varphi_{k,i}^{\pi}$ by

$$\varphi_{k,i}^{\pi} = p_{k,i1}^{\pi}\left(\varphi_{k,1}^{\pi}\right).$$

Using this construction, the property

$$\tilde{\rho_k}(g)\left(\varphi_{k,i}^{\pi}\right) = \sum_{j=1}^{d_\pi} \pi_{j,i}(g)\, \varphi_{k,j}^{\pi}\,.$$

holds. In the following two subsections, we calculate this basis explicitly for the octahedral group B_3 and the icosahedral group H_3 .

2.3.2 SOHS invariant under the octrahedral group

To calculate the basis of the coinvariant algebra, we are interested in the irreducible characters of the group. Information about these irreducible characters can be recorded in the form of a character table. For the octahedral group B_3 the character table is pictured in Table 2.2. A character is a *class function*, which is defined to be constant on the conjugacy classes of G. Each row is labeled by an irreducible character and each column is labeled by a conjugacy class. For each pair of an irreducible character and a conjugacy class the character table contains the corresponding constant. The number of conjugacy classes is equal to the number of inequivalent irreducible characters.

Robert S. Mulliken, Nobel laureate in Chemistry in 1966, suggests the Mulliken symbols, which give a scheme for labeling the irreducible characters. The name starts with a capital letter depending on the dimension of the character. One-dimensional characters, which are symmetric when rotating around the principal axis, start with letter A, whereas one-dimensional characters, which are asymmetric when rotating around the principal axis, are denoted by B. For two-, three-, four-, and five-dimensional characters the letters E, T, G, and H are used. To distinguish between $\chi(i) = 1$ and $\chi(i) = -1$, we use the index g (g from German *gerade* meaning *even*) and u (u from German *ungerade* meaning *odd*). Furthermore, the index can contain the number 1 or 2, to note whether the character is symmetric or asymmetric with respect to a reflection plane orthogonal to the principal axis.

The first column is always for the identity E (E from German *Einheit*) and therefore the dimension of each corresponding representation is given in the first column. The inverse operator i with $i(x) = -x$ is represented by the second conjugacy class. The other classes contain the remaining fundamental symmetry operations, which are reflections (denoted by σ from German *Spiegelung*), rotations (denoted by C), and rotation-reflections (denoted by S). The name of each of these conjugacy classes starts with the number of the symmetry operations, followed by the symbol of the operation. Furthermore, 360° divided by the index of this symbol is equal to the degree of the rotation. If the symbol of the operation has also an exponent, then the degree of the rotation has to be multiplied by this exponent. For example, the class C_4 corresponds to the class C_2^2.

	E	i	$3C_2$	$3\sigma_h$	$6C_2'$	$6\sigma_d$	$8C_3$	$6C_4$	$6S_4$	$8S_6$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	−1	1	−1	1	−1	1	1	−1	−1
A_{2g}	1	1	1	1	−1	−1	1	−1	−1	1
A_{2u}	1	−1	1	−1	−1	1	1	−1	1	−1
E_g	2	2	2	2	0	0	−1	0	0	−1
E_u	2	−2	2	−2	0	0	−1	0	0	1
T_{1g}	3	3	−1	−1	−1	−1	0	1	1	0
T_{1u}	3	−3	−1	1	−1	1	0	1	−1	0
T_{2g}	3	3	−1	−1	1	1	0	−1	−1	0
T_{2u}	3	−3	−1	1	1	−1	0	−1	1	0

Table 2.2: The character table of the octahedral group B_3.

The octahedral group B_3 has four one-dimensional characters (A_{1g}, A_{1u}, A_{2g}, A_{2u}), two two-dimensional characters (E_g,E_u) and four four-dimensional characters (T_{1g}, T_{1u}, T_{2g}, T_{2u}). The three clockwise rotation by 180° through the axis of the facet centers build the class $3C_2$ and the three reflections through planes which are parallel to pairs of facets generate the class $3\sigma_h$. The next conjugacy class named $6C_2'$ consists of the six clockwise rotation by 180° through the axis of the edge centers and $6\sigma_d$ represents the six reflections through the planes given by the diagonals of the facets. The class $8C_3$ contains the eight clockwise rotations by 120° through the diagonals of the cube. The six clockwise rotations by 90° through the axis of the facet centers build the class $6C_4$. The class $6S_4$ consists of the six rotation-reflections by 90° through the axis of the facet centers, and $8S_6$ consists of the eight rotation-reflections by 60° through the diagonals of the cube. Thus the group consists of 48 symmetry operations.

We are interested in the coinvariant algebra $\mathbb{C}[x]_{\mathsf{B}_3} = \mathbb{C}[x]/I$, where I is the ideal generated by the basic invariants of B_3. This reflection group has three basic invariants with degree 2, 4, and 6:

$$\theta_1 = x_1^2 + x_2^2 + x_3^2, \quad \theta_2 = x_1^4 + x_2^4 + x_3^4, \quad \theta_3 = x_1^6 + x_2^6 + x_3^6 \,.$$

Now we have all information to calculate its Poincaré series:

$$\begin{aligned} P_{\mathsf{B}_3}(t) &= (1-t)^{-3}(1-t^2)(1-t^4)(1-t^6) \\ &= 1 + 3t + 5t^2 + 7t^3 + 8t^4 + 8t^5 + 7t^6 + 5t^7 + 3t^8 + 1t^9, \end{aligned}$$

which gives us information about the subspaces of $\mathbb{C}[x]_{\mathsf{B}_3}$ and its dimension. Since the powers of t in the Poincaré series range from 0 to 9, we can decompose the coinvariant algebra into ten homogeneous subspaces

$$\mathbb{C}[x]_{\mathsf{B}_3} = \bigoplus_{k\geq 0} (\mathbb{C}[x]_{\mathsf{B}_3} \cap \mathrm{Hom}_k) = V_0 \oplus \ldots \oplus V_9$$

according to the grading by degree. Furthermore, the dimension of each subspace V_k is given by the coefficients of t^k in $P_{\mathsf{B}_3}(t)$.

Furthermore, from the character table we know that the group B_3 has ten irreducible characters and thus ten irreducible representations. The coinvariant algebra can also be decomposed into the following ten subspaces (one per irreducible representation)

$$\mathbb{C}[x]_{\mathsf{B}_3} = \bigoplus_{\pi \in \widehat{\mathsf{B}_3}} V^{\pi}.$$

The dimension and the degree of these subspaces can be obtained by the character table pictured in Table 2.2 or by the Poincaré series $P_{\mathsf{B}_3,\pi}(t)$ for each irreducible representation π of B_3 given in Table 2.3.

$A_{1g} : t^0$	$A_{1u} : t^3$	$A_{2g} : t^6$	$A_{2u} : t^9$
$E_g : 2(t^5 + t^7)$	$E_u : 2(t^2 + t^4)$		
$T_{1g} : 3(t^4 + t^6 + t^8)$	$T_{1u} : 3(t^3 + t^5 + t^7)$	$T_{2g} : 3(t^2 + t^4 + t^6)$	$T_{2u} : 3(t + t^3 + t^5)$

Table 2.3: Poincaré series $P_{\mathsf{B}_3,\pi}(t)$ for each irreducible representation π of B_3.

According to the Poincare series $P_{\mathsf{B}_3,\pi}(t)$ for each π in $\widehat{\mathsf{B}_3}$ or the character table, the group consists of four one-dimensional representations, two two-dimensional representations and four three-dimensional representations. Due to Theorem 2.11, a vector space with dimension equal to the order of G, can be decomposed into one subspace per irreducible representation and each of these subspaces can be decomposed into d_π many subspaces of dimension d_π. Thus, we get

$$\sum_{\pi \in \widehat{\mathsf{B}_3}} d_\pi^2 = 4 \cdot 1^2 + 2 \cdot 2^2 + 4 \cdot 3^2 = 48 = |\mathsf{B}_3|.$$

We also get this order by multiplying the degree of the irreducible representations

$$\deg \theta_1 \cdot \deg \theta_2 \cdot \deg \theta_3 = 2 \cdot 4 \cdot 6 = 48.$$

Let k_1^π be the smallest degree of the subspace V^π. As described in the previous section, we need to calculate an orthonormal basis for the vector subspace $V_{k_1^\pi}^\pi$, which is the image of $p^\pi(\mathbb{C}[x]_{\mathsf{B}_3} \cap \mathrm{Hom}_{k_1^\pi})$. Using this projection, we get a basis of $V_{k_1^\pi}^\pi$ and by applying the Gram-Schmidt orhonormalization to these basis elements, the orthonormal basis, which is pictured in Table 2.4, will be obtained.

Now that we have calculated the orthonormal basis of $V_{k_1^\pi}^\pi$ for all non-equivalent irreducible representations π of the group B_3, the next task will be the calculation of the remaining basis elements of the coinvariant algebra. For this, we apply the projection defined in (2.52), i.e.,

$$p_{k,ij}^\pi : \mathrm{Hom}_k \to \mathrm{Hom}_k \quad \text{with} \quad p_{k,ij}^\pi = \frac{d_\pi}{|\mathsf{B}_3|} \sum_{g \in \mathsf{B}_3} \pi_{ji}(g^{-1})\, \tilde{\rho}_k(g), \tag{2.53}$$

A_{1g}	1
A_{1u}	$x_1x_2x_3$
A_{2g}	$x_1^4x_2^2 - x_1^4x_3^2 - x_1^2x_2^4 + x_1^2x_3^4 + x_2^4x_3^2 - x_2^2x_3^4$
A_{2u}	$x_1^5x_2^3x_3 - x_1^5x_2x_3^3 - x_1^3x_2^5x_3 + x_1^3x_2x_3^5 + x_1x_2^5x_3^3 - x_1x_2^3x_3^5$
E_g	$x_1^3x_2x_3 - x_1x_2x_3^3$
	$\frac{\sqrt{3}}{3}x_1^3x_2x_3 - \frac{2\sqrt{3}}{3}x_1x_2^3x_3 + \frac{\sqrt{3}}{3}x_1x_2x_3^3$
E_u	$x_1^2 - x_3^2$
	$\frac{\sqrt{3}}{3}x_1^2 - \frac{2\sqrt{3}}{3}x_2^2 + \frac{\sqrt{3}}{3}x_3^2$
T_{1g}	$x_1^3x_2 - x_1x_2^3$
	$x_1^3x_3 - x_1x_3^3$
	$x_2^3x_3 - x_2x_3^3$
T_{1u}	$x_1^2x_2 - x_2x_3^2$
	$x_1^2x_3 - x_2^2x_3$
	$x_1x_2^2 - x_1x_3^2$
T_{2g}	x_1x_2
	x_1x_3
	x_2x_3
T_{2u}	x_1
	x_2
	x_3

Table 2.4: Orthonormal basis φ^{π}_{1j}, with $j = 1, \ldots, d_\pi$, of subspaces $V^{\pi}_{k_1^\pi}$.

By applying this approach, the obtained basis will satisfy condition (2.46), i.e.,

$$\tilde{\rho}_k(g)\varphi^{\pi}_{ij} = \big(\pi(g)_j\big)^{\mathsf{T}} \begin{pmatrix} \varphi^{\pi}_{i1} \\ \vdots \\ \varphi^{\pi}_{id_\pi} \end{pmatrix}, \; i = 1, \ldots, d_\pi, \tag{2.54}$$

for all $g \in \mathsf{B}_3$. Here, $\pi(g)_j$ denotes the j-th column of the unitary matrix $\pi(g) \in \mathrm{U}(d_\pi)$. The calculated basis is displayed in Table 2.5. We can use this basis for the SOS calculation described in the previous section. All irreducible unitary representations of the octahedral group B_3 are orthogonal. Therefore we can use Theorem 2.21 for the SOS calculation instead of the complex version.

A_{1g}	1
A_{1u}	$\theta_1^3 - 3\theta_1\theta_2 + 2\theta_3$
A_{2g}	$-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2$
A_{2u}	$-\theta_1^9 + 12\theta_1^7\theta_2 - 10\theta_1^6\theta_3 - 48\theta_1^5\theta_2^2 + 78\theta_1^4\theta_2\theta_3 + 66\theta_1^3\theta_2^3 - 34\theta_1^3\theta_3^2 - 150\theta_1^2\theta_2^2\theta_3$
	$-9\theta_1\theta_2^4 + 126\theta_1\theta_2\theta_3^2 + 6\theta_2^3\theta_3 - 36\theta_3^3$

E_g	$-2\theta_1^5 + 12\theta_1^3\theta_2 - 4\theta_1^2\theta_3 - 18\theta_1\theta_2^2 + 12\theta_2\theta_3$
	$-2\theta_1^4\theta_2 + 6\theta_1^3\theta_3 + 6\theta_1^2\theta_2^2 - 22\theta_1\theta_2\theta_3 + 12\theta_3^2$
	$\theta_1^7 - 9\theta_1^5\theta_2 + 10\theta_1^4\theta_3 + 19\theta_1^3\theta_2^2 - 36\theta_1^2\theta_2\theta_3 - 3\theta_1\theta_2^3 + 16\theta_1\theta_3^2 + 2\theta_2^2\theta_3$
E_u	$-2\theta_1^2 + 6\theta_2$
	$-2\theta_1\theta_2 + 6\theta_3$
	$\theta_1^4 - 6\theta_1^2\theta_2 + 8\theta_1\theta_3 + \theta_2^2$
T_{1g}	$12\theta_1\theta_3 - 12\theta_2^2$
	$2\theta_1^5 - 12\theta_1^3\theta_2 + 16\theta_1^2\theta_3 + 6\theta_1\theta_2^2 - 12\theta_2\theta_3$
	$2\theta_1^6 - 12\theta_1^4\theta_2 + 10\theta_1^3\theta_3 + 12\theta_1^2\theta_2^2 - 6\theta_1\theta_2\theta_3 - 6\theta_2^3$
	$2\theta_1^6 - 10\theta_1^4\theta_2 + 10\theta_1^3\theta_3 + 10\theta_1\theta_2\theta_3 - 12\theta_3^2$
	$\theta_1^7 - 3\theta_1^5\theta_2 + 2\theta_1^4\theta_3 - 9\theta_1^3\theta_2^2 + 24\theta_1^2\theta_2\theta_3 + 3\theta_1\theta_2^3 - 12\theta_1\theta_3^2 - 6\theta_2^2\theta_3$
	$4\theta_1^6\theta_2 - 3\theta_1^5\theta_3 - 21\theta_1^4\theta_2^2 + 32\theta_1^3\theta_2\theta_3 + 12\theta_1^2\theta_2^3 - 12\theta_1^2\theta_3^2 - 9\theta_1\theta_2^2\theta_3 - 3\theta_2^4$
T_{1u}	$-12\theta_1^3 + 48\theta_1\theta_2 - 36\theta_3$
	$-6\theta_1^4 + 24\theta_1^2\theta_2 - 12\theta_1\theta_3 - 6\theta_2^2$
	$-6\theta_1^3\theta_2 + 6\theta_1^2\theta_3 + 18\theta_1\theta_2^2 - 18\theta_2\theta_3$
	$-2\theta_1^5 + 6\theta_1^3\theta_2 + 2\theta_1^2\theta_3 - 6\theta_2\theta_3$
	$\theta_1^6 - 9\theta_1^4\theta_2 + 8\theta_1^3\theta_3 + 15\theta_1^2\theta_2^2 - 12\theta_1\theta_2\theta_3 - 3\theta_2^3$
	$\theta_1^7 - 6\theta_1^5\theta_2 + 5\theta_1^4\theta_3 + 3\theta_1^3\theta_2^2 + 6\theta_1\theta_2^3 - 9\theta_2^2\theta_3$
T_{2g}	$3\theta_1^2 - 3\theta_2$
	$6\theta_1\theta_2 - 6\theta_3$
	$-\theta_1^4 + 6\theta_1^2\theta_2 - 2\theta_1\theta_3 - 3\theta_2^2$
	$-2\theta_1^4 + 12\theta_1^2\theta_2 - 10\theta_1\theta_3$
	$-\theta_1^5 + 4\theta_1^3\theta_2 - 2\theta_1^2\theta_3 + 3\theta_1\theta_2^2 - 4\theta_2\theta_3$
	$-2\theta_1^4\theta_2 + \theta_1^3\theta_3 + 9\theta_1^2\theta_2^2 - 7\theta_1\theta_2\theta_3 - 3\theta_2^3 + 2\theta_3^2$
T_{2u}	$6\theta_1$
	$6\theta_2$
	$6\theta_3$
	$6\theta_3$
	$\theta_1^4 - 6\theta_1^2\theta_2 + 8\theta_1\theta_3 + 3\theta_2^2$
	$\theta_1^5 - 5\theta_1^3\theta_2 + 5\theta_1^2\theta_3 + 5\theta_2\theta_3$

Table 2.5: Matrices Q^π for the group B_3 given in upper triangular row-major order (in the consecutive order of row entries of upper triangular matrices).

If we would like to check whether a polynomial $p \in \mathbb{R}[x_1, x_2, x_3]_{30}^{\mathsf{B}_3}$ is SOS, we can try to find an SOS polynomial A with $p(x) = b(x)\, A\, b(x)^\mathsf{T}$, where $b(x)$ contains the monomial basis of $\mathbb{R}[x_1, x_2, x_3]$ up to degree 15. The desired matrix A has dimension $\binom{n+d}{d}$, so we have to find a positive semidefinite matrix of dimension 816. Alternatively, we can apply Theorem 2.21 to check the SOS property. Since the octahedral group B_3 has ten irreducible representations, we have to calculate ten positive semidefinite matrices instead of one. The

dimensions of these matrices are $31, 23, 11, 7, 27, 39, 34, 50, 50$, and 70. Thus the largest matrix has dimension 70. Hence, instead of calculating a symmetric matrix of dimension 816, we have to calculate symmetric matrices of dimension at most 70. Fortunately, the corresponding SDP can be solved by today's SDP solvers.

2.3.3 SOHS invariant under the icosahedral group

Since all irreducible representations of the icosahedral group are orthogonal, H_3-invariant polynomials have to be real. To apply Theorem 2.21 to these polynomials, we have to calculate a basis of the coinvariant algebra $\mathbb{C}[x]_{\mathsf{H}_3}$. To this end, we are interested in the irreducible representations of the group. Information about their properties are displayed in the character table given in Table 2.6. The structure of a character table and the symbols of its irreducible characters and conjugacy classes are explained in the beginning of Section 2.3.2.

	E	i	$15C_2$	15σ	$20C_3$	$12C_5$	$12C_5^2$	$20S_6$	$12S_{10}$	$12S_{10}^3$
A_g	1	1	1	1	1	1	1	1	1	1
A_u	1	−1	1	−1	1	1	1	−1	−1	−1
T_{1g}	3	3	−1	−1	0	τ	$\widehat{\tau}$	0	$\widehat{\tau}$	τ
T_{1u}	3	−3	−1	1	0	τ	$\widehat{\tau}$	0	$-\widehat{\tau}$	$-\tau$
T_{2g}	3	3	−1	−1	0	$\widehat{\tau}$	τ	0	τ	$\widehat{\tau}$
T_{2u}	3	−3	−1	1	0	$\widehat{\tau}$	τ	0	$-\tau$	$-\widehat{\tau}$
G_g	4	4	0	0	1	−1	−1	1	−1	−1
G_u	4	−4	0	0	1	−1	−1	−1	1	1
H_g	5	5	1	1	−1	0	0	−1	0	0
H_u	5	−5	1	−1	−1	0	0	1	0	0

Table 2.6: The character table of the icosahedral group H_3 with $\tau = (1 + \sqrt{5})/2$ and $\widehat{\tau} = (1 - \sqrt{5})/2$.

The three-dimensional icosahedral group H_3 has two one-dimensional characters (A_g, A_u), four three-dimensional characters ($T_{1g}, T_{1u}, T_{2g}, T_{2u}$), two four-dimensional characters (G_g, G_u), and two five-dimensional characters (H_g, H_u). Analogously to the character table of B_3, E represents the identity class and i the inverse operator. The fifteen rotations by 180° through the vertices build the class $15C_2$ and the fifteen reflections through planes through opposite edges generate the class 15σ. The next conjugacy class named $20C_3$ consists of the twenty clockwise rotations by 120° through the centers of the opposite faces and $12C_5$ represents the twelve clockwise rotations by 72° through each vertex. The class $15C_5^2$ consists of the fifteen clockwise rotations by 144° through the vertices. The twenty rotation-reflections by 60° through the axis of the facet centers build the class $20S_6$. The class $12S_{10}$ consists of the six rotation-reflections by 36° through the vertices, and $12S_{10}$

are the eight rotation-reflections by 108° through the vertices. The total number of these fundamental symmetry operations is 120, which is the order of the group H_3.

Due to the Poincaré series

$$\begin{aligned} P_{\mathsf{H}_3}(t) =& 1 + 3t + 5t^2 + 7t^3 + 9t^4 + 11t^5 + 12t^6 + 12t^7 + 12t^8 \\ &+ 12t^9 + 11t^{10} + 9t^{11} + 7t^{12} + 5^{13} + 3t^{14} + t^{15} \end{aligned}$$

as given before, the coinvariant algebra can be decomposed into 16 homogeneous subspaces

$$\mathbb{C}[x]_{\mathsf{H}_3} = \bigoplus_{k\geq 0} (\mathbb{C}[x]_{\mathsf{H}_3} \cap \mathrm{Hom}_k) = V_0 \oplus \ldots \oplus V_{15} \,,$$

according to the grading by degree. The dimension of each subspace V_k is given by the coefficient of t^k in $P_{\mathsf{H}_3}(t)$.

Furthermore, the icosahedral group has ten irreducible characters and thus ten irreducible representation. We can decompose the coinvariant algebra $\mathbb{C}[x]_{\mathsf{H}_3} = \mathbb{C}[x]/(\theta_1, \theta_2, \theta_3)$ with basic invariants of degree 2, 6, and 10:

$$\begin{aligned} \theta_1 =& x_1^2 + x_2^2 + x_3^2 \\ \theta_2 =& x_1^6 + x_2^6 + x_3^6 + \\ & \frac{54}{7} x_1^2 x_2^2 x_3^2 + \frac{39 - 3\sqrt{5}}{14} \left(x_1^4 x_2^2 + x_1^2 x_3^4 + x_2^4 x_3^2 \right) + \frac{39 + 3\sqrt{5}}{14} \left(x_1^2 x_2^4 + x_1^4 x_3^2 + x_2^2 x_3^4 \right) \\ \theta_3 =& x_1^{10} + x_2^{10} + x_3^{10} + \\ & \frac{147 - 21\sqrt{5}}{19} \left(x_1^6 x_2^4 + x_1^4 x_3^6 + x_2^6 x_3^4 \right) + \frac{147 + 21\sqrt{5}}{19} \left(x_1^4 x_2^6 + x_1^6 x_3^4 + x_2^4 x_3^6 \right) + \\ & \frac{153 - 27\sqrt{5}}{38} \left(x_1^8 x_2^2 + x_1^2 x_3^8 + x_2^8 x_3^2 \right) + \frac{153 + 27\sqrt{5}}{38} \left(x_1^2 x_2^8 + x_1^8 x_3^2 + x_2^2 x_3^8 \right) + \\ & \frac{630}{19} \left(x_1^4 x_2^4 x_3^2 + x_1^4 x_2^2 x_3^4 + x_1^2 x_2^4 x_3^4 \right) + \frac{504}{19} \left(x_1^2 x_2^2 x_3^6 + x_1^2 x_2^6 x_3^2 + x_1^6 x_2^2 x_3^2 \right). \end{aligned}$$

into one subspace per irreducible representation

$$\mathbb{C}[x]_{\mathsf{H}_3} = \bigoplus_{\pi \in \widehat{\mathsf{H}_3}} V^\pi.$$

To get some information about the dimension and the degree of these subspaces, we calculate the Poincaré series for each of the irreducible representations π, which are given in Table 2.1.

The icosahedral group consists of two one-dimensional, four three-dimensional, two four-dimensional, and two five-dimensional irreducible representations.

$$\sum_{\pi \in \widehat{\mathsf{H}_3}} d_\pi^2 = 2 \cdot 1^2 + 4 \cdot 3^2 + 2 \cdot 4^2 + 2 \cdot 5^2 = 120 = 2 \cdot 6 \cdot 120 = |\mathsf{H}_3|.$$

In Table 2.7, the orthogonal basis for $V^\pi_{k_1^\pi}$ with minimal degree k_1^π for each irreducible representation $\pi \in \widehat{\mathsf{H}_3}$ is presented. Using the projection described in (2.52) for H_3, i.e.,

$$p^\pi_{k,ij} : \mathrm{Hom}_k \to \mathrm{Hom}_k \quad \text{with} \quad p^\pi_{k,ij} = \frac{d_\pi}{|\mathsf{H}_3|} \sum_{g \in \mathsf{H}_3} \pi_{ji}\left(g^{-1}\right) \tilde{\rho}_k(g), \tag{2.55}$$

we get all remaining basis elements of $\mathbb{C}[x]_{\mathsf{H}_3}$, which are presented in Table 2.8.

A_g	1
A_u	$\frac{11\sqrt{5}+113}{2}(x_1x_2^5x_3^9 + x_1^9x_2x_3^5 + x_1^5x_2^9x_3) + \frac{-11\sqrt{5}+113}{2}(x_1^9x_2^5x_3 + x_1^5x_2x_3^9 + x_1x_2^9x_3^5)$ $-84(x_1^7x_2^7x_3 + x_1^7x_2x_3^7 + x_1x_2^7x_3^7) + (66\sqrt{5}-90)(x_1^7x_2^5x_3^3 + x_1^5x_2^3x_3^7 + x_1^3x_2^7x_3^5)$ $+(-66\sqrt{5}-90)(x_1^5x_2^7x_3^3 + x_1^3x_2^5x_3^7 + x_1^7x_2^3x_3^5) + 50(x_1^3x_2^9x_3^3 + x_1^3x_2^3x_3^9 + x_1^9x_2^3x_3^3)$ $+378x_1^5x_2^5x_3^5 + (-\sqrt{5}-13)(x_1^3x_2^{11}x_3 + x_1^{11}x_2x_3^3 + x_1x_2^3x_3^{11}) + x_1^{13}x_2x_3 + x_1x_2x_3^{13}$ $+x_1x_2^{13}x_3 + (\sqrt{5}-13)(x_1^3x_2x_3^{11} + x_1^{11}x_2^3x_3 + x_1x_2^{11}x_3^3)$
T_{1g}	$\sqrt{\frac{47}{3}}(-\frac{3}{47}x_1^7x_2 + \frac{-3\sqrt{5}+39}{94}x_1^5x_2^3 + \frac{9\sqrt{5}+9}{94}x_1^5x_2x_3^2 + \frac{-3\sqrt{5}-39}{94}x_1^3x_2^5 + \frac{30\sqrt{5}}{47}x_1^3x_2^3x_3^2$ $+\frac{-45\sqrt{5}-15}{94}x_1^3x_2x_3^4 + \frac{3}{47}x_1x_2^7 + \frac{9\sqrt{5}-9}{94}x_1x_2^5x_3^2 + \frac{-45\sqrt{5}+15}{94}x_1x_2^3x_3^4 + \frac{9}{47}\sqrt{5}x_1x_2x_3^6)$ $(-\frac{3}{47}x_1^7x_3 + \frac{-9\sqrt{5}+9}{94}x_1^5x_2^2x_3 + \frac{3\sqrt{5}+39}{94}x_1^5x_3^3 + \frac{45\sqrt{5}-15}{94}x_1^3x_2^4x_3 - \frac{30\sqrt{5}}{47}x_1^3x_2^2x_3^3$ $+\frac{3\sqrt{5}-39}{94}x_1^3x_3^5 - \frac{9\sqrt{5}}{47}x_1x_2^6x_3 + \frac{45\sqrt{5}+15}{94}x_1x_2^4x_3^3 + \frac{-9\sqrt{5}-9}{94}x_1x_2^2x_3^5 + \frac{3}{47}x_1x_3^7)$ $\sqrt{\frac{47}{3}}(-\frac{9\sqrt{5}}{47}x_1^6x_2x_3 + \frac{45\sqrt{5}+15}{94}x_1^4x_2^3x_3 + \frac{45\sqrt{5}-15}{94}x_1^4x_2x_3^3 + \frac{-9\sqrt{5}-9}{94}x_1^2x_2^5x_3$ $-\frac{30\sqrt{5}}{47}x_1^2x_2^3x_3^3 + \frac{-9\sqrt{5}+9}{94}x_1^2x_2x_3^5 + \frac{3}{47}x_2^7x_3 + \frac{3\sqrt{5}-39}{94}x_2^5x_3^3 + \frac{3\sqrt{5}+39}{94}x_2^3x_3^5 - \frac{3}{47}x_2x_3^7)$
T_{2u}	x_1
	x_2
	x_3
T_{1u}	$\sqrt{\frac{28}{3}}(-\frac{3}{28}x_1^3 + \frac{-9\sqrt{5}+9}{56}x_1x_2^2 + \frac{9\sqrt{5}+9}{56}x_1x_3^2)$
	$\sqrt{\frac{28}{3}}(\frac{-9\sqrt{5}-9}{56}x_1^2x_2 + \frac{3}{28}x_2^3 + \frac{9\sqrt{5}-9}{56}x_2x_3^2)$
	$\sqrt{\frac{28}{3}}(\frac{-9\sqrt{5}+9}{56}x_1^2x_3 + \frac{9\sqrt{5}+9}{56}x_2^2x_3 - \frac{3}{28}x_3^3)$
T_{2g}	$\alpha(\frac{-3\sqrt{5}-9}{16}x_1^5x_2 + \frac{3\sqrt{5}+15}{16}(2x_1^3x_2^3 + x_1x_2x_3^4) + \frac{3\sqrt{5}}{4}x_1^3x_2x_3^2 - \frac{3}{8}x_1x_2^5 + \frac{-9\sqrt{5}-15}{8}x_1x_2^3x_3^2)$
	$\alpha(-\frac{3}{8}x_1^5x_3 + \frac{-9\sqrt{5}-15}{8}x_1^3x_2^2x_3 + \frac{3\sqrt{5}+15}{16}(x_1^3x_3^3 + x_1x_2^4x_3) + \frac{3\sqrt{5}}{4}x_1x_2^2x_3^3 + \frac{-3\sqrt{5}-9}{16}x_1x_3^5)$
	$\alpha(\frac{-3\sqrt{5}-15}{16}(x_1^4x_2x_3 + 2x_2^3x_3^3) - \frac{3\sqrt{5}}{4}x_1^2x_2^3x_3 + \frac{9\sqrt{5}+15}{8}x_1^2x_2x_3^3 + \frac{3\sqrt{5}+9}{16}x_2^5x_3 + \frac{3}{8}x_2x_3^5)$
G_g	$\sqrt{\frac{-61}{4}}\frac{4}{61}(-x_1^4 + 3x_1^2x_2^2 + 3x_1^2x_3^2 - x_2^4 + 3x_2^2x_3^2 - x_3^4)$
	$\sqrt{\frac{-61}{4}}(\frac{2\sqrt{5}-10}{61}x_1^3x_2 + \frac{2\sqrt{5}+10}{61}x_1x_2^3 - \frac{12\sqrt{5}}{61}x_1x_2x_3^2)$
	$\sqrt{\frac{-61}{4}}(\frac{2\sqrt{5}+10}{61}x_1^3x_3 - \frac{12\sqrt{5}}{61}x_1x_2^2x_3 + \frac{2\sqrt{5}-10}{61}x_1x_3^3)$
	$\sqrt{\frac{-61}{4}}(-\frac{12\sqrt{5}}{61}x_1^2x_2x_3 + \frac{2\sqrt{5}-10}{61}x_2^3x_3 + \frac{2\sqrt{5}+10}{61}x_2x_3^3)$
G_g	$\sqrt{7}(-\frac{1}{7}x_1^3 + \frac{\sqrt{5}+3}{14}x_1x_2^2 + \frac{-\sqrt{5}+3}{14}x_1x_3^2)$
	$\sqrt{7}(\frac{\sqrt{5}-3}{14}x_1^2x_2 + \frac{1}{7}x_2^3 + \frac{-\sqrt{5}-3}{14}x_2x_3^2)$

	$\sqrt{7}(\frac{\sqrt{5}+3}{14}x_1^2x_3 + \frac{-\sqrt{5}+3}{14}x_2^2x_3 - \frac{1}{7}x_3^3)$
	$-\sqrt{7}\frac{2\sqrt{5}}{7}x_1x_2x_3$
H_g	$-\frac{15}{44}\sqrt{\frac{44}{15}}(x_1^2 - x_3^2)$
	$-\frac{15}{22}\sqrt{\frac{44}{15}}x_1x_2$
	$-\frac{15}{22}\sqrt{\frac{44}{15}}x_1x_3$
	$\sqrt{\frac{11}{5}}\frac{5}{22}(x_1^2 - 2x_2^2 + x_3^2)$
	$-\frac{15}{22}\sqrt{\frac{44}{15}}x_2x_3$
H_u	$\sqrt{\frac{264}{5}}(-\frac{5}{264}x_1^5 + \frac{-5\sqrt{5}+25}{264}x_1^3x_2^2 + \frac{5\sqrt{5}+25}{264}x_1^3x_3^2 + \frac{5\sqrt{5}-15}{528}x_1x_2^4 - \frac{5}{44}x_1x_2^2x_3^2 - \frac{5\sqrt{5}+15}{528}x_1x_3^4)$
	$\sqrt{\frac{264}{5}}(\frac{5\sqrt{5}+15}{528}x_1^4x_2 - \frac{5\sqrt{5}+25}{264}x_1^2x_2^3 + \frac{5}{44}x_1^2x_2x_3^2 + \frac{5}{264}x_2^5 + \frac{5\sqrt{5}-25}{264}x_2^3x_3^2 + \frac{-5\sqrt{5}+15}{528}x_2x_3^4)$
	$\sqrt{\frac{264}{5}}(\frac{5\sqrt{5}-15}{528}x_1^4x_3 - \frac{5}{44}x_1^2x_2^2x_3 + \frac{-5\sqrt{5}+25}{264}x_1^2x_3^3 - \frac{5\sqrt{5}+15}{528}x_2^4x_3 + \frac{5\sqrt{5}+25}{264}x_2^2x_3^3 - \frac{5}{264}x_3^5)$
	$\sqrt{\frac{11}{20}}\frac{20}{11}(-x_1^3x_2x_3 + x_1x_2x_3^3)$
	$\sqrt{\frac{33}{80}}\frac{40}{33}(x_1^3x_2x_3 - 2x_1x_2^3x_3 + x_1x_2x_3^3)$

Table 2.7: Orthonormal basis φ^{π}_{1j}, with $j = 1, \ldots, d_\pi$, of subspaces $V^{\pi}_{k_1^\pi}$ with $\alpha = \sqrt{\frac{-4\sqrt{5}+12}{3}}$.

A_g	1
A_u	$-\frac{54329344}{10125}\theta_1^{15} + \frac{245088256}{10125}\theta_1^{12}\theta_2 + \frac{505856}{375}\theta_1^{10}\theta_3 - \frac{148746752}{3375}\theta_1^9\theta_2^2 - \frac{1498112}{375}\theta_1^7\theta_2\theta_3$ $+\frac{81639488}{2025}\theta_1^6\theta_2^3 + \frac{652688}{375}\theta_1^5\theta_3^2 + \frac{96824}{75}\theta_1^4\theta_2^2\theta_3 - \frac{1394981}{81}\theta_1^3\theta_2^4 - \frac{192052}{75}\theta_1^2\theta_2\theta_3^2$ $+\frac{6517}{3}\theta_1\theta_2^3\theta_3 + \frac{16807}{9}\theta_2^5 + \frac{6859}{25}\theta_3^3$
T_{1g}	$-\frac{18176}{45}\theta_1^8 + \frac{42112}{45}\theta_1^5\theta_2 - \frac{684}{5}\theta_1^3\theta_3 - \frac{4753}{9}\theta_1^2\theta_2^2 + 133\theta_2\theta_3$
	$\frac{-273664\sqrt{5}-206080}{225}\theta_1^9 + \frac{740768\sqrt{5}+428960}{225}\theta_1^6\theta_2 + \frac{-17708\sqrt{5}-29260}{75}\theta_1^4\theta_3 +$
	$\frac{-121667\sqrt{5}-31115}{45}\theta_1^3\theta_2^2 + \frac{7049\sqrt{5}+11305}{30}\theta_1\theta_2\theta_3 + \frac{3773\sqrt{5}-1715}{6}\theta_2^3$
	$\frac{85312\sqrt{5}-150208}{45}\theta_1^{10} + \frac{-232736\sqrt{5}+397152}{45}\theta_1^7\theta_2 + \frac{-34333\sqrt{5}+96995}{15}\theta_1^5\theta_3 + \frac{-6498\sqrt{5}+17689}{10}\theta_3^2$
	$\frac{1132831\sqrt{5}-2219553}{180}\theta_1^4\theta_2^2 + \frac{42959\sqrt{5}-119833}{12}\theta_1^2\theta_2\theta_3 + \frac{-65856\sqrt{5}+154693}{18}\theta_1\theta_2^3$
	$\frac{-366592\sqrt{5}-239616}{45}\theta_1^{10} + \frac{988288\sqrt{5}+577920}{45}\theta_1^7\theta_2 - \frac{162944}{15}\theta_1^5\theta_3 + \frac{-860048\sqrt{5}-54096}{45}\theta_1^4\theta_2^2$ $+\frac{-2394\sqrt{5}+46018}{3}\theta_1^2\theta_2\theta_3 + \frac{102557\sqrt{5}-153321}{18}\theta_1\theta_2^3 + \frac{3971\sqrt{5}-22743}{10}\theta_3^2$
	$\frac{27597952\sqrt{5}-54052480}{675}\theta_1^{11} + \frac{-28899248\sqrt{5}+56311920}{225}\theta_1^8\theta_2 + \frac{-285266\sqrt{5}+876090}{25}\theta_1^6\theta_3$ $+\frac{13457997\sqrt{5}-26980625}{90}\theta_1^5\theta_2^2 + \frac{3979493\sqrt{5}-13534745}{300}\theta_1^3\theta_2\theta_3 + \frac{-18292876\sqrt{5}+38915065}{270}\theta_1^2\theta_2^3$

$$+\frac{-292049\sqrt{5}+734635}{50}\theta_1\theta_3^2+\frac{585599\sqrt{5}-1149785}{60}\theta_2^2\theta_3$$

$$\frac{-60654112\sqrt{5}+125407648}{675}\theta_1^{12}+\frac{39500496\sqrt{5}-76098064}{225}\theta_1^9\theta_2+\frac{33156729\sqrt{5}-75230101}{450}\theta_1^7\theta_3+$$

$$\frac{-89263153\sqrt{5}+74398317}{1800}\theta_1^6\theta_2^2+\frac{-168351267\sqrt{5}+386584583}{1800}\theta_1^4\theta_2\theta_3+\frac{-65763733\sqrt{5}+166406107}{540}\theta_1^3\theta_2^3$$

$$+\frac{3231311\sqrt{5}-7187149}{100}\theta_1^2\theta_3^2+\frac{-7999152\sqrt{5}+17170433}{180}\theta_1\theta_2^2\theta_3+\frac{4235364\sqrt{5}-9654421}{36}\theta_2^4$$

T_{2u} θ_1

$$\frac{-7\sqrt{5}+9}{2}\theta_1^3+\frac{7\sqrt{5}-7}{2}\theta_2$$

$$\frac{-21\sqrt{5}+579}{11}\theta_1^5+\frac{21\sqrt{5}-777}{11}\theta_1^2\theta_2+19\theta_3$$

$$\frac{-113\sqrt{5}-51}{30}\theta_1^5+\frac{28\sqrt{5}+126}{15}\theta_1^2\theta_2+\frac{19\sqrt{5}-57}{10}\theta_3$$

$$\frac{46955\sqrt{5}-53543}{495}\theta_1^7+\frac{-93310\sqrt{5}+120526}{495}\theta_1^4\theta_2+\frac{855\sqrt{5}+551}{110}\theta_1^2\theta_3+\frac{17003\sqrt{5}-27587}{198}\theta_1\theta_2^2$$

$$\frac{3627738\sqrt{5}-10764242}{5445}\theta_1^9+\frac{-2655912\sqrt{5}+7900928}{1815}\theta_1^6\theta_2+\frac{100092\sqrt{5}-362748}{605}\theta_1^4\theta_3+$$

$$\frac{281946\sqrt{5}-786058}{363}\theta_1^3\theta_2^2+\frac{-1596\sqrt{5}+6384}{11}\theta_1\theta_2\theta_3-\frac{1715}{9}\theta_2^3$$

T_{1u} $36\theta_1^3-35\theta_2$

$$\frac{28\sqrt{5}-4}{3}\theta_1^4+\frac{-28\sqrt{5}+7}{3}\theta_1\theta_2$$

$$-14\theta_1^5+\frac{49}{2}\theta_1^2\theta_2-\frac{19}{2}\theta_3$$

$$\frac{1336\sqrt{5}-3352}{15}\theta_1^5+\frac{-1792\sqrt{5}+4564}{15}\theta_1^2\theta_2+\frac{152\sqrt{5}-399}{5}\theta_3$$

$$\frac{742\sqrt{5}-3178}{15}\theta_1^6+\frac{-2128\sqrt{5}+9247}{30}\theta_1^3\theta_2+\frac{133\sqrt{5}-627}{10}\theta_1\theta_3+\frac{49\sqrt{5}-196}{6}\theta_2^2$$

$$\frac{-2063}{9}\theta_1^7+\frac{12397}{36}\theta_1^4\theta_2-\frac{133}{2}\theta_1^2\theta_3-\frac{1715}{36}\theta_1\theta_2^2$$

T_{2g} $$\frac{416\sqrt{5}-1248}{15}\theta_1^6+\frac{-812\sqrt{5}+2436}{15}\theta_1^3\theta_2+\frac{19\sqrt{5}-57}{10}\theta_1\theta_3+\frac{49\sqrt{5}-147}{2}\theta_2^2$$

$$\frac{-16384\sqrt{5}+40960}{225}\theta_1^8+\frac{45248\sqrt{5}-113120}{225}\theta_1^5\theta_2+\frac{-1216\sqrt{5}+3040}{25}\theta_1^3\theta_3+\frac{-5978\sqrt{5}+14945}{45}\theta_1^2\theta_2^2$$

$$+\frac{266\sqrt{5}-665}{5}\theta_2\theta_3$$

$$\frac{-405392\sqrt{5}+875920}{225}\theta_1^{10}+\frac{1118558\sqrt{5}-2420670}{225}\theta_1^7\theta_2+\frac{1888011\sqrt{5}-4358315}{900}\theta_1^5\theta_3$$

$$+\frac{-5428367\sqrt{5}+11967515}{900}\theta_1^4\theta_2^2+\frac{-738948\sqrt{5}+1700405}{225}\theta_1^2\theta_2\theta_3+\frac{62083\sqrt{5}-139944}{18}\theta_1\theta_2^3$$

$$+\frac{29963\sqrt{5}-68590}{50}\theta_3^2$$

$$\frac{1536\sqrt{5}-3584}{45}\theta_1^{10}+\frac{-1344\sqrt{5}+3136}{5}\theta_1^7\theta_2+\frac{1368\sqrt{5}-3192}{5}\theta_1^5\theta_3+\frac{4116\sqrt{5}-9604}{15}\theta_1^4\theta_2^2$$

$$+\frac{-2394\sqrt{5}+5586}{5}\theta_1^2\theta_2\theta_3+\frac{1029\sqrt{5}-2401}{18}\theta_1\theta_2^3+\frac{1083\sqrt{5}-2527}{10}\theta_3^2$$

$$\frac{-34098688\sqrt{5}+77295104}{2025}\theta_1^{12}+\frac{40026168\sqrt{5}-90747272}{675}\theta_1^9\theta_2+\frac{955776\sqrt{5}-2117968}{225}\theta_1^7\theta_3$$

$$+\frac{-217640213\sqrt{5}+492955043}{2700}\theta_1^6\theta_2^2+\frac{-5170641\sqrt{5}+11390519}{900}\theta_1^4\theta_2\theta_3+\frac{38828629\sqrt{5}-87777473}{810}\theta_1^3\theta_2^3$$

$$+\frac{262447\sqrt{5}-588791}{150}\theta_1^2\theta_3^2+\frac{-354711\sqrt{5}+816487}{180}\theta_1\theta_2^2\theta_3+\frac{-290521\sqrt{5}+655473}{36}\theta_2^4$$

$$\begin{aligned}
&\tfrac{9361491200\sqrt{5}-21038935248}{30375}\theta_1^{14} + \tfrac{-1486873360\sqrt{5}+3339562226}{1125}\theta_1^{11}\theta_2 \\
&\quad + \tfrac{-3487480400\sqrt{5}+7717928877}{40500}\theta_1^{9}\theta_3 + \tfrac{90696080090\sqrt{5}-203504641011}{40500}\theta_1^{8}\theta_2^2 \\
&\quad + \tfrac{4029194435\sqrt{5}-8919263157}{20250}\theta_1^{6}\theta_2\theta_3 + \tfrac{-43953224959\sqrt{5}+98505697689}{24300}\theta_1^{5}\theta_2^3 \\
&\quad + \tfrac{-202295375\sqrt{5}+451108849}{4500}\theta_1^{4}\theta_3^2 + \tfrac{-158557679\sqrt{5}+343726131}{4050}\theta_1^{3}\theta_2^2\theta_3 \\
&\quad \tfrac{1910031515\sqrt{5}-4276197807}{3240}\theta_1^{2}\theta_2^4 + \tfrac{23276197\sqrt{5}-51962701}{450}\theta_1\theta_2\theta_3^2 + \tfrac{-31379355\sqrt{5}+70298879}{360}\theta_2^3\theta_3
\end{aligned}$$

G_g

$$-\tfrac{32}{3}\theta_1^4 + \tfrac{35}{3}\theta_1\theta_2$$

$$\tfrac{160\sqrt{5}+128}{3}\theta_1^5 + \tfrac{-217\sqrt{5}-182}{3}\theta_1^2\theta_2 + (19\sqrt{5}+19)\theta_3$$

$$\tfrac{-224}{3}\theta_1^6 + 126\theta_1^3\theta_2 - \tfrac{19}{2}\theta_1\theta_3 - \tfrac{245}{6}\theta_2^2$$

$$\tfrac{416}{9}\theta_1^8 - \tfrac{952}{9}\theta_1^5\theta_2 + \tfrac{95}{6}\theta_1^3\theta_3 + \tfrac{2009}{36}\theta_1^2\theta_2^2 - \tfrac{133}{12}\theta_2\theta_3$$

$$\tfrac{512\sqrt{5}-1824}{15}\theta_1^6 + \tfrac{-364\sqrt{5}+3423}{15}\theta_1^3\theta_2 + \tfrac{114\sqrt{5}-38}{5}\theta_1\theta_3 + \tfrac{-98\sqrt{5}-294}{3}\theta_2^2$$

$$\tfrac{2528\sqrt{5}-832}{45}\theta_1^7 + \tfrac{-3346\sqrt{5}+2324}{45}\theta_1^4\theta_2 + \tfrac{209\sqrt{5}+114}{10}\theta_1^2\theta_3 + \tfrac{-49\sqrt{5}-784}{18}\theta_1\theta_2^2$$

$$\begin{aligned}
&\tfrac{13984\sqrt{5}+16064}{45}\theta_1^9 + \tfrac{-34776\sqrt{5}-39536}{45}\theta_1^6\theta_2 + \tfrac{2071\sqrt{5}+2546}{30}\theta_1^4\theta_3 + \tfrac{103929\sqrt{5}+113974}{180}\theta_1^3\theta_2^2 + \\
&\tfrac{-3059\sqrt{5}-3724}{60}\theta_1\theta_2\theta_3 + \tfrac{-2401\sqrt{5}-2401}{18}\theta_2^3
\end{aligned}$$

$$\tfrac{-576}{5}\theta_1^8 + \tfrac{2716}{15}\theta_1^5\theta_2 - \tfrac{133}{15}\theta_1^3\theta_3 - \tfrac{539}{12}\theta_1^2\theta_2^2 - \tfrac{133}{12}\theta_2\theta_3$$

$$\tfrac{-9856}{135}\theta_1^{10} + \tfrac{7616}{45}\theta_1^7\theta_2 - \tfrac{2774}{15}\theta_1^5\theta_3 + \tfrac{343}{60}\theta_1^4\theta_2^2 + \tfrac{8113}{30}\theta_1^2\theta_2\theta_3 - \tfrac{30527}{216}\theta_1\theta_2^3 - \tfrac{361}{8}\theta_3^2$$

$$\begin{aligned}
&\tfrac{36544}{45}\theta_1^{12} - \tfrac{356608}{135}\theta_1^9\theta_2 + \tfrac{3173}{15}\theta_1^7\theta_3 + \tfrac{533071}{180}\theta_1^6\theta_2^2 - \tfrac{21679}{60}\theta_1^4\theta_2\theta_3 - \tfrac{234269}{180}\theta_1^3\theta_2^3 + \\
&\tfrac{38171}{240}\theta_1\theta_2^2\theta_3 + \tfrac{69629}{432}\theta_2^4
\end{aligned}$$

G_u

$$-\tfrac{32}{3}\theta_1^3 + \tfrac{35}{3}\theta_2$$

$$16\theta_1^5 - \tfrac{49}{2}\theta_1^2\theta_2 + \tfrac{19}{2}\theta_3$$

$$\tfrac{7200\sqrt{5}+76768}{909}\theta_1^6 + \tfrac{-9765\sqrt{5}-123347}{909}\theta_1^3\theta_2 + \tfrac{285\sqrt{5}+2527}{101}\theta_1\theta_3 + \tfrac{245}{9}\theta_2^2$$

$$\tfrac{11328\sqrt{5}+41768}{135}\theta_1^7 + \tfrac{-69384\sqrt{5}-269899}{540}\theta_1^4\theta_2 + \tfrac{684\sqrt{5}+2299}{30}\theta_1^2\theta_3 + \tfrac{2352\sqrt{5}+12397}{108}\theta_1\theta_2^2$$

$$\tfrac{168}{5}\theta_1^7 - \tfrac{2737}{60}\theta_1^4\theta_2 + \tfrac{171}{10}\theta_1^2\theta_3 - \tfrac{49}{12}\theta_1\theta_2^2$$

$$\begin{aligned}
&\tfrac{-49776\sqrt{5}-93584}{909}\theta_1^8 + \tfrac{241269\sqrt{5}+565187}{1818}\theta_1^5\theta_2 + \tfrac{-5472\sqrt{5}-10906}{303}\theta_1^3\theta_3 + \tfrac{-144795\sqrt{5}-427672}{1818}\theta_1^2\theta_2^2 \\
&\quad + \tfrac{11970\sqrt{5}+38969}{606}\theta_2\theta_3
\end{aligned}$$

$$\begin{aligned}
&\tfrac{-95712\sqrt{5}-226588}{135}\theta_1^9 + \tfrac{2018184\sqrt{5}+4937275}{1080}\theta_1^6\theta_2 - \tfrac{64752\sqrt{5}+149093}{360}\theta_1^4\theta_3 - \tfrac{1515864\sqrt{5}+3878399}{1080}\theta_1^3\theta_2^2 \\
&\quad + \tfrac{35112\sqrt{5}+86317}{180}\theta_1\theta_2\theta_3 + \tfrac{16464\sqrt{5}+45619}{72}\theta_2^3
\end{aligned}$$

$$\begin{aligned}
&\tfrac{-281741760\sqrt{5}-863222464}{1377135}\theta_1^9 + \tfrac{146457990\sqrt{5}+567389326}{459045}\theta_1^6\theta_2 - \tfrac{6528780\sqrt{5}+17098252}{51005}\theta_1^4\theta_3 \\
&\quad + \tfrac{9472680\sqrt{5}-19720148}{91809}\theta_1^3\theta_2^2 + \tfrac{1280790\sqrt{5}+3672662}{10201}\theta_1\theta_2\theta_3 - \tfrac{59270400\sqrt{5}+115184545}{275427}\theta_2^3
\end{aligned}$$

$$\frac{-145953192\sqrt{5}-348596056}{40905}\theta_1^{10} + \frac{464994327\sqrt{5}+1129687601}{54540}\theta_1^7\theta_2 + \frac{3548003\sqrt{5}+7216105}{6060}\theta_1^5\theta_3$$
$$-\frac{23723693\sqrt{5}+58514428}{3636}\theta_1^4\theta_2^2 + \frac{-4355617\sqrt{5}-9240042}{3030}\theta_1^2\theta_2\theta_3 + \frac{65393979\sqrt{5}+157923374}{32724}\theta_1\theta_2^3$$
$$+\frac{1274691\sqrt{5}+2836016}{3030}\theta_3^2$$
$$\frac{-16222176\sqrt{5}-35079878}{2025}\theta_1^{11} + \frac{68530448\sqrt{5}+133728539}{10800}\theta_1^8\theta_2 + \frac{5104388\sqrt{5}+10360339}{900}\theta_1^6\theta_3 +$$
$$\frac{68158216\sqrt{5}+168589253}{5400}\theta_1^5\theta_2^2 - \frac{19693044\sqrt{5}+41821717}{1350}\theta_1^3\theta_2\theta_3 - \frac{14887572\sqrt{5}+36813161}{1620}\theta_1^2\theta_2^3$$
$$+\frac{1481544\sqrt{5}+2991607}{900}\theta_1\theta_3^2 + \frac{11887008\sqrt{5}+27193579}{2160}\theta_2^2\theta_3$$

H_g

$$\frac{4}{3}\theta_1^2$$
$$-\theta_1^3 + \frac{35}{16}\theta_2$$
$$-\frac{7}{3}\theta_1^4 + \frac{161}{48}\theta_1\theta_2$$
$$\frac{7}{9}\theta_1^5 - \frac{49}{36}\theta_1^2\theta_2 + \frac{95}{64}\theta_3$$
$$\frac{231}{20}\theta_1^6 - \frac{1533}{80}\theta_1^3\theta_2 + \frac{16397}{3840}\theta_1\theta_3 + \frac{4263}{1024}\theta_2^2$$
$$-\frac{31}{12}\theta_1^4 + \frac{175}{48}\theta_1\theta_2$$
$$-\frac{15}{4}\theta_1^5 + \frac{77}{16}\theta_1^2\theta_2 - \frac{19}{128}\theta_3$$
$$-\frac{7}{24}\theta_1^6 - \frac{21}{32}\theta_1^3\theta_2 + \frac{551}{512}\theta_1\theta_3 + \frac{4165}{6144}\theta_2^2$$
$$\frac{739}{72}\theta_1^7 - \frac{10549}{576}\theta_1^4\theta_2 + \frac{1805}{512}\theta_1^2\theta_3 + \frac{48461}{9216}\theta_1\theta_2^2$$
$$-\frac{89}{20}\theta_1^6 + \frac{427}{80}\theta_1^3\theta_2 - \frac{57}{160}\theta_1\theta_3 + \frac{49}{192}\theta_2^2$$
$$-\frac{71}{120}\theta_1^7 - \frac{1421}{1440}\theta_1^4\theta_2 + \frac{1767}{2560}\theta_1^2\theta_3 + \frac{29155}{18432}\theta_1\theta_2^2$$
$$\frac{6827}{720}\theta_1^8 - \frac{103901}{5760}\theta_1^5\theta_2 + \frac{43681}{15360}\theta_1^3\theta_3 + \frac{1173011}{184320}\theta_1^2\theta_2^2 - \frac{2527}{122880}\theta_2\theta_3$$
$$\frac{218}{135}\theta_1^8 - \frac{7861}{2160}\theta_1^5\theta_2 + \frac{133}{160}\theta_1^3\theta_3 + \frac{7987}{6912}\theta_1^2\theta_2^2 + \frac{665}{1024}\theta_2\theta_3$$
$$\frac{5897}{720}\theta_1^9 - \frac{19565}{1536}\theta_1^6\theta_2 + \frac{82973}{46080}\theta_1^4\theta_3 + \frac{76979}{61440}\theta_1^3\theta_2^2 + \frac{2158457}{1474560}\theta_1\theta_2\theta_3 + \frac{691831}{1179648}\theta_2^3$$
$$\frac{141653}{14400}\theta_1^{10} - \frac{264873}{25600}\theta_1^7\theta_2 + \frac{31977}{12800}\theta_1^5\theta_3 - \frac{4207483}{614400}\theta_1^4\theta_2^2 + \frac{2664123}{1638400}\theta_1^2\theta_2\theta_3 + \frac{8189125}{2359296}\theta_1\theta_2^3$$
$$+\frac{5285401}{19660800}\theta_3^2$$

H_u

$$\frac{448}{3}\theta_1^5 - \frac{616}{3}\theta_1^2\theta_2 + 57\theta_3$$
$$\frac{1248\sqrt{5}-2720}{5}\theta_1^6 + \frac{-2436\sqrt{5}+5740}{5}\theta_1^3\theta_2 + \frac{171\sqrt{5}+95}{10}\theta_1\theta_3 + \frac{441\sqrt{5}-1225}{2}\theta_2^2$$
$$\frac{24128\sqrt{5}-54336}{15}\theta_1^7 + \frac{-47096\sqrt{5}+107352}{15}\theta_1^4\theta_2 + \frac{551\sqrt{5}-1007}{5}\theta_1^2\theta_3 + (1421\sqrt{5}-3332)\theta_1\theta_2^2$$
$$\frac{12992512\sqrt{5}-29577600}{225}\theta_1^8 + \frac{-29413664\sqrt{5}+67006800}{225}\theta_1^5\theta_2 + \frac{432288\sqrt{5}-985150}{25}\theta_1^3\theta_3$$
$$+\frac{3237479\sqrt{5}-7382340}{45}\theta_1^2\theta_2^2 + \frac{-81263\sqrt{5}+185535}{5}\theta_2\theta_3$$
$$\frac{72650528\sqrt{5}-162710112}{45}\theta_1^9 + \frac{-178550428\sqrt{5}+399904596}{45}\theta_1^6\theta_2 + \frac{13365607\sqrt{5}-29931213}{30}\theta_1^4\theta_3$$

$$+\frac{239629453\sqrt{5}-536752713}{90}\theta_1^3\theta_2^2+\frac{-6496784\sqrt{5}+14549934}{15}\theta_1\theta_2\theta_3+\frac{-964859\sqrt{5}+2161929}{3}\theta_2^3$$

$$\frac{26208\sqrt{5}-61408}{15}\theta_1^7+\frac{-51156\sqrt{5}+121156}{15}\theta_1^4\theta_2+\frac{1197\sqrt{5}-2337}{10}\theta_1^2\theta_3+\frac{3087\sqrt{5}-7497}{2}\theta_1\theta_2^2$$

$$\frac{12510592\sqrt{5}-28122880}{225}\theta_1^8+\frac{-28224224\sqrt{5}+63454160}{225}\theta_1^5\theta_2+\frac{408158\sqrt{5}-915420}{25}\theta_1^3\theta_3$$

$$+\frac{6189043\sqrt{5}-13919185}{90}\theta_1^2\theta_2^2+\frac{-152551\sqrt{5}+342475}{10}\theta_2\theta_3$$

$$\frac{357958848\sqrt{5}-801263680}{225}\theta_1^9+\frac{-878913336\sqrt{5}+1967205800}{225}\theta_1^6\theta_2+\frac{32869981\sqrt{5}-73593935}{75}\theta_1^4\theta_3$$

$$+\frac{235563531\sqrt{5}-527124997}{90}\theta_1^3\theta_2^2+\frac{-6385463\sqrt{5}+14297101}{15}\theta_1\theta_2\theta_3+\frac{-1887529\sqrt{5}+4218557}{6}\theta_2^3$$

$$\frac{1693705184\sqrt{5}-3787860832}{45}\theta_1^{10}+\frac{-21859861828\sqrt{5}+48887989780}{225}\theta_1^7\theta_2+\frac{829053239\sqrt{5}-1854036435}{50}\theta_1^5\theta_3$$

$$+\frac{15064043246\sqrt{5}-33689691770}{225}\theta_1^4\theta_2^2+\frac{-1007541367\sqrt{5}+2253166965}{50}\theta_1^2\theta_2\theta_3$$

$$+\frac{-51641051\sqrt{5}+115500105}{9}\theta_1\theta_2^3+\frac{46835057\sqrt{5}-104731515}{25}\theta_3^2$$

$$\frac{368851328\sqrt{5}-825444480}{225}\theta_1^9+\frac{-907003216\sqrt{5}+2029747440}{225}\theta_1^6\theta_2+\frac{33736666\sqrt{5}-75492510}{75}\theta_1^4\theta_3$$

$$+\frac{121976386\sqrt{5}-272962242}{45}\theta_1^3\theta_2^2+\frac{-6555836\sqrt{5}+14670432}{15}\theta_1\theta_2\theta_3+\frac{-994700\sqrt{5}+2225727}{3}\theta_2^3$$

$$\frac{2953684096\sqrt{5}-6605545600}{75}\theta_1^{10}+\frac{-4580798320\sqrt{5}+10244330544}{45}\theta_1^7\theta_2+\frac{1315287274\sqrt{5}-2941519770}{75}\theta_1^5\theta_3$$

$$+\frac{15794253643\sqrt{5}-35321218065}{225}\theta_1^4\theta_2^2+\frac{-1604288959\sqrt{5}+3587845905}{75}\theta_1^2\theta_2\theta_3$$

$$+\frac{-53534411\sqrt{5}+119706657}{9}\theta_1\theta_2^3+\frac{50450111\sqrt{5}-112826940}{25}\theta_3^2$$

$$\frac{75715610496\sqrt{5}-169308883712}{75}\theta_1^{11}+\frac{-630884869664\sqrt{5}+1410731127344}{225}\theta_1^8\theta_2$$

$$+\frac{42327530326\sqrt{5}-94648999244}{75}\theta_1^6\theta_3+\frac{972238541267\sqrt{5}-2174036688173}{450}\theta_1^5\theta_2^2$$

$$+\frac{-58719975076\sqrt{5}+131304228188}{75}\theta_1^3\theta_2\theta_3+\frac{-25972330097\sqrt{5}+58077179489}{90}\theta_1^2\theta_2^3$$

$$+\frac{2011259155\sqrt{5}-4497384569}{25}\theta_1\theta_3^2+\frac{302790992\sqrt{5}-677073474}{5}\theta_2^2\theta_3$$

$$\frac{695144135168\sqrt{5}-1554407364352}{675}\theta_1^{11}+\frac{-644002014208\sqrt{5}+1440045581856}{225}\theta_1^8\theta_2$$

$$+\frac{43239175368\sqrt{5}-96687242636}{75}\theta_1^6\theta_3+\frac{496757391942\sqrt{5}-1110787534346}{225}\theta_1^5\theta_2^2$$

$$+\frac{-60039573944\sqrt{5}+134254318212}{75}\theta_1^3\theta_2\theta_3+\frac{-39973239208\sqrt{5}+89380532549}{135}\theta_1^2\theta_2^3$$

$$+\frac{2056498592\sqrt{5}-4598562761}{25}\theta_1\theta_3^2+\frac{936312286\sqrt{5}-2093598353}{15}\theta_2^2\theta_3$$

$$\frac{102484099009216\sqrt{5}-229161983510080}{3375}\theta_1^{12}+\frac{-103712003920168\sqrt{5}+231907635997240}{1125}\theta_1^9\theta_2$$

$$+\frac{18203575800549\sqrt{5}-40704542676695}{1125}\theta_1^7\theta_3+\frac{192334395907241\sqrt{5}-430073674278955}{2250}\theta_1^6\theta_2^2$$

$$+\frac{-27575163543228\sqrt{5}+61660097771440}{1125}\theta_1^4\theta_2\theta_3+\frac{-15950451341027\sqrt{5}+35666340525725}{675}\theta_1^3\theta_2^3$$

$$+\frac{542807423231\sqrt{5}-1213757793755}{250}\theta_1^2\theta_3^2+\frac{908322350082\sqrt{5}-2031073882600}{225}\theta_1\theta_2^2\theta_3+$$

$$\frac{18838942290\sqrt{5}-42125180048}{9}\theta_2^4$$

$$\frac{3017661092856288\sqrt{5}-6747698145436256}{3375}\theta_1^{13}+\frac{-9757682133208212\sqrt{5}+21818849408711684}{3375}\theta_1^{10}\theta_2$$

$$+\frac{1018019538640689\sqrt{5}-2276361853755053}{2250}\theta_1^8\theta_3+\frac{3379828161239544\sqrt{5}-7557528462019018}{1125}\theta_1^7\theta_2^2$$
$$+\frac{-858802528101924\sqrt{5}+1920341613573908}{1125}\theta_1^5\theta_2\theta_3+\frac{-1433089424148543\sqrt{5}+3204486519902213}{1350}\theta_1^4\theta_2^3$$
$$+\frac{21805257173562\sqrt{5}-48758058158054}{375}\theta_1^3\theta_3^2+\frac{48419759670870\sqrt{5}-108269912096318}{225}\theta_1^2\theta_2^2\theta_3$$
$$+\frac{2747035841550\sqrt{5}-6142560966430}{27}\theta_1\theta_2^4+\frac{-739662143766\sqrt{5}+1653935302474}{75}\theta_2\theta_3^2$$

Table 2.8: Matrices Q^π for the group H_3 given in upper triangular row-major order (in the consecutive order of row entries of upper triangular matrices).

Chapter Three

New upper bounds for the density of translative packings of three-dimensional convex bodies with tetrahedral symmetry

This chapter is based on the paper: "M. Dostert, C. Guzmán, F. M. de Oliveira Filho, and F. Vallentin, *New upper bounds for the density of translative packings of three-dimensional convex bodies with tetrahedral symmetry*, arXiv:1510.02331 [math.MG], *Discrete and Computational Geometry*, 2017, 30 pages".

3.1 Formulation as a polynomial optimization problem

Theorem 1.2 contains a characterization of a suitable Schwartz function f, such that $f(0)$ gives an upper bound for the density of every translative packing of a given convex body in $\mathbb{R}^n$. Thus, based on this characterization, we can formulate an optimization problem with objective function $f(0)$ and linear constraints to ensure that f satisfies the conditions given in Theorem 1.2. Since the obtained problem has infinitely many linear constraints and we optimize over $\mathcal{S}(\mathbb{R}^n)$, thus an infinite dimensional set, it is an infinite dimensional linear program.

$$\begin{aligned}
\delta(\mathcal{K}) \leq \min\ & f(0) && (3.1)\\
& f \in \mathcal{S}(\mathbb{R}^n) && (3.2)\\
& \widehat{f}(0) \geq \operatorname{vol}\mathcal{K} && (3.3)\\
& \widehat{f}(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\} && (3.4)\\
& f(x) \leq 0 \text{ whenever } \mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset && (3.5)
\end{aligned}$$

As explained in Section 2.1.1, SDPs has been well studied and there exists techniques to solve these kind of problems efficiently. Thus, we relax the above optimization problem

to an SDP. In Section 2.1.2, we explained how to relax a polynomial optimization problem to an SDP, therefore we first relax the infinite dimensional linear program to a polynomial optimization problem, and then we relax the obtained problem to an SDP. To be able to formulate this problem as a polynomial optimization problem, we would like to optimize over the set of polynomials $\mathbb{R}[x]_{\leq 2d}$ of a fixed maximum degree $2d$, instead of optimizing over the space of Schwartz functions. To do so, we use the following equation for the Fourier transform $\widehat{f}$ of the optimization variable f to specify it by a real polynomial $g \in \mathbb{C}[x]_{\leq 2d}$ multiplied with the Gaussian density

$$\widehat{f}(u) = g(u)e^{-\pi\|u\|^2}. \tag{3.6}$$

All derivatives $D^\beta \widehat{f}(x)$ exist for all $x \in \mathbb{R}^n$ and for all $\beta \in \mathbb{N}^n$. Moreover,

$$\sup\left\{\left|x^\alpha D^\beta \widehat{f}(x)\right| : x \in \mathbb{R}^n\right\} < \infty$$

holds for all $\alpha, \beta \in \mathbb{N}^n$. Thus, the Fourier transform $\widehat{f}$ is a Schwartz function, which implies that the function f is also a Schwartz function [35, Chapter 9.4, Theorem 9.7]. In particular, the function f is a feasible solution for the Cohn-Elkies bound, if it satisfies conditions (3.3) to (3.5). By applying equation (3.6), we obtain the following polynomial optimization problem:

$$\begin{aligned}
\delta(\mathcal{K}) \leq \min \int_{\mathbb{R}^n} g(u)e^{-\pi\|u\|^2} & && (3.7)\\
g \in \mathbb{R}[x]_{2d} & && (3.8)\\
g(0) \geq \mathrm{vol}\mathcal{K} & && (3.9)\\
g(u) \geq 0 \ \text{ for all } u \in \mathbb{R}^n \setminus \{0\} & && (3.10)\\
\int_{\mathbb{R}^n} g(u)e^{-\pi\|u\|^2} e^{2\pi i u\cdot x} du \leq 0 \ \text{ whenever } \mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset & && (3.11)
\end{aligned}$$

Since we restrict the function f to be of the form (3.6), the polynomial optimization problem is a relaxation of the Cohn-Elkies program. However, since those weighted polynomials lie dense in the Schwartz space [50, Chapter III], the optimal value of the polynomial optimization problem is equal to the optimal value of the original problem. Since $\widehat{f}(0) = g(0)$, condition (3.9) corresponds to condition (3.3). Furthermore, the Fourier transform $\widehat{f}$ is nonnegative if and only if the polynomial g is nonnegative. Therefore, we can replace condition (3.4) by condition (3.10). However, for computing the objective value and for checking condition (3.5), we have to compute the function f from the polynomial g, which means we determine f from its Fourier transform $\widehat{f}$. In Section 3.2, we will explain this calculation in detail.

We can simplify the above polynomial optimization problem by using symmetries. Note, that the Gaussian part $e^{-\pi\|u\|^2}$ of $\widehat{f}$ is invariant under any orthogonal transformation. Furthermore, conditions (3.3) and (3.4) are invariant under any invertible linear transformation. For the last condition (3.5), we will consider the *symmetry group* of a convex body $\mathcal{K} \subseteq \mathbb{R}^n$, which is defined by

$$S(\mathcal{K}) = \{A \in O(n) : A\mathcal{K} = \mathcal{K}\}.$$

The *Minkowski difference* of $A, B \subseteq \mathbb{R}^n$ is given by

$$A - B = \{a - b : a \in A, b \in B\}\,.$$

To prove that condition (3.5) is invariant under the symmetry group $S(\mathcal{K} - \mathcal{K})$, we have to check whether $\mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset$ if and only if $\mathcal{K}^\circ \cap (A^{-1}x + \mathcal{K}^\circ) = \emptyset$ for all $A \in S(\mathcal{K} - \mathcal{K})$. To do so, we consider an arbitrary element of the symmetry group $A \in S(\mathcal{K} - \mathcal{K})$, then

$$\begin{aligned}
\mathcal{K}^\circ \cap (A^{-1}x + \mathcal{K}^\circ) = \emptyset &\iff A\mathcal{K}^\circ \cap (x + A\mathcal{K}^\circ) = \emptyset \\
&\iff x \notin A\mathcal{K}^\circ - A\mathcal{K}^\circ \\
&\iff x \notin A(\mathcal{K}^\circ - \mathcal{K}^\circ) \\
&\iff x \notin \mathcal{K}^\circ - \mathcal{K}^\circ \\
&\iff \mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset\,.
\end{aligned}$$

Lemma 3.1. *Let (P) be the linear program given in (3.1) to (3.5) for a solid $\mathcal{K}$. Let (P') be the linear program, which we obtain by adding the condition*

$$f \text{ is invariant under the group } S(\mathcal{K} - \mathcal{K})$$

to (P). Then, the optimal value of (P) is equal to the optimal value of (P').

Proof. Let f be a feasible function for (P) and $S(\mathcal{K} - \mathcal{K})$ be the symmetry group of the Minkowski difference of $\mathcal{K}$. For a function $f \in \mathcal{S}(\mathbb{R}^n)$, we define the Reynolds operator similar as (2.22):

$$Mf(x_1, \ldots, x_n) = \frac{1}{|G|} \sum_{g \in G} f\left(g^{-1}(x_1, \ldots, x_n)\right).$$

Then, we get a function $\tilde{f} = Mf$ invariant under $S(\mathcal{K} - \mathcal{K})$. Furthermore, this function is a Schwartz function if f is a Schwartz function. The linearity of the Fourier transforms implies that $\tilde{f}$ satisfies conditions (3.3) and (3.4). Since the intersection $\mathcal{K}^\circ \cap (A^{-1}x + \mathcal{K}^\circ)$ is empty if and only if the intersection $\mathcal{K}^\circ \cap (x + \mathcal{K}^\circ)$ is empty, we know that $f(x) \leq 0$ holds if and only if $f(A^{-1}x) \leq 0$ holds for all $A \in S(\mathcal{K} - \mathcal{K})$. This implies that each summand of $\tilde{f}(x) = \frac{1}{|G|} \sum_{g \in G} f\left(g^{-1}x\right)$ is nonpositive, and thus, condition (3.5) is satisfied. Consequently, the function $\tilde{f}$ is a feasible solution for (P'). Furthermore, by applying the Reynolds operator the value at the point $x = 0$ will not change, because we are averaging, and therefore, the optimal values of (P) and (P') coincide. □

Consequently, we can assume that f is invariant under $S\,(\mathcal{K} - \mathcal{K})$:

$$f(A^{-1}x) = f(x) \quad \text{for all } A \in S\,(\mathcal{K} - \mathcal{K})\ .$$

If the function f is invariant under the symmetry group $S(\mathcal{K} - \mathcal{K})$, then its Fourier transform $\widehat{f}$ is invariant under this group, too. Furthermore, since the Gaussian part of the formula for $\widehat{f}$ is invariant under any orthogonal transformation, the polynomial g, which defines $\widehat{f}$, is invariant under the symmetry group, too. For the convex bodies $\mathcal{K}$ with $S(\mathcal{K} - \mathcal{K})$ equal to the octahedral group B_3 or to the icosahedral group H_3, the invariant polynomial g is a real polynomial as we mentioned in Section 2.3.2 and Section 2.3.3.

3.2 Computation of the Fourier transform

To compute the antitransform f from $\widehat{f}$, we have to compute the Fourier transform of $u \mapsto \widehat{f}(-u)$. First, we explain how to obtain the function f from an arbitrary complex polynomial g and then, we give a simplification of this computation by using some properties of the polynomial g of the considered optimization problem. We can decompose the set of complex polynomials of degree at most d into the following direct sum

$$\mathbb{C}[x]_{\leq d} = \bigoplus_{j=0}^{d} \mathrm{Hom}_j = \bigoplus_{j=0}^{d} \bigoplus_{\substack{r,k \\ 2r+k=j}} \|x\|^{2r} \mathrm{Harm}_k \ , \tag{3.12}$$

where

$$\mathrm{Harm}_k = \left\{ h \in \mathrm{Hom}_k : \Delta\, h = \left(\frac{\partial^2}{\partial^2 x_1} + \cdots + \frac{\partial^2}{\partial^2 x_n} \right) h = 0 \right\}$$

is the set of *(homogeneous) harmonic polynomials* of degree k. This means, harmonic polynomials of degree k are the kernel of the *Laplace operator*

$$\mathrm{Harm}_k = \ker \Delta, \quad \Delta : \mathrm{Hom}_k \to \mathrm{Hom}_{k-2} \ ,$$

with

$$\Delta h(x_1, \ldots, x_n) = \sum_{i=1}^{n} \frac{\partial^2 h}{\partial^2 x_i} \ ,$$

where

$$\dim \mathrm{Harm}_k = \dim \mathrm{Hom}_k - \dim \mathrm{Hom}_{k-2} = \binom{n+k-1}{k} - \binom{n+k-3}{k-2} . \tag{3.13}$$

A proof of the decomposition of the complex polynomials into harmonic polynomials is, for example, presented by Stein and Weiss in [69, Theorem IV.2.10]. For the computation of f, we need *Laguerre polynomials* $L_n^{\alpha}(x)$ of degree $n \in \mathbb{Z}_{\geq 0}$ in the variable x and with parameter $\alpha \in \mathbb{R}$ greater than -1, which are defined by

$$L_n^{\alpha}(x) = \frac{1}{n} x^{-\alpha} e^{x} \frac{d^n}{dx^n} \left(e^{-x} x^{n+\alpha} \right) \ .$$

The Fourier transform of the function $u \mapsto \widehat{f}(-u)$ is equal to f. Therefore, we will compute this Fourier transform to obtain f from $\widehat{f}$, which is specified by a polynomial $g \in \mathbb{C}[x]_{\leq d}$. If we express g by harmonic polynomials, we can apply Proposition 3.2 to compute f.

Proposition 3.2. *Let*

$$f(x) = h_k(x) \|x\|^{2r} e^{-\pi \|x\|^2}$$

be a Schwartz function with $h_k \in \mathrm{Harm}_k$. The Fourier transform of f is

$$\widehat{f}(u) = (i^{-k} h_k(u)) \cdot \pi^{-r} r! L_r^{n/2+k-1}(\pi \|u\|^2) e^{-\pi \|u\|^2},$$

where $L_r^{n/2+k-1}$ is the Laguerre polynomial of degree r with parameter $n/2 + k - 1$.

Proposition 3.2 shows that the function $x \mapsto h_k(x)e^{-\pi\|x\|^2}$ is an eigenfunction of the Fourier transform with eigenvalue i^{-k}. This means, by applying Proposition 3.2 the function f with Fourier transform $\widehat{f}(u) = g(u)e^{-\pi\|u\|^2}$ can be computed from the polynomial g by solving a system of linear equations. Dunkl uses a similar computation and he even gives in [32] explicit algebraic solutions.

To prove Proposition 3.2, we have to give some definitions and lemmas. The *Gamma function* of a complex number $x \in \mathbb{C}$ with real part $\mathrm{Re}(x) > 0$ is defined by

$$\Gamma(x) = \int_0^\infty t^{x-1}e^{-t}dt\,. \tag{3.14}$$

Furthermore, we need the *Bessel function* $J_k(t)$ with real number $k \geq -1/2$ and $t \in \mathbb{R}_{>0}$ given by the formula

$$J_k(t) = \frac{(t/2)^k}{\Gamma(k+1/2)\,\Gamma(1/2)} \int_{-1}^1 e^{its}(1-s)^{k-1/2}ds\,. \tag{3.15}$$

The *hypergeometric series* ${}_1F_1\left(\begin{smallmatrix}a\\b\end{smallmatrix}; x\right)$ is defined as

$${}_1F_1\left(\begin{matrix}a\\b\end{matrix}; x\right) = \sum_{k=0}^\infty \frac{(a)_k}{(b)_k}\frac{x^k}{k!}\,, \tag{3.16}$$

where $a, b, x \in \mathbb{C}$ are arbitrary complex numbers satisfying $b \notin \mathbb{Z}_{\leq 0}$ and $(q)_n$ is defined as

$$(q)_n = \begin{cases} 1, & \text{if } n = 0\,, \\ \prod_{k=0}^{n-1}(q+k), & \text{if } n > 0\,. \end{cases}$$

The proof of Proposition 3.2 can be divided into three steps. First, we express the Fourier transform of f in terms of a Bessel function. Then, we describe the Bessel function by the hypergeometric series. In the last step, we replace the hypergeometric series by the Laguerre polynomials, and so, we get the equation of Proposition 3.2. In the following, we explain each of these steps in more detail, and then, we give the proof for Proposition 3.2.

The relation between the Fourier transform of f and the Bessel function is described in the following lemma.

Lemma 3.3. *Suppose $n \geq 2$ and $f \in L^2(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$ has the form*

$$f(x) = f_0(\|x\|)P(x),$$

where $P(x)$ is a harmonic function of degree k and $f_0(\|x\|)$ is a radial function. Then, the Fourier transform $\widehat{f}$ has the form $\widehat{f}(x) = F_0(\|u\|)P(x)$, where

$$F_0(r) = 2\pi i^{-k}r^{-(n/2+k-1)} \int_0^\infty f_0(s)J_{n/2+k-1}(2\pi rs)\cdot s^{n/2+k}ds\,. \tag{3.17}$$

Stein and Weiss present in [69] a proof of Lemma 3.3. The function in Proposition 3.2 is described by the equation $f(x) = h_k(x)\|x\|^{2r}e^{-\pi\|x\|^2}$, where $h_k(x)$ is a harmonic polynomial

of degree k. Since $x \to \|x\|^{2r} e^{-\pi\|x\|^2}$ is a radial function and $h_k(x) \in \mathrm{Harm}_k$, we can apply Lemma 3.3 to the function f. As there exists a monomial basis for the complex homogeneous polynomials of degree k, such that all coefficients of the monomials in this basis are real, we can compute a basis for Harm_k with real coefficients, too.

Lemma 3.4 describes how to replace the Bessel function by the hypergeometric series.

Lemma 3.4. *For $Re(x) > 0$,*

$$\int_0^\infty J_v(at) t^{\mu-1} e^{-p^2t^2} dt = \frac{\Gamma(\frac{\mu+\nu}{2})(\frac{a}{2p})^\nu e^{-a^2/4p^2}}{2p^\mu \Gamma(\nu+1)} {}_1F_1\left(\begin{matrix}\frac{\nu-\mu}{2}+1\\ \nu+1\end{matrix}; \frac{a^2}{4p^2}\right). \tag{3.18}$$

In [3], Andrew, Askey, and Roy give a proof for Lemma 3.4. Furthermore, they present a relation between finite hypergeometric series and Laguerre polynomials. This relation is given in Lemma 3.5.

Lemma 3.5. *The Laguerre polynomial $L_n^\alpha(x)$ can be expressed in terms of a hypergeometric series as*

$$L_n^\alpha(x) = \frac{(\alpha+1)_n}{n!} \sum_{k=0}^n \frac{(-n)_k x^k}{(\alpha+1)_k k!} = \frac{(\alpha+1)_n}{n!} {}_1F_1\left(\begin{matrix}-n\\ \alpha+1\end{matrix}; x\right).$$

The tedious verification of this formula has been, for example, carried out by Pütz [64]. First, he proves by induction over n the equation

$$\frac{d^n}{dx^n}(e^{-x}x^{n+\alpha}) = \sum_{k=0}^n \left(\frac{(-1)^{n-k}}{(n-k)!}\left(\prod_{l=k+1}^n l \prod_{m=0}^{k-1}(n+\alpha-m)\right)\right).$$

Then he splits the right-hand side into two parts and shows that

$$(-1)^{n-k}\prod_{l=k+1}^n l = (-n)_{n-k} \quad \text{and} \quad \prod_{m=0}^{k-1}(n+\alpha-m) = \frac{(\alpha+1)_m}{(\alpha+1)_{n-k}}.$$

Combining these results with the definition of the Laguerre polynomial, we obtain

$$\begin{aligned} L_n^\alpha(x) &= \frac{x^{-a}e^x}{n!}\sum_{l=0}^n \left(\frac{(-n)_l}{(l)!}\frac{(\alpha+1)_n}{(\alpha+1)_l}\right) e^{-x}x^{\alpha+l} \\ &= \frac{(\alpha+1)_n}{n!}\sum_{k=0}^n \frac{(-n)_k x^k}{(\alpha+1)_k k!} = \frac{(\alpha+1)_n}{n!}{}_1F_1\left(\begin{matrix}-n\\ \alpha+1\end{matrix}; x\right) \end{aligned}$$

the equations of Lemma 3.5. By using Lemma 3.3, Lemma 3.4, and Lemma 3.5, we can give a proof for Proposition 3.2.

Proof. Let $f(x) = h_k(x)\|x\|^{2r}e^{-\pi\|x\|^2}$ be a Schwartz function with $h_k \in \mathrm{Harm}_k$. As mentioned before, the function $f_0(\|x\|) = \|x\|^{2r}e^{-\pi\|x\|^2}$ has the property that $f_0(x)$ just depends on the norm $\|x\|$, and thus, f_0 is a radial function. By definition, h_k is a harmonic polynomial of degree k, thus, we can apply Lemma 3.3 and obtain

$$\begin{aligned} \widehat{f}(u) &= 2\pi i^{-k}\|u\|^{-(n/2+k-1)} \int_0^\infty f_0(s) J_{n/2+k-1}(2\pi\|u\|us)\cdot s^{n/2+k} ds \ \cdot h_k(u) \\ &= (i^{-k}h_k(u))\cdot 2\pi\|u\|^{-(n/2+k-1)} \int_0^\infty J_{n/2+k-1}(2\pi s\|u\|) s^{n/2+k+2r} e^{-\pi s^2} ds. \end{aligned}$$

To describe the Bessel function by hypergeometric series, we apply Lemma 3.4 by setting $a = 2\pi\|u\|,\ p = \sqrt{\pi},\ \mu = n/2 + 2r + k + 1$, and $\nu = n/2 + k - 1$ and using the equations

$$\frac{a}{2p} = \sqrt{\pi}\|u\|, \quad \frac{a^2}{4p^2} = \pi\|u\|^2, \quad \frac{\mu+\nu}{2} = n/2 + r + k, \quad \frac{\nu-\mu}{2} + 1 = -r.$$

This implies

$$\begin{aligned}
&\int_0^\infty J_{n/2+k-1}(2\pi s\|u\|)s^{n/2+k+2r}e^{-\pi s^2}ds \\
&= \frac{\Gamma(n/2+r+k)(\sqrt{\pi}\|u\|)^{n/2+k-1}e^{-\pi\|u\|^2}}{2(\sqrt{\pi})^{n/2+2r+k+1}\Gamma(n/2+k)}\,{}_1F_1\left(\begin{matrix}-r\\ n/2+k\end{matrix};\pi\|u\|^2\right) \\
&= \frac{\|u\|^{n/2+k-1}\Gamma(n/2+r+k)e^{-\pi\|u\|^2}}{2(\sqrt{\pi})^{2r+2}\Gamma(n/2+k)}\,{}_1F_1\left(\begin{matrix}-r\\ n/2+k\end{matrix};\pi\|u\|^2\right).
\end{aligned}$$

In the last step, we just worked with the part of the Fourier transform $\widehat{f(u)}$ which contains the integral. Now we consider the whole remaining equation

$$\begin{aligned}
\widehat{f(u)} &= (i^{-k}h_k(u)) \cdot \frac{2\pi \cdot \|u\|^{n/2+k-1}\Gamma(n/2+r+k)e^{-\pi\|u\|^2}}{\|u\|^{n/2+k-1}\cdot 2\pi^{r+1}\Gamma(n/2+k)}\,{}_1F_1(\tfrac{-r}{n/2+k};\pi\|u\|^2) \\
&= (i^{-k}h_k(u)) \cdot \pi^{-r}\frac{\Gamma(n/2+r+k)}{\Gamma(n/2+k)}\,{}_1F_1\left(\begin{matrix}-r\\ n/2+k\end{matrix};\pi\|u\|^2\right)e^{-\pi\|u\|^2}.
\end{aligned}$$

By applying Lemma 3.5, we replace the hypergeometric series by the Laguerre polynomial $L_n^\alpha(x)$ with $\alpha = n/2 + k - 1,\ n = r$, and $x = \pi\|u\|^2$, and obtain

$${}_1F_1\left(\begin{matrix}-r\\ n/2+k\end{matrix};\pi\|u\|^2\right)e^{-\pi\|u\|^2} = \frac{r!}{(n/2+k)_r}L_r^{n/2+k-1}(\pi\|u\|^2)\,.$$

Finally, we can describe the Fourier transform $\widehat{f(u)}$ by using the Laguerre polynomial $L_r^{n/2+k-1}(\pi\|u\|^2)$. Thus,

$$\begin{aligned}
\widehat{f(u)} &= (i^{-k}h_k(u)) \cdot \pi^{-r}\frac{\Gamma(n/2+r+k)}{\Gamma(n/2+k)}\,{}_1F_1\left(\begin{matrix}-r\\ n/2+k\end{matrix};\pi\|u\|^2\right)e^{-\pi\|u\|^2} \\
&= (i^{-k}h_k(u)) \cdot \pi^{-r}\frac{\Gamma(n/2+r+k)}{\Gamma(n/2+k)}\frac{r!}{(n/2+k)_r}L_r^{n/2+k-1}(\pi\|u\|^2)\,.
\end{aligned}$$

We use the property $\Gamma(x+1) = x\Gamma(x)$ of the Gamma function, and therefore,

$$\frac{\Gamma(n/2+k+r)}{\Gamma(n/2+k)} = \prod_{j=0}^{r-1}(n/2+k+j)\,\frac{\Gamma(n/2+k)}{\Gamma(n/2+k)} = (n/2+k)_r$$

holds for $r \in \mathbb{Z}$. By using

$$\frac{\Gamma(n/2+r+k)}{\Gamma(n/2+k)}\frac{1}{(n/2+k)_r} = 1\,,$$

we obtain the desired result

$$\widehat{f(u)} = \left(i^{-k}h_k(u)\right) \cdot \pi^{-r}r!L_r^{n/2+k-1}\left(\pi\|u\|^2\right)e^{-\pi\|u\|^2}\,.$$

□

To compute the inverse Fourier transform of $\widehat{f}$, we write $\widehat{f}$ as a sum over polynomials of the form $h_k(x)\|x\|^{2r}e^{-\pi\|u\|^2}$, where h_k is a harmonic polynomial of degree k. Due to the linearity of the Fourier transform operator, it is sufficient to compute the inverse Fourier transform of each of these summands for obtaining the inverse Fourier transform of $\widehat{f}$. For this computation, we use Proposition 3.2.

From Section 3.1, we know that the polynomial g is invariant under a pseudo-finite reflection group G. By using this property, we can reduce the dimension of the harmonic subspaces. To do so, we have to define the set of *G-invariant harmonic polynomials*

$$\mathrm{Harm}_k^G = \left\{h \in \mathrm{Hom}_k^G : \Delta h = 0\right\} .$$

Thus, the space of G-invariant complex polynomials can be decomposed as

$$\mathbb{C}[x]_{\leq d}^G = \bigoplus_{j=0}^{d} \mathrm{Hom}_j^G = \bigoplus_{j=0}^{d} \bigoplus_{\substack{r,k \\ 2r+k=j}} \|x\|^{2r}\,\mathrm{Harm}_k^G .$$

Using this decomposition, we can compute the antitransform $\widehat{f}$ from f by applying Proposition 3.2 in the same way as by using the decomposition of $\mathbb{C}[x]$. The benefit of taking the G-invariance into account is, that the dimension of the harmonic subspaces is smaller, and therefore, the computation of f should be faster. To compare the dimensions, we can use the *harmonic Molien-Poincáre series*, given by Goethals and Seidel in [39].

Theorem 3.6. *Let $G \subset O_n(\mathbb{R})$ be a finite reflection group. Then, the harmonic Molien-Poincáre series is given by*

$$\sum_{k=0}^{\infty} \dim \mathrm{Harm}_k^G \cdot t^k = \prod_{i=2}^{n} (1 - t^{d_i})^{-1} ,$$

where $d_1 \leq \ldots \leq d_n$ are the degrees of the primary invariants of G.

Example 3.7. By applying the formula for the dimension of Harm_k given in (3.13) to 3-variate polynomials, we obtain $2k + 1$. We will compare this dimension to the dimension of the subspaces $\mathrm{Harm}_k^{\mathsf{B}_3}$ and $\mathrm{Harm}_k^{\mathsf{H}_3}$. Since B_3 and H_3 are finite reflection groups, we can apply Theorem 3.6:

$$\begin{aligned}\sum_{k=0}^{\infty} \dim \mathrm{Harm}_k^{\mathsf{B}_3} \cdot t^k &= \frac{1}{(1-t^4)(1-t^6)} \\ &= 1 + t^4 + t^6 + t^8 + t^{10} + t^{12} + t^{14} + 2t^{16} + 2t^{18} + 2t^{20} + 2t^{22} + \\ &\quad 3t^{24} + 2t^{26} + 3t^{28} + 3t^{30} + 3t^{32} + 3t^{34} + 4t^{36} + 3t^{38} + 3t^{40} + \ldots\end{aligned}$$

$$\begin{aligned}\sum_{k=0}^{\infty} \dim \mathrm{Harm}_k^{\mathsf{H}_3} \cdot t^k &= \frac{1}{(1-t^6)(1-t^{10})} \\ &= 1 + t^6 + t^{10} + t^{12} + t^{18} + t^{20} + t^{22} + t^{24} + t^{26} + t^{26} + \\ &\quad t^{28} + 2t^{30} + t^{32} + t^{34} + 2t^{36} + t^{38} + 2t^{40} + \ldots\end{aligned}$$

We consider for example $\mathbb{C}[x]^G_{\leq 40}$

$$\sum_{k=0}^{40} \dim \mathrm{Harm}_k = \sum_{k=0}^{40} 2k+1 = 1681 \,,$$

but

$$\sum_{k=0}^{40} \dim \mathrm{Harm}_k^{\mathsf{B}_3} = 42 \quad \text{and} \quad \sum_{k=0}^{40} \dim \mathrm{Harm}_k^{\mathsf{H}_3} = 20 \,.$$

The computation of the invariant harmonic spaces is more work than the computation of the harmonic spaces. However, for the groups B_3 and H_3, the computation of the Fourier antitransform f was much faster by exploiting the group invariance.

3.3 Semidefinite formulation

In Section 3.1 we relaxed the infinite dimensional linear program from Cohn and Elkies to a polynomial optimization problem, in which we optimize over polynomials $g \in \mathbb{R}[x]_{\leq 2d}$ invariant under a finite pseudo-reflection group G. The next task is to relax the polynomial optimization problem to an SDP, which is solvable by using current SDP solvers. In Section 2.1.2 we explained how to relax a polynomial optimization problem in order to obtain an SDP. The problem is that if the dimension of the matrices in the SDP is too large, we cannot use current SDP solvers. Thus, on the one hand we have to find a relaxation of the polynomial optimization problem described as an SDP, and on the other hand, we need to use the G-invariance of g to simplify the problem in such a way, that we can use a solver. Furthermore, we have to find a way to formulate the infinitely many nonpositivity constraints as suitable constraints in the SDP.

3.3.1 Representation of the function f

To transform the objective function in (3.7) and condition (3.11) into standard form for the SDP, we have to give a *good* representation of the function f. Since its definition depends on the polynomial g, the next task is to describe this polynomial. Due to the constraint (3.10) it has to be nonnegative, which we know from Section 2.1.2 is difficult to check. Therefore, we restrict $g(x)$ to be equal to $\tilde{g}(x, \overline{x})$, where $\tilde{g}$ is an SOHS polynomial.

An example of a B_3-invariant polynomial is the Robinson polynomial

$$x_1^6 + x_2^6 + x_3^6 - \left(x_1^4x_2^2 + x_1^2x_2^4 + x_1^4x_3^2 + x_1^2x_3^4 + x_2^4x_3^2 + x_2^2x_3^4\right) + 3x_1^2x_2^2x_3^2,$$

which is nonnegative, but it is not SOS. A proof is given by Reznick in [66]. Furthermore, this implies that it is not SOHS, too, since B_3-invariant polynomials are SOS if and only if they are SOHS. Thus, even for B_3-invariant polynomials with three variables and degree six, the set of SOS polynomials is a strict subset of the set of nonnegative polynomials. One possibility to describe g with degree at most $2d$ offers Theorem 2.20:

$$g(z, \overline{w}) = \sum_{\pi \in \widehat{G}} \langle P^\pi(z, \overline{w}), R^\pi \rangle \,, \tag{3.19}$$

with

$$P^\pi(z,\overline{w}) = \left(v^\pi(z)\ \overline{v^\pi(w)}^{\mathsf{T}}\right) \otimes Q^\pi(z,\overline{w})\ ,$$

and

$$[Q^\pi]_{kl}(z,\overline{w}) = \sum_{i=1}^{d_\pi} \varphi^\pi_{ki}(z)\ \overline{\varphi^\pi_{li}(w)}$$

where φ^π_{ij} are the basis elements of the coinvariant algebra as described in Section 2.3.1, R^π is Hermitian positive semidefinite, and $v^\pi(x)$ contains all monomials in the basic invariants up to degree $d - \min\{\deg \varphi^\pi_{ii}(x) : i \in [d_\pi]\}$. Since the solutions we get from the SDP solvers can be slightly infeasible, we will use a derived representation of g to formulate problems, which are numerically more stable and whose solutions can be rigorously shown to be correct. Before explaining this representation, we have to give some definitions. For each irreducible representation $\pi \in \widehat{G}$, we define a d_π-dimensional symmetric matrix Φ^π by

$$\Phi^\pi_{ij} = \varphi^\pi_{ij}\ , \qquad \text{and thus} \qquad Q^\pi = \Phi^\pi(\overline{\Phi^\pi})^{\mathsf{T}}$$

holds. Since each row of Φ^π contains homogeneous polynomials of the same degree, we define the degree of a row i of Φ^π by

$$\deg \Phi^\pi_i = \deg \Phi^\pi_{i1}\ .$$

Furthermore, let $\mathcal{B}$ be some basis of $\mathbb{C}[x]^G$ consisting of homogeneous polynomials and set

$$\mathcal{I}^t_\pi = \{(a,r) \in \mathcal{B} \times [d_\pi] : \deg a + \deg \Phi^\pi_r \le t\}\ .$$

We define a matrix

$$V^{\pi,t}_{(a,r)(b,s)}(z,\overline{w}) = a(z)\ \overline{b(w)}\ Q^\pi_{rs}(z,\overline{w})$$

with indices in $\mathcal{I}^t_\pi$. The degree of each entry can be calculated by

$$\deg V^{\pi,t}_{(a,r)(b,s)} = \deg a + \deg b + \deg Q^\pi_{r,s} = \deg a + \deg b + \deg \Phi^\pi_r + \deg \Phi^\pi_s \le 2t\ .$$

By using the above matrix, we can describe an SOHS polynomial $g \in \mathbb{C}[z,\overline{w}]^G_{\le 2d}$ by

$$g(z,\overline{w}) = \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(z,\overline{w}), \tilde{R}^\pi \right\rangle\ , \tag{3.20}$$

where $\tilde{R}^\pi$ is a Hermitian positive semidefinite matrix of dimension $\left|\mathcal{I}^d_\pi\right|$.

Lemma 3.8. *The parameterization of a G invariant SOHS polynomial in (3.19) is equivalent to the parameterization in (3.20).*

Proof. Let g be a polynomial described by the equation in (3.20). Since for each $(b,r) \in \mathcal{I}^d_\pi$ it follows $b \in v^\pi(x)$, the polynomial g can be expressed by using the P^π matrices instead of the $V^{\pi,d}$ matrices. To obtain a larger Hermitian positive semidefinite matrix R^π from $\tilde{R}^\pi$, such that the equation (3.19) holds, we set all new entries of R^π equal to zero. Since we can obtain the matrix R^π from the matrix $\tilde{R}^\pi$ by applying a basis change matrix, the new matrix is still positive semidefinite.

Conversely, let g be a polynomial in (3.19). Each $p \in P^\pi$ is contained in $V^{\pi,d}$ if $\deg p \leq \deg g$, otherwise $R^\pi_{ij} p = 0$ for all i, j with $p = P^\pi_{ij}$. Thus, the old representation (3.19) can be transformed into the new representation (3.20), by setting

$$\tilde{R}^\pi_{ij} = \sum_{(k,l)\in\mathcal{M}_{ij}} R^{kl}, \text{ with } \mathcal{M}_{ij} = \left\{(k,l) : P^\pi_{kl} = V^{\pi,d}_{ij}\right\} .$$

Since the matrix R^π is Hermitian positive definite and the matrix $\tilde{R}^\pi$ can be obtained by applying a basis change matrix to R^π, the new matrix $\tilde{R}^\pi$ is Hermitian positive semidefinite, too. □

The benefit of the new parameterization of g is that we use smaller matrices where $\tilde{R}^\pi$ has less zero entries than R^π in order to obtain strictly feasible solutions which can be easier checked to be rigorous. For the infinite dimensional linear program of Cohn-Elkies the function f, which we expressed in terms of a polynomial g, has to be real-valued, therefore we define a real-valued nonnegative function g from an SOHS by

$$g(x) = g(x, \overline{x}) = \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x, \overline{x}), H^\pi \right\rangle \tag{3.21}$$

and a matrix

$$V^{\pi,d}(x) = V^{\pi,d}(x, \overline{x}) .$$

In case all the irreducible representations of the group are orthogonal, the representation of g in (3.20) is equal to

$$g(x) = \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), R^\pi \right\rangle, \tag{3.22}$$

where R^π is a positive semidefinite matrix, $Q^\pi = \Phi^\pi(\Phi^\pi)^\mathsf{T}$, $\mathcal{B}$ contains a basis of $\mathbb{R}[x]^G$, and

$$V^{\pi,t}_{(a,r)(b,s)}(x) = a(x)\, b(x)\, Q^\pi_{rs}(x) .$$

Using the new representation of g, we obtain a suitable representation of the function f in the SDP. By applying Proposition 3.2, the function f can be computed from $\widehat{f}$ by a linear transformation $\mathcal{F} : \mathbb{R}[x]^G \to \mathbb{R}[x]^G$, such that

$$f(x) = \mathcal{F}[g](x) e^{-\pi\|x\|^2}$$

holds. We represent the polynomial g as in (3.21) with the matrix $V^{\pi,d}(x)$, and thus, we obtain

$$f(x) = e^{-\pi\|u\|^2} \sum_{\pi\in\widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), R^\pi \right\rangle , \tag{3.23}$$

where we apply $\mathcal{F}$ to the matrix $V^{\pi,d}(x)$ by applying it to all its entries.

3.3.2 Nonpositivity condition

By using the above representation of f and g, we can directly transform the objective function and the constraints of the polynomial optimization problem into an SDP, except of the nonpositivity constraint in (3.11), which states

$$f(x) \leq 0 \quad \text{whenever } x \notin \mathcal{K}^\circ - \mathcal{K}^\circ.$$

For this, we divide the domain $\mathbb{R}^3 \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ)$ into a bounded and unbounded part. We deal with the nonpositivity in the bounded part by using sample points, whereas the nonpositivity in the unbounded part can be ensured by using an SOHS condition. We start with the unbounded part: Let s be a G-invariant polynomial, such that

$$\mathcal{K}^\circ - \mathcal{K}^\circ \subseteq \left\{x \in \mathbb{R}^3 : s(x) < 0\right\},$$

where $\left\{x \in \mathbb{R}^3 : s(x) < 0\right\}$ is a bounded set. For example, if we consider $\mathcal{K} = B_3^p$ with p being an even positive integer, then $\mathcal{K} - \mathcal{K} = 2B_3^p$ and so we take $s(x) = x_1^p + x_2^p + x_3^p - 2$. If p is odd or not an integer, then we use the next larger even integer p' for defining $s(x)$. For polytopes, we may use $s(x) = \|x\|^2 - \delta^2$, where δ is the maximal norm of a vector in $\mathcal{K} - \mathcal{K}$, which means $\delta = \max\{\|x\| : x \in \mathcal{K} - \mathcal{K}\}$. By using nonnegative polynomials p_1 and p_2 derived from SOHS polynomials like in (3.21), we can formulate a condition to ensure that f is nonpositive in $\{x \in \mathbb{R}^3 : s(x) \geq 0\}$:

$$f(x) = -s(x)p_1(x) - p_2(x)\,, \tag{3.24}$$

then f is nonpositive if s, p_1, and p_2 are nonnegative. Since p_1 and p_2 are nonnegative, for $s(x) \geq 0$ the function $f(x)$ is nonpositive. Since s and f are G-invariant, we can assume p_1 and p_2 are G-invariant without loss of generality. Therefore, we can represent the G-invariant nonnegative polynomials in the program similar to the representation of the polynomial g. On the one hand, we should not choose too small degrees for p_1 and p_2 to make sure that the equality (3.24) may hold. On the other hand, if the degree of p_2 is higher than the degree of f, the matrices in our parameterization cannot be positive definite. A matrix A is *positive definite* if and only if all its eigenvalues are strictly positive. In Chapter 4, we will see that for positive semidefinite matrices, which are not positive definite, it is more difficult to prove that the results give bounds for the maximal packing density. Therefore, we have to be careful with the choice of the degree of p_1 and p_2. Since, we fix the maximal degree of g to be $2d$, the function $f = \mathcal{F}[g]$ has maximal degree $2d$, too. As s is G-invariant, it has even degree, which we define to be $2d_s$ with $d_s \in \mathbb{N}$. Hence, we limit the maximal degrees

$$\deg p_1 \leq 2(d - d_s) \quad \text{and} \quad \deg p_2 \leq 2d\,.$$

To describe the polynomials p_1 and p_2 similar to g, we use a parameterization for p_1 containing Hermitian positive semidefinite matrices S_1^π and for the parameterization of p_2 we use Hermitian positive semidefinite matrices S_2^π. We can formulate the constraint

$$f(x) + s(x)p_1(x) + p_2(x) = 0$$

by the following linear condition

$$\sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), R^\pi \right\rangle + \sum_{\pi \in \widehat{G}} \left\langle s(x)V^{\pi,d-d_s}(x), S_1^\pi \right\rangle + \sum_{\pi \in \widehat{G}} \left\langle V^{\pi,d}(x), S_2^\pi \right\rangle = 0\,. \tag{3.25}$$

By adding the condition in (3.25) to the SDP, we ensure that f is nonpositive in $\{x \in \mathbb{R}^3 : s(x) \geq 0\}$. Since the nonpositivity condition (3.11) has to hold on

$$\mathbb{R}^3 \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ) = \{x \in \mathbb{R}^3 : s(x) \geq 0\} \cup \{x \in \mathbb{R}^3 : s(x) < 0\} \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ) \,,$$

we still have to deal with the bounded part

$$\mathcal{D} = \{x \in \mathbb{R}^3 : s(x) < 0\} \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ) \,.$$

For example for $\mathcal{K} = B_3^p$ where p is not an even integer, we used the next larger even integer p' in the unbounded part, and so we still have to check the condition for $2B_3^{p'} \setminus 2B_3^p$. We have to take twice the superball, because $B_3^p - B_3^p = 2B_3^p$. In Figure 3.1, a superball $2B_3^p$ with $p = 1.2$ is pictured in a superball $2B_3^{p'}$ with $p' = 2$. Analogously, for polytopes, we have still to check the nonpositivity condition for the points in $\delta B_3^2 \setminus (\mathcal{K} - \mathcal{K})$. For $\mathcal{K}$ equal to a regular tetrahedron, the Minkowski difference $\mathcal{K} - \mathcal{K}$ is a cuboctahedron. In Figure 3.2, a cuboctahedron inside of the ball δB_3^2 is pictured.

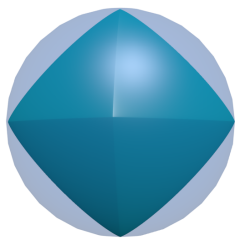


Figure 3.1: $2B_3^{1.2}$ in $2B_3^2$.

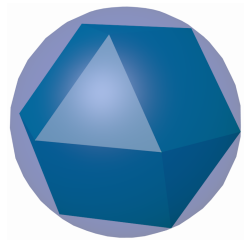


Figure 3.2: Cuboctahedron in δB_3^2.

We take a subset $\mathcal{S}$ of points in $\mathcal{D}$ and add linear constraints to the SDP, which ensure that f is nonpositive for all elements of the sample set $\mathcal{S}$. We would like to find a finite set of points $\mathcal{S}$, such that, if f is nonpositive on this set, it will probably also be nonpositive on $\mathcal{D}$. For this, we have to find a *good* set of sample points. Since the polynomial g is G-invariant, and so, the function $\mathcal{F}[g]$ is G-invariant, too, we can restrict the sample points (x_1, x_2, x_3) to the fundamental domain of G. For example for $G = \mathsf{B}_3$, we choose

$$\mathcal{S} \subseteq \mathcal{D} \cap \{x \in \mathbb{R}^3 : 0 \leq x_1 \leq x_2 \leq x_3\} \,.$$

The choice of the sample points is important for the quality of the result. Pütz developed in his master's thesis [64] two further methods for calculating a sample set other than the one we use in [30]. For each of these three sample methods, he solved the SDP with $d = 13$ for the truncated icosahedron. Afterwards, he verified these results. In Section 3.4.3, where the verification of the sample conditions be explained, we will present the obtained results by Pütz.

To ensure the nonpositivity of f on a certain sample set $\mathcal{S} \subseteq \mathcal{D}$, we add the condition

$$\sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), R^\pi \right\rangle \leq 0 \text{ for all } x \in \mathcal{S} \,. \tag{3.26}$$

Furthermore, the number of sample conditions in the SDP corresponds to the number of sample points, thus, the sample set should not become too large. However, no sample method guarantees that if the nonpositivity condition holds for the sample points, it will also hold for all elements in the bounded part $\mathcal{D}$. Thus, after solving the SDP, we have to verify the obtained solution to ensure, that the nonpositivity condition indeed holds for the required part.

3.3.3 Full formulation

We formulate a relaxation of the polynomial optimization problem (3.7) - (3.11) as an SDP. For this, we start by considering the objective function $f(0)$. Since we describe the function f by (3.23), we obtain the objective function

$$f(0) = \sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](0), R^{\pi} \right\rangle .$$

We modify the first condition (3.9) $g(0) \geq \operatorname{vol} \mathcal{K}$ to $g(0) \geq 1$, therefore we have to scale $f(0)$ by multiplying with the volume of $\mathcal{K}$ to obtain an upper bound for the density. In (3.21) we set $x = 0$ to obtain $g(0)$, and so, the first condition will be transformed to

$$\sum_{\pi \in \widehat{G}} \left\langle V^{\pi,d}(0), R^{\pi} \right\rangle \geq 1.$$

In the relaxation, we replace the nonnegativity condition (3.10) for g by an SOHS condition. By the chosen description of g this property holds. In the SDP we have to fix the maximal degree of g by $2d$, where we choose d to be an odd positive integer. In Chapter 4, we will explain why the verification is easier if d is odd. The last condition is the nonpositivity condition on f, which we transformed into an SOHS condition (3.25) and a sample condition (3.26).

Finally, we can give a relaxation of the program of Cohn and Elkies as an SDP

$$\begin{aligned}
\min \ & \sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](0), R^{\pi} \right\rangle \\
\text{(a)} \ & \sum_{\pi \in \widehat{G}} \left\langle V^{\pi,d}(0), R^{\pi} \right\rangle \geq 1, \\
\text{(b)} \ & \sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), R^{\pi} \right\rangle + \sum_{\pi \in \widehat{G}} \left\langle s(x) V^{\pi,d-d_s}(x), S_1^{\pi} \right\rangle \\
& \qquad\qquad + \sum_{\pi \in \widehat{G}} \left\langle V^{\pi,d}(x), S_2^{\pi} \right\rangle = 0, \\
\text{(c)} \ & \sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), R^{\pi} \right\rangle \leq 0 \qquad \text{for all } x \in \mathcal{S}, \\
& R^{\pi}, S_1^{\pi}, \text{ and } S_2^{\pi} \text{ are Hermitian positive semidefinite,}
\end{aligned} \tag{3.27}$$

where $G = \mathcal{S}(\mathcal{K} - \mathcal{K})$. If the irreducible representations of the group are orthogonal, the matrices R^{π}, S_1^{π}, and S_2^{π} are real-valued positive semidefinite matrices.

3.4 Rigorous verification

We formulated an SDP in (3.27), which is a relaxation of the infinite dimensional linear program of Cohn and Elkies. Now we can solve the program by using an SDP solver. To transform the SDP into valid input data, we have to use floating numbers. Since we are not able to describe the SDP with rationals, we use floating numbers in the input, and thus, the solver use floating numbers in the computation. Therefore, the solution we obtain is likely infeasible. We would like to find solutions which are just slightly infeasible, such that we can transform them into feasible solutions.

To obtain a rigorous bound for the maximal packing density, we apply the following steps:

1. Solve the SDP in (3.27) by using an SDP solver.
2. Transform the obtained solution into a strictly feasible solution for the SDP.
3. Check whether the new solution is also feasible for the Cohn Elkies program:
   (a) Check the normalization and SOS condition.
   (b) Check the nonpositivity condition on the bounded part $\mathcal{D}$.

If the last step fails, then we have to use a larger sample set or we have to go back in step two.

Since we computed upper bounds for three-dimensional convex bodies having tetrahedral or icosahedral symmetry, the corresponding solutions of the SDP are real-valued positive semidefinite matrices. In this section, we describe the verification process for the case, in which the solution matrices are real-valued.

3.4.1 Solving the semidefinite program

To be able to transform the numerical solution of the SDP solver into a feasible solution, it should just slightly violate the conditions. Therefore, we are interested in solutions, whose matrices $\left(R^\pi, S_1^\pi, S_2^\pi\right)$ have minimal eigenvalues which are much larger than the maximal violation of any constraint. The eigenvalues of a semidefinite matrix are all nonnegative, but they can be *zero* or due to numerical instability they can be negative. If all eigenvalues are strictly positive the matrix is called a *positive definite matrix*. The interior of the cone of positive semidefinite matrices consists of the positive definite matrices, and thus, the solutions just consisting of positive definite matrices are equal to the strictly feasible solutions. Since, we need solution matrices with strictly positive eigenvalues, we would like to find a strictly feasible solution. If we choose d to be even, we never obtained a strictly feasible solution of the SDP in our calculations. Therefore, we restrict d to be odd. Furthermore, we have to be careful with the choice of the right degrees d and d_s. As mentioned in Section 3.3.2, the degree of the polynomial p_2 has to be less or equal to the degree of the function $\mathcal{F}[g]$, otherwise the representation cannot contain positive definite matrices, and thus, the solutions will not be strictly feasible.

First, we explain how we can get a strictly feasible solution of the given SDP: Many solvers use positive definite matrices in their calculation, like for example by using the

interior point method. After the calculation, the solution will be rounded to get a solution which lies on the boundary of the cone of positive semidefinite matrices. Thus, the solution is not strictly feasible anymore. However, after the calculation we get an estimate z^* of the optimal value of the SDP. Using this estimate, we can turn the SDP into a feasibility problem to obtain strictly feasible solutions. For this, we define a small positive error η, in our computations we usually used $\eta = 10^{-5}$. To obtain a feasibility problem instead of an optimization problem, the objective function of the SDP will be removed. To make sure that $f(0)$ is almost z^*, which means $f(0) \leq z^* + \eta$, we add the constraint

$$\sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](0), R^\pi \right\rangle \leq z^* + \eta$$

to the new problem. Thus, for getting a strictly feasible solution, we sacrifice a bit of the optimal value. The advantage of feasibility problems is, that solvers usually return strictly feasible solutions, which means the minimal eigenvalues of the resulting matrices are strictly positive.

To translate our solution into a feasible solution, the minimal eigenvalues of these matrices should be larger than the maximal violation of any constraint. The resulting matrices of the optimization problem lie on the boundary of the positive semidefinite cone, whereas the resulting matrices of the feasibility problem lie in the interior, thus the minimal eigenvalues of the new matrices depend on η. If the minimal eigenvalues are smaller than the violation, we have to increase η even if this means that the optimal value becomes worse.

For the calculation it is important to use an SDP solver with high-precision floating-point numbers to obtain a solution of the optimization problem which is just slightly infeasible. Solvers with double-precision floating-point arithmetic have failed due to numerical instability problems. For our calculations we used the SDPA-GMP solver [36].

3.4.2 Checking the normalization and SOS condition

From the computation of the feasibility problem with a suitable η, we get positive definite matrices $\left(R^\pi, S_1^\pi, S_2^\pi\right)$ with minimal eigenvalues much larger than the maximal constraint violation. We compute a bound for the minimal eigenvalues of each of these matrices: Let A be one of these matrices, then we use binary search to find λ_A close to the minimal eigenvalues, such that $A - \lambda_A I$ has a Cholesky decomposition LL^T. For this calculation, we use high-precision floating-point arithmetic. We define a new matrix $\tilde{A} = LL^\mathsf{T} + \lambda_A I$. Now we have positive definite matrices $\left(\tilde{R}^\pi, \tilde{S}_1^\pi, \tilde{S}_2^\pi\right)$ and a bound on their minimal eigenvalues. For the representation of the new solution $\left(\tilde{R}^\pi, \tilde{S}_1^\pi, \tilde{S}_2^\pi\right)$, we use interval arithmetic with high-precision floating-point arithmetic [65].

We can easily compute the objective value

$$\sum_{\pi \in \widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](0), \tilde{R}^\pi \right\rangle.$$

The next task is to compute the violation of each constraint. We start with the normalization constraint (a): If a solution violates this constraint, we multiply it with a positive number such that this constraint is satisfied, by using interval arithmetic. If a solution violates the

SOS constraint (b), we compute the absolute value of the coefficient of

$$r(x) = \sum_{\pi\in\widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), \tilde{R}^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle s(x)V^{\pi,d-d_s}(x), \tilde{S}_1^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), \tilde{S}_2^{\pi} \right\rangle \tag{3.28}$$

with largest absolute value. In order to satisfy condition (b) the polynomial $r(x)$ has to be equal to zero. Thus, the absolute value of the coefficient of $r(x)$ with largest absolute value gives an upper bound on the violation of this constraint. As mentioned before, we need a common basis for the polynomials in the SOS constraint and since all contained polynomials are invariant, we use a basis of $\mathbb{R}[x]^G$. Therefore, we can represent the matrices $V^{\pi,d}$ and V^{π,d_s} by using rationals and these can be approximated by interval arithmetic. The SOS constraints also contain the Fourier antitransform $\mathcal{F}[V^{\pi,d}]$ with powers of π, therefore we need irrationals, but these can be approximated by interval arithmetic, too.

Since we are interested in feasible solutions, we have to turn the matrices $\left(\tilde{R}^{\pi}, \tilde{S}_1^{\pi}, \tilde{S}_2^{\pi}\right)$ into a solution, for which the polynomial $r(x)$ is identically zero. From the definition of $r(x)$ in (3.28), we know that the degree of $r(x)$ is at most $2d$ and that $r(x)$ has to be a G-invariant polynomial. Furthermore, due to the construction of the matrices $V^{\pi,d}$ and $V^{\pi,d-d_s}$, we can formulate the polynomial $r(x)$ as a linear combination of the entries of these matrices. This means, for each irreducible representation $\pi \in \widehat{G}$, there exists a matrix T^{π}, so that

$$r(x) = \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), T^{\pi} \right\rangle \tag{3.29}$$

holds. Thus if we take the difference of the right-hand sides of (3.28) and (3.29), we get

$$\sum_{\pi\in\widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), \tilde{R}^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle s(x)V^{\pi,d-d_s}(x), \tilde{S}_1^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), \tilde{S}_2^{\pi} \right\rangle - \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), T^{\pi} \right\rangle = 0\,,$$

which is equivalent to

$$\sum_{\pi\in\widehat{G}} \left\langle \mathcal{F}[V^{\pi,d}](x), \tilde{R}^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle s(x)V^{\pi,d-d_s}(x), \tilde{S}_1^{\pi} \right\rangle + \sum_{\pi\in\widehat{G}} \left\langle V^{\pi,d}(x), \tilde{S}_2^{\pi} - T^{\pi} \right\rangle = 0\,.$$

Consequently, the SOS condition (b) is satisfied for $\left(\tilde{R}^{\pi}, \tilde{S}_1^{\pi}, \tilde{S}_2^{\pi} - T^{\pi}\right)$. Furthermore, by modifying the third matrix, the objective value will not change. Since the matrices have to be positive semidefinite to be feasible for the SDP, we have to check whether $\tilde{S}_2^{\pi} - T^{\pi}$ is positive semidefinite.

To ensure the positive semidefiniteness, the entries of T^{π} have to be small enough compared to the minimal eigenvalues of $\tilde{S}_2^{\pi}$. Hence, we need a restriction on the maximal value of the entries of T^{π}. For this, we use the *Frobenius norm*, which is defined by $\|A\| = \langle A, A\rangle^{1/2}$ for a matrix A. Moreover, we need $\lambda_{\tilde{S}_2^{\pi}}$, which is any lower bound on the minimal eigenvalues of the matrix $\tilde{S}_2^{\pi}$. We can compute this bound by using binary search as mentioned before. Now, we can restrict the entries of the matrix T^{π} by

$$\|T^{\pi}\| \leq \lambda_{\tilde{S}_2^{\pi}}\,. \tag{3.30}$$

Thus the SOS condition is satisfied, if T^{π} satisfies (3.30) for all $\pi \in \widehat{G}$. To estimate $\|T^{\pi}\|$ we use the following approach without computing the matrix T^{π} explicitly.

To determine an estimate, we have to find a maximal linearly independent subset $\mathcal{B}$ of the polynomials inside the set of all entries of the matrices $V^{\pi,d}$. Let $\mathcal{M}$ be the set consisting of all monomials appearing in $\mathcal{B}$. Then, we can create a $|\mathcal{M}| \times |\mathcal{B}|$ matrix A, such that each entry $(m, a) \in \mathcal{M} \times \mathcal{B}$ contains the coefficient of the monomial m in the polynomial a. We consider a submatrix $\widehat{A}$ of A consisting of $|\mathcal{B}|$ linearly independent rows of A.

For the upper bound, we have to use the *infinity norm for matrices*, which is defined for an $n \times m$ matrix A by

$$\|A\|_\infty = \max_{i=1,\dots n} \sum_{j=1}^{m} \left|A_{ij}\right|.$$

Furthermore, we need the *infinity norm for polynomials*, given by

$$\|p(x)\|_\infty = \max\left\{|\lambda_i| : i \in \{1, \dots, m\}\right\},$$

for a polynomial $p(x) = \sum_{i=1}^{m} \lambda_i m_i$, with coefficients λ_i and monomials m_i.

Proposition 3.9. *Let T^π, $\widehat{A}$, and r be defined as above, then*

$$\|T^\pi\| \leq \left|\mathcal{I}_\pi^d\right| \left\| \widehat{A}^{-1} \right\|_\infty \|r\|_\infty,$$

holds for all $\pi \in \widehat{G}$.

Proof. The matrix T^π has to satisfy

$$r(x) = \sum_{\pi \in \widehat{G}} \left\langle V^{\pi,d}(x), T^\pi \right\rangle,$$

therefore, the matrix T^π is indexed by the elements of $\mathcal{I}_\pi^d$ similarly to $V^{\pi,d}(x)$. Hence,

$$\|T^\pi\| = \langle T^\pi, T^\pi \rangle^{1/2} = \left(\sum_{(a,r) \in \mathcal{I}_\pi^d} \sum_{(b,s) \in \mathcal{I}_\pi^d} \left|T^\pi_{(a,r),(b,s)}\right|^2 \right)^{1/2}.$$

The monomials of $r(x)$ with non-zero coefficient, are contained in some entries of the matrix $V^{\pi,d}$, and thus, the monomials of $r(x)$ are elements of $\mathcal{M}$. The polynomials in $\mathcal{B}$ can appear multiple times in $V^{\pi,d}(x)$. The entries of T^π can be estimated by the matrix $\widehat{A}$

$$\left|T^\pi_{(a,r),(b,s)}\right| \leq \left| \sum_{j=1}^{|\mathcal{B}|} \widehat{A}^{-1}_{ij} \lambda_i \right|,$$

for $V^\pi_{(a,r),(b,s)} = b_i(x)$, where λ_i is the largest coefficient of all monomials contained in $b_i(x)$. Furthermore,

$$\left| \sum_{j=1}^{|\mathcal{B}|} \widehat{A}^{-1}_{ij} \lambda_i \right| \leq \sum_{j=1}^{|\mathcal{B}|} \left| \widehat{A}^{-1}_{ij} \lambda_i \right|.$$

Since all coefficients are upper bounded by $\|r\|_\infty$, which means $|\lambda_i| \leq \|r\|_\infty$, it follows

$$\sum_{j=1}^{|\mathcal{B}|} \left| \widehat{A}^{-1}_{ij} \lambda_i \right| \leq \|r\|_\infty \sum_{j=1}^{|\mathcal{B}|} \left| \widehat{A}^{-1}_{ij} \right| \leq \left\| \widehat{A}^{-1} \right\|_\infty \|r\|_\infty$$

and consequently, we obtain

$$\|T^\pi\| \leq \left|\mathcal{I}_\pi^d\right| \left\| \widehat{A}^{-1} \right\|_\infty \|r\|_\infty .$$

□

Due to Proposition 3.9 the inequality in (3.30) is satisfied if

$$\left|\mathcal{I}_\pi^d\right| \left\| \widehat{A}^{-1} \right\|_\infty \|r\|_\infty \leq \lambda_{\tilde{S}_2^\pi}$$

holds for all $\pi \in \widehat{G}$. For checking this inequality, we compute the inverse $\widehat{A}^{-1}$ by using rational arithmetic. To break these $|\widehat{G}|$ many conditions down to just one condition, we take the cardinality of the largest index set

$$i_{\max} = \max\left\{ \left|\mathcal{I}_\pi^d\right| : \pi \in \widehat{G} \right\}$$

and the minimal eigenvalue $\lambda_{\min} = \min\left\{\lambda_{\tilde{S}_2^\pi} : \pi \in \widehat{G}\right\}$, and consider the stronger condition

$$i_{\max} \, \| \widehat{A}^{-1} \|_\infty \|r\|_\infty \leq \lambda_{\min}.$$

If this condition is not satisfied by our solution, we have some options to get a better solution: we can increase the error η to increase the right-hand side, or we take more sample points, or we increase the precision of the input data, or we fix a different degree d.

3.4.3 Checking sample conditions

We have to check whether our solution satisfies the nonpositivity condition (3.11), which states that the function f has to be nonpositive in $\mathbb{R}^n \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ)$. To transform this condition into linear constraints for the SDP, we divided it into two conditions. For the first part we checked the feasibility in the previous subsection. Now the second part is left. Since the solution is feasible for the SDP if this condition is just satisfied by the sample points in $\mathcal{S} \subset \mathcal{D}$, the condition is probably not satisfied for all elements in

$$\mathcal{D} = \{x \in \mathbb{R}^3 : s(x) < 0\} \setminus (\mathcal{K}^\circ - \mathcal{K}^\circ\} ,$$

and thus, the obtained solution is probably not feasible for the Cohn Elkies program. The problem is that it is difficult to detect the boundary of $\mathcal{D}$ by using sampling. However, we can find a small value $\alpha > 1$, such that

$$f(x) \leq 0 \quad \text{for all } x \in \mathcal{D}' = \{x \in \mathbb{R}^3 : s(x) < 0\} \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ) . \tag{3.31}$$

By modifying the set $\mathcal{D}$ to $\mathcal{D}'$, the solid we want to pack will increase from $\mathcal{K}$ to $\alpha\mathcal{K}$. Therefore, we have to multiply α^3, or in general α^n, with $f(0)$, the upper bound we obtain by solving the SDP. Since, the upper bound should be as small as possible, we have to find small $\alpha > 1$ satisfying (3.31). By testing the function f in a fine grid of points, we can determine an estimate of α. The required factor α depends on the considered sample set $\mathcal{S}$. Therefore, we explain our sample method and the two further sample methods developed by Pütz [64].

Sample methods

As mentioned before, we just have to consider the intersection of $\mathcal{D}$ with the fundamental domain of G, due to the G-invariance of $\mathcal{F}[g]$. We denote the fundamental domain of G by $F(G)$. In our approach, we use a uniform sample, which is a general method and can be used for arbitrary convex bodies $\mathcal{K} \subseteq \mathbb{R}^n$. Before defining this sample method, we first explain the idea of it. We take sample points of the intersection of $F(G)$ and $\mathcal{D}$, such that they are uniformly distributed with a distance of $\varepsilon \in \mathbb{R}_{>0}$. The set $\mathcal{D}$ is bounded and contained in the cube $[s(0), -s(0)]^n$, therefore it is sufficient to restrict the grid to this domain. The *uniform sample* $\mathcal{S}$ is defined by

$$\mathcal{S} = \mathcal{G} \cap \mathcal{D} \cap F(G) \,,$$

with grid

$$\mathcal{G} = \left\{ x \in \mathbb{R}^n : x = \varepsilon \cdot k \text{ for all } k \in \mathbb{Z}^n, \text{ such that } |k_i| \leq \frac{-s(0)}{\varepsilon} \text{ for all } i \in [n] \right\} \,,$$

and grid size $\varepsilon \in \mathbb{R}_{>0}$. We would like to detect the boundary of $\mathcal{K} - \mathcal{K}$ to obtain a feasible solution or at least to obtain a solution which requires a small factor α to get a feasible solution. In the uniform sample the sample points are uniformly distributed, thus for obtaining a fine grid at the boundary, we have to use a small grid size ε, but then the sample set would become large. Thus, it would be better to develop a sample method with more sample points near the boundary than for the other parts of the considered region.

Therefore, Pütz developed two different methods for computing a sample set $\mathcal{S}$, in which the sample points are not uniformly distributed. These sample methods can just be used for $\mathcal{K} - \mathcal{K}$ being a polytope. One way to obtain sample points such that there are more sample points at the boundary, is by distributing the sample points in such a way that they lie in planes which are parallel to the faces of $\mathcal{K} - \mathcal{K}$. Therefore, for each face of $\mathcal{K} - \mathcal{K}$, we need two orthonormal vectors r_1 and r_2 spanning the plane and one vertex v of the considered face. The sample points in a plane spanned by r_1 and r_2 with grid size $\varepsilon \in \mathbb{R}_{>0}$ can be calculated by $\varepsilon(k_1 r_1 + k_2 r_2)$. Since the faces are at most twice the square spanned by these orthonormal vectors, it is sufficient to compute sample points for k_1 and k_2 in $[0, \ldots, \lfloor 2/\varepsilon \rfloor]$, where we define $[0, \ldots, k]$ to be the set of integers $\{0\} \cup [k]$. We denote the set of values for k_1 and k_2 by M_1. To translate these points in the considered plane we have to add them to a point contained in that plane. For this we consider the vector v which lies in the considered face of the solid. In order to obtain a point on each plane we want to sample, we copy v to each of these planes by multiplying it with a factor δ and k_3. If we would like to consider, for example, 10 planes above a face, then we choose the range of k_3 equal to $[0, \ldots, 10]$. We denote this set by M_3. Furthermore, we need a factor δ for the distance between each plane and the next plane above. If the face we are considering is close to the sphere, we might not get enough sample points between the face and the sphere. Therefore, we multiply v also with a scaling factor $\lambda_v \in (0, 1]$ to obtain a sample set which is not too small. Due to numerical errors, a point can be mistakenly associated to the interior of $\mathcal{K} - \mathcal{K}$. To avoid this, we add μ to the factor of v. Pütz set in his computations $\mu = 0.00005$. The *plane sample* S with parameters ε, δ, and μ, is defined by

$$S = \mathcal{G} \cap \mathcal{D} \cap F(G),$$

with

$$\mathcal{G} = \bigcup_{(v,r_1,r_2,\lambda_v)\in F} \{(1+\mu+\delta\cdot\lambda_v k_3)\, v + \varepsilon\,(k_1 r_1 + k_2 r_2) : k_1, k_2 \in M_1, k_3 \in M_3\},$$

where F contains all fourtuples (v, r_1, r_2, λ_v) for each face of the intersection $F(G)\cap(\mathcal{K}-\mathcal{K})$, which lives in a face of $(\mathcal{K}-\mathcal{K})$. For the groups B_3 and H_3, which we consider in our approach, there exists at most three of these faces. To apply this sample method, for each face of $\mathcal{K}-\mathcal{K}$, we have to determine the orthonormal vectors r_1 and r_2 and a point v lying on that face. For the solids $\mathcal{K}-\mathcal{K}$ invariant under B_3 or H_3, each face of $(\mathcal{K}-\mathcal{K})\cap F(G)$ contains one vertex v lying on a face of $\mathcal{K}-\mathcal{K}$, with orthogonal edges originating from v. By scaling these edges to have norm 1, we obtain the desired orthonormal vectors.

In the plane sample the sample points are not uniformly distributed in the considered space, but they are uniformly distributed in each plane. By decreasing the distance between the sample points lying close to the boundary or by increasing the distance for the points in the center of the faces, we might obtain a better sample set without considering a large set of sample points. Therefore, Pütz derived a generalized version of the plane sample method, in which the distance of the samples in the centers of the faces increase. For this we additionally need the length l_1 and l_2 of the edges from which we obtain the orthonormal vectors r_1 and r_2. Thus, for each face of $\mathcal{K}-\mathcal{K}$, we consider a sixtupel $(v, r_1, r_2, \lambda_v, l_1, l_2)$. For $i \in \{1,2\}$, the range of k_i, denoted by M_i, is equal to $[0,\dots,d_i]$ with $d_i = \lfloor l_i/\varepsilon \rfloor$. To increase the distance in the centers of the faces, we define a function for $j \in \{1,2\}$ by

$$f_{j,\lambda} : [0, d_j] \to [0,1]$$

with

$$f_{j,\lambda}(x) = \frac{1}{2}\left(1 + \frac{\arctan(\lambda(2x/d_j - 1))}{\arctan(\lambda)}\right).$$

In the new sample method, we apply this function to the elements of k_1 and k_2 to obtain the desired sample set. The *generalized plane sample* $\mathcal{S}$ with parameters ε, μ, δ, and λ in $\mathbb{R}_{>0}$ is defined by

$$S = \mathcal{G} \cap D \cap F[G],$$

with

$$\mathcal{G} = \bigcup_{(v,r_1,r_2,\lambda_v,l_1,l_2)\in F} \{(1+\mu+\delta\cdot\lambda_v k_3)\, v + (1+\delta\cdot\lambda_v k_3)\,(f_{1,\lambda}(k_1) l_1 r_1 + f_{2,\lambda}(k_2) l_2 r_2) : k_i \in M_i, i \in [3]\}.$$

In Table 3.1, one can see how the choice of the parameter λ in the function $f_{i,\lambda}$ influences the number of sample points and the obtained numerical result.

For the truncated icosahedron, Pütz solved the SDP with $d = 13$ three times by using each time a different sample method. Afterwards, he transformed the numerical results into rigorous bounds. Table 3.2 contains for each of these sample methods, the number of sample points, the obtained rigorous upper bound, and the required value for α. In this case, the generalized plane sample is the best sampling, because it contains the least number of sampling points, the factor α is small, and in particular, the obtained upper bound is better than in the other two cases.

For the truncated icosahedron, the sample points of the uniform sample, the plane sample, and the generalized plane sample are pictured in Figure 3.3.

Parameter λ	Points	Numerical result
0.0001	576	0.367795...
0.5	572	0.367783...
1	567	0.367742...
1.5	562	0.367667...
2	552	0.367578...
2.5	550	0.367462...

Table 3.1: Number of sample points and obtained numerical results for the tetrahedron using generalized plane sample with different values of λ [64].

Sample method	Points	Upper bound	Factor α
Uniform sample	546	0.856190	1.0180
Plane sample	411	0.835740	1.0002
Generalized plane sample	400	0.835536	1.0002

Table 3.2: Number of sample points, rigorous bounds, and required blow-up factor α, for the truncated icosahedron and $d = 13$ [64].

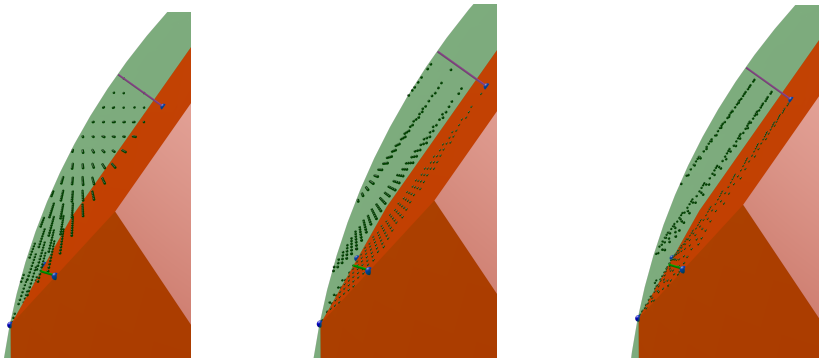


Figure 3.3: Left: Uniform sample, center: plane sample, right: generalized plane sample for truncated icosahedron [64]

Checking sample conditions on bounded part

The next task is to check whether the function f is indeed nonpositive in $\mathcal{D}'$: Since, we are interested in rigorous results, we evaluate f, which is equal to $\mathcal{F}[g]$, by using interval arithmetic. We consider a cube of side length $\delta_{\max} = \max_{x \in \mathcal{K}-\mathcal{K}} \|x\|_2$, which is the maximal norm of elements in $\mathcal{K} - \mathcal{K}$, thus, the cube is defined by $[-\delta_{\max}, \delta_{\max}]^3$. By this definition, the set $\mathcal{D}$ is contained in the initial cube, and therefore, its subset $\mathcal{D}'$ is contained in this cube, too. The idea is, that we divide the cube, into many smaller cubes, and check the nonnegativity condition for each of these smaller cubes, which intersect with the set $\mathcal{D}'$. If f is nonpositive on each of these cubes, it has to be nonpositive on $\mathcal{D}'$.

To do so, we choose $\delta < \delta_{\max}$ and divide the initial cube into a set of smaller cubes $[-\delta, \delta]^3$. Furthermore, let C be the set of all cubes containing at least one element (x_1, x_2, x_3) in $\mathcal{D}'$ with $0 \leq x_1 \leq x_2 \leq x_3$. Because of the invariance of $\mathcal{F}[g]$, it is again sufficient to consider just the fundamental domain $\{x \in \mathbb{R}^3 : 0 \leq x_1 \leq x_2 \leq x_3\}$. Since $\mathcal{D}'$ is contained in the initial cube, C covers $\mathcal{D}'$ in the fundamental domain. Furthermore, the set C is finite.

Let $\mathcal{K}$ be the regular tetrahedron, then $\mathcal{K} - \mathcal{K}$ corresponds to the cuboctahedron. In Figure 3.4 the cuboctahedron is pictured together with the initial set of cubes. For the regular tetrahedron, we choose $\alpha = 1.02$ and $s(x) = \|x\|^2 - 1$. In Figure 3.5, the set $\{x \in \mathbb{R}^3 : s(x) < 1\}$ is pictured, too, which is equal to the interior of the unit ball and is colored in green.

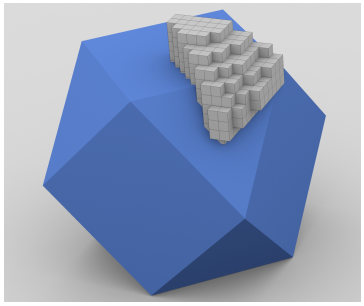


Figure 3.4: Cuboctahedra with initial set of cubes [30]

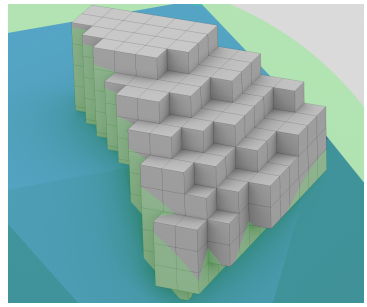


Figure 3.5: Cuboctahedra with initial set of cubes and unit ball [30]

To ensure that the nonpositivity condition is satisfied on $\mathcal{D}'$, we have to check whether it is satisfied on C, which means

$$\mathcal{F}[g](x) \leq 0\,,$$

for all $x \in \bigcup_{C \in \mathcal{C}}$. To check this condition, we compute an upper bound ν_C of the norm of the gradient of $\mathcal{F}[g]$ for all cubes $C \in \mathcal{C}$:

$$\|\nabla \mathcal{F}[g](x)\| \leq \nu_C \quad \text{for all } x \in C.$$

We can easily compute ν_C by using interval arithmetic: The coefficients of $\mathcal{F}[g]$ are represented by intervals. Moreover, the cubes are also represented by intervals, since they are a product of three intervals $C = [x_1, y_1] \times [x_2, y_2] \times [x_3, y_3]$. By using interval arithmetic,

we can now compute the gradient $\nabla\mathcal{F}[g]([x_1, y_1] \times [x_2, y_2] \times [x_3, y_3])$ and get the intervals $([l_1, u_1], [l_2, u_2], [l_3, u_3])$, such that for all $(x_1, x_2, x_3) \in C$

$$(l_1, l_2, l_3) \leq \nabla\mathcal{F}[g]\,(x_1, x_2, x_3) \leq (u_1, u_2, u_3)$$

holds. From this, we can compute ν_C by

$$\nu_C = \left\| \ (\max\{|l_i|, |u_i|\})_{i\in[3]} \ \right\|.$$

For a fixed $N \geq 1$, we divide each side of the cube C into N intervals and so we get a grid of points inside of C. Let x_C denote the lower-left corner of the cube C, then the set of points we consider is defined by

$$C_N = \{x_c + (a, b, c)\,\delta/N : 0 \leq a, b, c \leq N, a, b, c \in \mathbb{N}\}.$$

Since by definition of $\mathcal{D}'$, this set contains no elements of $\alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ and the set C contains at least one element of $\mathcal{D}'$, there exists an element of $C_N \subset C$, which is not contained in $\alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$. We define the maximal minimal distance from a point in $C \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ to a grid point in $C_N \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ by $d(C, N)$:

$$d(C, N) = \max_{x\in C\setminus\alpha(\mathcal{K}^\circ-\mathcal{K}^\circ)} \min_{y\in C_N\setminus\alpha(\mathcal{K}^\circ-\mathcal{K}^\circ)} \|x - y\|.$$

Moreover, we define

$$\mu(C, N) = \max\{\mathcal{F}[g](x) : x \in C_N \setminus \alpha\,(\mathcal{K}^\circ - \mathcal{K}^\circ)\}.$$

By using $d(C, N)$ and $\mu(C, N)$, we can check whether $\mathcal{F}[g]$ is nonpositive in C: If $\mu(C, N) > 0$ the required condition fails. Therefore, we hope that $\mu(C, N)$ is nonpositive for our choice of α. In that case, let $x \in C \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ and let $x' \in C_N \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ be the closest point to x. By applying the mean value theorem, we obtain

$$\left|\, \mathcal{F}[g](x) - \mathcal{F}[g](x') \,\right| \leq \nu_C \ \left\|x - x'\right\| \leq \nu_C \ d(C, N)\,.$$

Consequently, the function $\mathcal{F}[g]$ is nonpositive, if

$$\nu_C d(C, N) \leq |\,\mu(C, N)\,| \leq \left|\, \mathcal{F}[g](x') \,\right| \tag{3.32}$$

holds. Hence, we obtain the sufficient condition

$$\nu_C\ d(C, N) \leq |\,\mu(C, N)\,| \leq \left|\, \mathcal{F}[g](x') \,\right| \quad \text{for all } x' \in C_N \setminus \alpha\,(\mathcal{K}^\circ - \mathcal{K}^\circ) \tag{3.33}$$

for the condition in (3.31). In order to check this condition, we estimate $d(C, N)$. To do so, we first assume $C \cap \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ) = \emptyset$: Let $x \in C$, then there exists a grid point $\tilde{x} \in C$, such that $x \in \tilde{x} + [0, \delta/N]^3$. To maximize the distance, we assume that the distance of x to all its neighboring grid points is the same, which implies

$$x = \tilde{x} + \delta/(2N)\mathbf{1}_3,$$

with $\mathbf{1}_3 = (1, 1, 1)^\mathsf{T}$ is the central point in the cube $\tilde{x} + [0, \delta/N]^3$. Thus, in this case the distance of x to one of its neighbors is equal to

$$d(x, \tilde{x}) = \|\tilde{x} + \delta/(2N)\mathbf{1}_3 - \tilde{x}\| = \delta/(2N)\ \|\mathbf{1}_3\| = \delta/(2N)\ \sqrt{3}.$$

Assume $C \cap \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ) \neq \emptyset$: Let $x \in C$ and let $\tilde{x}$ be a grid point such that $x \in \tilde{C} = \tilde{x} + [0, \delta/N]^3$. If $\tilde{C} \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$ contains no grid point of C_N, then it is empty. Therefore, we can assume that there exists a grid point in $y \in \tilde{C} \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$. The distance between a point $x \in \tilde{C}$ and $y \in \tilde{C} \setminus (\alpha\mathcal{K}^\circ - \alpha\mathcal{K}^\circ)$ increases if we choose x to be close to $\alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$. However, since x and y are both elements of $\tilde{C}$, their largest distance is bounded above by the diagonal of the cube $\tilde{C}$ which is equal to

$$d(\tilde{x}, \tilde{x} + \delta/N\mathbf{1}_3) = \|\delta/N\mathbf{1}_3\| = \delta/N\,\sqrt{3}.$$

Thus, we can estimate $d(C, N)$ by

$$d(C, N) \leq \begin{cases} \sqrt{3}\,(\delta/N)\,, & \text{if } C \cap \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ) \neq 0, \\ \sqrt{3}\,(\delta/(2N))\,, & \text{otherwise.} \end{cases}$$

In our approach, we run over all cubes $C \in \mathcal{C}$ starting with $N = 2$. In every iteration, we check the condition in (3.33) for the currently considered cube. If this condition is not satisfied, we increase N and check it again. We repeat this procedure until the condition is satisfied. After we applied this procedure to every cube in $\mathcal{C}$, we know that the function $\mathcal{F}[g]$ is nonpositive everywhere in the domain $\mathcal{D}'$, in case the approach terminates. Since we use interval arithmetic for evaluating the function, the obtained results are rigorous.

The disadvantage of using interval arithmetic is that the computations need much more time. If we take for example a dense grid with $N = 1000$, then the computation would take several months. Since the size of the grid required by a cube is proportional to ν_C, which is better the smaller the cube is, we can improve on the grid size by taking small values for δ. But, if we change δ globally, we increase the total number of cubes, and thus, we may slowing down our calculations.

We improved our approach as follows: We fix a threshold, which is in our computation equal to 30 and if the grid size required by a cube becomes larger than the threshold, we split the cube into eight smaller cubes. To do so, we split each side of the cube into two halves. Since just one point of the cube has to be contained in $\mathcal{D}'$, some of the new smaller cubes may have no intersection with $\mathcal{D}'$. For the further calculations, we just consider the new cubes with at least one point in $\mathcal{D}'$. Since these cubes are smaller, we get a better grid size. We fix a maximal depth to limit the number of splittings of one cube. By reaching the grid size, we increase N, but it could be that N will just become a little bit larger. This case should be avoided, because then, we have to evaluate the function $\mathcal{F}[g]$ more often than if the increasing step would be larger. The problem is that evaluating the function is computationally very expensive, since we are using interval arithmetic.

To speed up our approach, we first use double-precision floating-point arithmetic for the function evaluation to get an estimate of the required grid size of each cube. Afterwards, we use this estimate to rerun the checking process by evaluating the function $\mathcal{F}[g]$ using interval arithmetic. The benefit of this precalculation is the reduction of the number of evaluations of $\mathcal{F}[g]$ with interval arithmetic.

Algorithm 1 describes the precalculation process by using double values. Furthermore, Algorithm 2 describes the checking process by using interval arithmetic.

Algorithm 1 Precalculation using double values

Require: $\mathcal{K}$, α, `max_depth`, `split_threshold`
  $\mathcal{D}' = \{x \in \mathbb{R}^3 : s(x) < 0\} \setminus \alpha(\mathcal{K}^\circ - \mathcal{K}^\circ)$
  $C = \{C \subseteq \mathbb{R}^3 : C \text{ cube of side length } \delta, \exists x \in C \cap \mathcal{D}' : 0 \le x_1 \le x_2 \le x_3\}$
  `cube_list` $= \emptyset$
  for cube $C \in C$ **do**
    calculate ν_C
    $N = 2$; `depth` $= 0$
    while `depth` $\le$ `max_depth` **do**
      $C_N = \{x_C + (a, b, c)\ \delta/N : 0 \le a, b, c \le N\}$
      calculate $d(C, N)$
      calculate $\mu(C, N)$
      if $\mu(C, N) > 0$ **then**
        throw `NonNegativeValue`
      end if
      if $\nu_C d(C, N) \le |\mu(C, N)|$ **then**
        add(C, `grid_size`) to `cube_list`
        break // nonpositivity constraint satisfied for C
      else if $N <$ `split_threshold` **then**
        increase N
      else
        split C into 8 new cubes
        add every new cube which intersects the domain $\mathcal{D}'$ to C
        $N = 2$
        increase `depth`
      end if
    end while
    if `depth` $>$ `max_depth` **then**
      throw `MaxGridSizeExceeded`
    end if
  end for
  return `cube_list`

Algorithm 2 Check nonnegativity of $\mathcal{F}[g]$ using mpfi values

Require: `cube_list`
  for (C, `grid_size`) $\in$ `cube_list` **do**
    if $\mu(C,$ `grid_size`$) \ge 0$ **then**
      throw `NonNegativeValue`
    end if
  end for

3.4.4 Rigorous bounds

In [30], we published new upper bounds for three-dimensional convex bodies with tetrahedral symmetry by using the described approach. In our computations, we used the uniform sample method for checking the nonpositivity condition in the bounded part. By using the plane and generalized plane sample method, Pütz was able to improve some of our upper bounds. Furthermore, Pütz adapted our approach for three-dimensional convex bodies having icosahedral symmetry. In Table 3.3 the best obtained rigorous upper bounds with the corresponding factor α are given.

Body	Upper bound	Factor α
Regular octahedron (B_3^1)	0.972912750	1.0010
B_3^3	0.823611150	1.0020
B_3^4	0.874257405	1.0000
B_3^5	0.922441815	1.0050
B_3^6	0.933843309	1.0000
Regular tetrahedron	0.368333384	1.0005
Truncated cube	0.980578583	1.0003
Truncated tetrahedron	0.717085879	1.0009
Rhombicuboctahedron	0.876796420	1.0004
Regular icosahedron	0.879603500	1.0003
Regular dodecahdron	0.918311372	1.0001
Truncated icosahedron	0.834557102	1.0005
Rhombicosidodecahedron	0.843685241	1.0002
Truncated icosidodecahedron	0.860265927	1.0005
Truncated cuboctahedron	0.881501128	1.0005
Regular icosidodecahedron	0.883236750	1.0005
Truncated dodecahedron	0.911427019	1.0002

Table 3.3: List of rigorous upper bounds together with the factor α we needed in the verification.

3.5 Further implementation details

For computing rigorous bounds, we have to transform the problem into an SDP in standard form, then we use a solver for returning a numerical result, and afterwards we turn it into a solution which we verify to be rigorous.

For the first part, a basis for $V^{\pi,d}$ and $\mathcal{F}[V^{\pi,d}]$ is needed. Since, $V^{\pi,d}$ depends on the basis vectors φ^π of the coinvariant algebra $\mathbb{C}[x]_G$, we first compute this basis by using Magma

[12]. The advantage of Magma is, that it provides useful methods like the computation of the basic invariants and the character table.

Based on the obtained basis for the coinvariant algebra, we implemented a Sage script [70] for calculating a basis of $\mathbb{C}[x]^G_{\leq 40}$. Furthermore, in this program its Fourier inverse will be computed as described in Section 3.2. For formulating the program as an SDP, we need to get a common basis for $\mathbb{C}[x]^G_{\leq 40}$, $\mathbb{C}[x]_G$, and its inverses, which we also get by this Sage program.

The last step to express the program as an SDP is to compute the sample points, which we implemented as a C++ program. Then, we can transform this into an SDP in standard form by using the C++ library SDPSL [28], a semidefinite programming specification library. Now we can solve the program by using the SDPA-GMP solver to obtain a numerical result. Besides this library a further advantage of using C++ is that we can use multiple kernels, and thus, we can speed up our calculations. Moreover, the program has to work with large files and for transforming them into a format supported by the SDP solver, we have to formulate it by using floating-point numbers, since it cannot be described by rationals. Therefore, by using the C++ program, we can translate the exact values computed in the steps before into high-precision floating-point numbers.

The verification consists of the normalization and SOS checking in Section 3.4.2, and the sample checking in Section 3.4.3. For three-dimensional convex bodies with tetrahedral symmetry, the solutions, as well as the verification scripts and problems are available as ancillary files from the `arXiv.org` e-print archive [30]. We started the verification process by checking the normalization and SOS condition implemented as a Sage script named verify.sage, which runs in Sage 6.2. Further details about this program are explained in the file README_SOSChecking. Besides the normalization and SOS checking, this program produces input files for the sample checking, containing the function $\mathcal{F}[g]$ described by interval arithmetic.

The last step is the sample checking, which is implemented as a C++11 program called checker. To obtain rigorous bounds, we have to use interval arithmetic for this calculation. That can be realized by using the MPFI library [65] supported by C++. A detailed documentation about this program, including the description of all classes and methods is given in the file docu.pdf. Moreover, in README_SampleChecking we explain how to use the sample checking program.

Chapter Four

Lattice packings of superballs

4.1 Formulation as a polynomial optimization problem

In Section 3, we determined upper bounds for the translative packing density of three-dimension convex bodies having tetrahedral symmetry. To determine the optimal translative packing density one also needs lower bounds. Since lattice packings are in particular translative packings, any lattice packing density is a lower bound of the optimal translative packing density. Lattice packings are well studied and there are multiple results known. Theorem 1.3 provides a characterization of the basis vectors b_1, b_2, b_3 of a lattice Λ, for 2Λ being an optimal packing lattice in dimension three. These vectors are called *contact points*, since they are lying on the intersection of the boundary of a superball with the boundary of a neighboring superball.

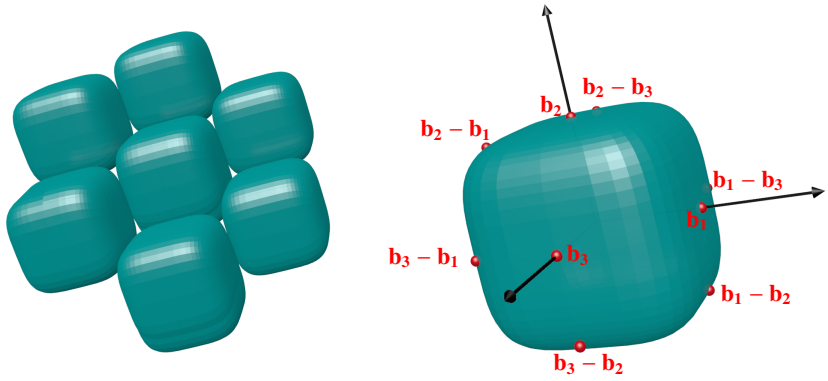


Figure 4.1: Left: A part of a lattice packing for B_3^4 satisfying Case 1 of Theorem 1.3. Right: Nine of twelve contact points of the packing on the left-hand side. The contact points are labeled in red.

Example 4.1. On the left-hand side in Figure 4.1, a lattice packing of three-dimensional superballs with $p = 4$ is given. In this packing, each solid has twelve contacting neighbors. One superball with six of its contacting neighbors is pictured. For the sake of clarity, there

are three contacting neighbors in front of the superball and three contacting neighbors behind the superball missing. The corresponding packing lattice 2Λ has a basis $2b_1, 2b_2, 2b_3$ such that

$$\pm b_1,\ \pm b_2,\ \pm b_3,\ \pm(b_1 - b_2),\ \pm(b_1 - b_3),\ \pm(b_2 - b_3)$$

are lattice points of Λ which lie on the boundary of B_3^4. Thus, they are defining the contact points and building the set $\mathcal{U}_B^1$ with matrix B consisting of the columns b_1, b_2, and b_3. Furthermore, the lattice points

$$\pm(-b_1 + b_2 + b_3),\ \pm(b_1 - b_2 + b_3),\ \pm(b_1 + b_2 - b_3)$$

lie outside of the superball. Therefore, in this example, Case 1 of Theorem 1.3 is satisfied. On the right-hand side in Figure 4.1, a superball with nine of its twelve contact points is shown. The remaining contact points are $-b_1$, $-b_2$, and $-b_3$, which lie behind the solid. The contacting neighbors pictured on the left-hand side correspond to the contact points $b_i - b_j$ for $i, j \in [3]$ with $i \neq j$ on the right-hand side.

In [61], Minkowski gives necessary conditions for the optimality of a lattice packing based on the supporting hyperplanes of the solid. From this, Betke and Henk were able to formulate in [9] an implementable algorithm for computing an optimal lattice packing of an arbitrary three-dimensional polytope. The characterizations of Minkowski are defined for any three-dimensional centrally-symmetric convex bodies, but they stated in [9]:

> Of course, given an arbitrary convex body $\mathcal{K}$ we do not know how to exploit [these necessary conditions], but if we consider only polytopes then for the supporting hyperplanes, we may always choose the supporting hyperplanes of the facets of the polytope. As a polytope has only finitely many facets we obtain the following frame of an algorithm for the computation of a critical lattice of a polytope.

Thus, for non-polytopes like superballs we cannot apply the approach of Betke and Henk. If $2\Lambda^*$ is an optimal lattice, Λ^* is called a *critical lattice*. Besides polytopes, Theorem 1.3 can also be used for computing an optimal lattice packing for three-dimensional round balls. Following Minkowski, we consider $\mathcal{K} = 1/2\, B_3^2$ a three-dimensional round ball with radius $1/2$. Due to Theorem 1.3, there exists an optimal lattice $2\Lambda^*$ for $\mathcal{K}$, such that the basis vectors of the corresponding critical lattice Λ satisfy exactly one of the three cases of Theorem 1.3. Let $b_1, b_2, b_3 \in \mathbb{R}^3$ be basis vectors of an optimal lattice $2\Lambda^*$, then we have to check whether $1/2\, b_1$, $1/2\, b_2$, and $1/2\, b_3$, basis vectors of Λ, satisfy Case 1, Case 2, or Case 3. Alternatively, we can check this for the basis vectors b_1, b_2, and b_3 and consider the solid $2\mathcal{K} = B_3^2$ a three-dimensional unit ball.

Moreover, a point $y_B = (y_1, y_2, y_3)_B^\mathsf{T}$ is a point in the basis b_1, b_2, and b_3, which are contained as columns in the matrix B, thus, $y_B = y_1 b_1 + y_2 b_2 + y_3 b_3$. A point y_B is lying on the boundary of B_3^2, if its norm $\|y_B\|_2$ is equal to the radius which is one. The square of the ℓ_3^2 norm of y_B can be calculated as

$$\begin{aligned}
\|y_B\|_2^2 &= \|y_1 b_1 + y_2 b_2 + y_3 b_3\|_2^2 \\
&= (b_{11} y_1 + b_{12} y_2 + b_{13} y_3)^2 + (b_{21} y_1 + b_{22} y_2 + b_{23} y_3)^2 + (b_{31} y_1 + b_{32} y_2 + b_{33} y_3)^2 \\
&= \alpha_{11} y_1^2 + 2\alpha_{12} y_1 y_2 + 2\alpha_{13} y_1 y_3 + \alpha_{22} y_2^2 + \alpha_{33} y_3^2,
\end{aligned}$$

with

$$\alpha_{ij} = b_{1i}b_{1j} + b_{2i}b_{2j} + b_{3i}b_{3j} \quad \text{for } i, j \in [3].$$

We define the function h, which maps a point $y \in \mathbb{R}^3$ to $\|y_B\|_2^2$, the ℓ_3^2 norm squared of y with respect to the basis B. Formally, this function is defined by

$$h : \mathbb{R}^3 \to \mathbb{R},$$

with

$$h(y_1, y_2, y_3) = \alpha_{11}y_1^2 + 2\alpha_{12}y_1y_2 + 2\alpha_{13}y_1y_3 + \alpha_{22}y_2^2 + \alpha_{33}y_3^2 \,. \tag{4.1}$$

If the lattice packing satisfies Case 2 of Theorem 1.3, the lattice points

$$\pm b_1, \ \pm b_2, \ \pm b_3, \ \pm (b_1 + b_2), \ \pm (b_1 + b_3), \ \pm (b_2 + b_3)$$

are elements of the boundary of $\mathcal{K}$. The set of these points in the basis B is $\{x_B : x \in L\}$, where

$$L = \left\{ \pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \ \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \ \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \ \pm \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \ \pm \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \ \pm \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right\}.$$

If these points lie on the boundary, the following equation holds

$$h(y_1, y_2, y_3) = 1 \quad \text{for all } (y_1, y_2, y_3)^\mathsf{T} \in L \,. \tag{4.2}$$

Then, we obtain

$$h(y_1, y_2, y_3) = y_1^2 - y_1y_2 - y_1y_3 - y_2y_3 + y_2^2 + y_3^2 \tag{4.3}$$

$$= \left(y_1 - \frac{1}{2}y_2 - \frac{1}{2}y_3\right)^2 + \frac{3}{4}(y_2 - y_3)^2 \,, \tag{4.4}$$

which describes a cylinder instead of a round sphere. Thus, this leads to a contradiction.

In Case 3, equation (4.2) and equation $h(1, 1, 1) = 1$ has to be satisfied. Therefore,

$$h(y_1, y_2, y_3) = 1 \quad \text{for all } (y_1, y_2, y_3)^\mathsf{T} \in L \cup \left\{\pm(1, 1, 1)^\mathsf{T}\right\}$$

has to hold. If we calculate $h(1, 1, 1)$ using the equation (4.3), we obtain $h(1, 1, 1) = 0$, and thus, this leads to a contradiction, too.

If we consider Case 1 of Theorem 1.3, we can do a similar calculation and obtain

$$h(y_1, y_2, y_3) = y_1^2 + y_1y_2 + y_1y_3 + y_2y_3 + y_2^2 + y_3^2.$$

To satisfy this condition, the matrix $M = (\alpha_{ij})_{i,j\in[3]}$ is

$$M = \begin{pmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{pmatrix}.$$

Note that $\det M = (\det B)^2$, where B is the matrix with columns equal to the basis vectors b_1, b_2, b_3. Since the determinant of M is equal to $1/2$, the determinant of B is $1/\sqrt{2}$. This is also equal to the volume of the fundamental domain of the corresponding packing lattice. Thus, we can calculate the lattice packing density. To do so, we have to divide the volume of the three-dimensional ball with radius $1/2$, which is equal to $\pi/6$, by the determinant of B, and thus, we obtain the optimal lattice packing density $\pi/\sqrt{18}$. Furthermore, Hales and Ferguson proved that this is also the optimal density for general packings of balls in dimension three [43].

Using the characterization of the contact points given in Theorem 1.3, we formulate a polynomial optimization problem for finding an optimal lattice for packing superballs. Theorem 1.3 states that there exists an optimal lattice such that for the corresponding critical lattice Case 1, Case 2, or Case 3 is satisfied. Thus, we have to calculate a best lattice for each of these three cases. By taking a best of these three resulting lattices, we obtain an optimal lattice. Since the only difference between these three cases is the set $\mathcal{U}_B$ and the points which have to lie outside of the considered solid $\mathcal{K}$, we just formulate a polynomial optimization problem for Case 1. For the other two cases, a polynomial optimization problem can be formulated in the same way.

We assume that Case 1 of Theorem 1.3 holds. Besides the lattice points which have to lie on the boundary of $\mathcal{K}$, there are also lattice points which have to lie outside of $\mathcal{K}$. We define a set $\widetilde{\mathcal{U}}_B^1$ consisting of these points

$$\widetilde{\mathcal{U}}_B^1 = \{(-1,1,1)_B, (1,-1,1)_B, (1,1,-1)_B\}.$$

Moreover, we define the function h mapping $y \in \mathbb{R}^3$ to $\|y_B\|_3^p$. For $p = 2$, this function is given in (4.1). For general values of p, it is

$$\begin{aligned} h(y_1,y_2,y_3) &= \|(y_1,y_2,y_3)_B\|_p^p \\ &= |y_1b_{11} + y_2b_{21} + y_3b_{31}|^p + |y_1b_{12} + y_2b_{22} + y_3b_{32}|^p + |y_1b_{13} + y_2b_{23} + y_3b_{33}|^p. \end{aligned}$$

Due to the absolute value, $h(y_1, y_2, y_3)$ is not a polynomial, unless p is an even integer, then it is equal to

$$(y_1b_{11} + y_2b_{21} + y_3b_{31})^p + (y_1b_{12} + y_2b_{22} + y_3b_{32})^p + (y_1b_{13} + y_2b_{23} + y_3b_{33})^p.$$

If p is not an even integer, and thus, $h(y_1, y_2, y_3)$ is not a polynomial, it is more complicated to formulate the problem as a polynomial optimization problem. One possibility would be to split the problem into many optimization problems depending on the sign of the optimization variables. However, for the rest of this section, we consider the case where p is an even integer.

Since our goal is to formulate an optimization problem for Case 1 of Theorem 1.3, the polynomial h has to satisfy

$$h(y_1,y_2,y_3) = 1 \quad \text{for all } (y_1,y_2,y_3) \in \mathcal{U}_B^1, \tag{4.5}$$

$$h(y_1,y_2,y_3) > 1 \quad \text{for all } (y_1,y_2,y_3) \in \widetilde{\mathcal{U}}_B^1. \tag{4.6}$$

Hence, a basis $b_1, b_2, b_3 \in \mathbb{R}^3$ satisfying (4.5) and (4.6) is a feasible lattice for Case 1.

To describe the objective function, we consider the lattice packing density: A lattice Λ is called a *packing lattice* for a solid $\mathcal{K}$ if for all $x, y \in \Lambda$ with $x \neq y$, the intersection of the interior of $x + \mathcal{K}$ and $y + \mathcal{K}$ is empty. An optimal packing lattice for $\mathcal{K}$ is denoted by $\Lambda^*(\mathcal{K})$, and thus, the corresponding lattice packing density is

$$\delta(\mathcal{K}) = \frac{\text{vol}(\mathcal{K})}{\det \Lambda^*(K)},$$

where $\det \Lambda^*(\mathcal{K})$ is the absolute value of the determinant of the matrix whose columns are the basis vectors of $\Lambda^*(\mathcal{K})$. Consequently, finding the densest lattice packing is equivalent to the problem of finding a packing lattice with minimal determinant. The absolute value of the determinant of a lattice with basis vectors b_1, b_2, b_3, or in general $b_1, \ldots, b_n$, is equal to the volume of the parallelepiped generated by these basis vectors called *fundamental domain*. Therefore, the volume of the fundamental domain of a lattice is given by the absolute value of the determinant of the matrix B whose columns are equal to the basis vectors. For transforming the problem into a polynomial optimization problem in standard form, we cannot take the absolute value of a polynomial into account. However, we can avoid this problem by taking the minimum of $(\det B)^2$ or alternatively, we can add a constraint that the determinant has to be positive. Since the optimal lattice has to have a nonzero determinant, we have to add this constraint to the optimization problem, too.

Let $x \in \mathbb{R}^9$ be a vector consisting of the elements in B, such that $x^\mathsf{T} = (b_{11}, b_{12}, \ldots, b_{33})$. Furthermore, let $d(x)$ be a polynomial equal to the determinant of the matrix B whose columns coincide with b_1, b_2, and b_3, thus,

$$d(x) = x_2x_6x_7 - x_3x_5x_7 + x_3x_4x_8 - x_1x_6x_8 - x_2x_4x_9 + x_1x_5x_9. \tag{4.7}$$

Our goal is to find a packing lattice 2Λ with basis vectors $2b_1, 2b_2, 2b_3 \in \mathbb{R}^3$ such that b_1, b_2, b_3 satisfy Case 1 of Theorem 1.3 and the absolute value of the determinant of 2Λ is minimal. Since, the determinant of the packing lattice 2Λ is minimal if and only if the determinant of the critical lattice Λ is minimal, we optimize over $x \in \mathbb{R}^9$ defining a critical lattice. Thus, we have to minimize $|d(x)|$. Since $d(x)$ has to be nonnegative, we use $p_0(x) = d(x)^2$ as the objective function of the desired optimization problem. To formulate the problem as a polynomial optimization problem defined in (2.4) – (2.5), we have to express the inequality conditions as nonnegativity conditions. To do so, we define the polynomial $p_u(x)$ for $u \in \mathcal{U}_B^1 \cup \widetilde{\mathcal{U}}_B^1$ to be equal to $h(u) - 1$ with respect to the basis contained in x.

Finally, we formulate a polynomial optimization problem with optimal value $p_{\min}$ to compute an optimal lattice for Case 1

$$p_{min} = \min\ p_0(x) \tag{4.8}$$
$$x \in \mathbb{R}^9 \tag{4.9}$$
$$p_u(x) = 0\ \forall u \in \mathcal{U}_B^1 \tag{4.10}$$
$$p_u(x) > 0\ \forall u \in \widetilde{\mathcal{U}}_B^1 \tag{4.11}$$

If Case 1 of Theorem 1.3 holds, the optimal value p_{min} is equal to $(\det \Lambda^*(K))^2$. We replace the strict inequality conditions by non-strict inequality conditions in order to obtain

a semidefinite program (SDP) by using a sum of squares (SOS) relaxation as explained in Section 2.1.2. Therefore, we have also to check whether the computed solutions are feasible for problem (4.8) – (4.11), which means we have to check whether they even satisfy the strictly inequality conditions.

The optimization variable $x \in \mathbb{R}^9$ contains the elements of basis vectors $b_1, b_2, b_3 \in \mathbb{R}^3$ defining a lattice. Thus, we have to optimize over nine variables. We apply SOS relaxations to the polynomial optimization problem in order to obtain a semidefinite program (SDP), which can be solved by SDP solvers. In Section 2.1.2, we explained the SOS relaxation of a polynomial optimization problem.

If we split equation (4.10) into $p_u(x) \leq 0$ and $-p_u(x) \leq 0$ for all $u \in \mathcal{U}_B^1$, we get the following SDP by using SOS relaxations:

$$\begin{aligned} p_{sos,i,j} = \max\ & \Lambda \\ & \Lambda \in \mathbb{R}_{>0} \\ & p_0(x) - \Lambda \in \Sigma_{9,2i} + \sum_{u \in \mathcal{U}_B^1} p_u(x)\, \Sigma_{9,2j} - p_u(x)\, \Sigma_{9,2j} + \sum_{u \in \widetilde{\mathcal{U}}_B^1} p_u(x)\, \Sigma_{9,2j}, \end{aligned}$$

where $\Sigma_{m,k}$ denotes the set of SOS polynomials with m variables and degree at most k. To compute an optimal solution for superballs with $p = 4$, the polynomials p_u for $u \in \mathcal{U}_B^1 \cup \widetilde{\mathcal{U}}_B^1$ have degree four. Furthermore, the polynomial $p_0(x)$ has degree six. If we consider $i = 3$ and $j = 1$, the positive semidefinite matrices of the cone $\Sigma_{9,6}$ have dimension 220 and the matrices of the cone $\Sigma_{9,2}$ have dimension 10. We can solve this SDP with the interior point method by using CSDP, a C library for semidefinite programs [11]. The obtained objective value is $p_{sos,3,1} = 0.64432\ldots$. Since our goal is to determine the density of a critical lattice, $p_{\min}$ is equal to the volume of its fundamental domain squared. As $p_{sos,i,j} \leq p_{\min}$ for $i, j \in \mathbb{N}$, we obtain lower bounds for $p_{\min}$ by solving the SDP. The optimal lattice packing density is equal to $\operatorname{vol} B_3^4/(8\sqrt{p_{\min}})$ and thus by using the upper bound for the density computed in Section 3, we get $p_{\min} \geq 0.8590$. Furthermore, if we had $p_{\min} = 0.64432\ldots$, the corresponding density would be equal to $1.0094\ldots$. This implies, that $p_{sos,3,1}$ is not equal to $p_{\min}$. Thus, using the SOS relaxation with $i = 3$ and $j = 1$ to determine $p_{\min}$ is not useful. However, by increasing the degrees i and j the solution of the corresponding SDP might be equal to $p_{\min}$. If we set $j = 2$, the ten-dimensional matrices increase to dimension 55. The SDP solver had to interrupt its computation after around 10 hours, which might be because of memory problems. For $j = 3$, the dimension of these matrices is equal to 220 and the solver immediately stops with the message that the SDP is too large. It might be possible to determine $p_{\min}$ by solving the SDP $p_{sos,i,j}$, but we probably have to choose larger values for i and j, and then the corresponding SDP is not solvable in practice.

In the previous step, we split the equality condition (4.10) into inequality conditions in order to apply SOS relaxations to the polynomial optimization problem. Alternatively, we can use the condition

$$p(x) \text{ is SOS in } \mathbb{R}[x]/I,$$

where I is the ideal generated by the polynomials $p_u(x)$ for $u \in \mathcal{U}_B^1$. Thus, $p(x)$ has to be

SOS, if $p_u(x) = 0$ for all $u \in \mathcal{U}_B^1$. The corresponding SDP is then given as

$$p_{sos,i,j} = \max \Lambda \tag{4.12}$$
$$\Lambda > 0 \tag{4.13}$$
$$p_0(x) - \Lambda \text{ is SOS in } \mathbb{R}[x]/I \tag{4.14}$$
$$p_0(x) - \Lambda \in \Sigma_{9,2i} + \sum_{u \in \overline{\mathcal{U}}_B^1} p_u(x)\, \Sigma_{9,2j}. \tag{4.15}$$

For checking condition (4.14) the solver has to compute a *Gröbner basis* for the ideal I. For more details about Gröbner bases, we refer the interested reader to Becker and Weispfenning [7], Buchberger [14, 15], and Cox, Little, and O'Shea [22]. For superballs with $p = 4$, the calculation of the Gröbner basis is too expensive, and thus, this SDP is not solvable.

4.2 Shortest vector problem

In the previous section, we saw that we can formulate a polynomial optimization problem to find an optimal lattice packing of superballs if p is an even integer. Unfortunately, we could not solve this problem by using SOS relaxations. Thus, we compute lattice packings and check, whether these packings are locally optimal. For this, we first have to check whether a given lattice is a packing lattice.

As defined before, a lattice $\Lambda \subseteq \mathbb{R}^n$ described by its basis vectors $b_1, \dots, b_n$ is a packing lattice for $\mathcal{K}$, if and only if, for all $x, y \in \Lambda$ the intersection of the interior of $x+\mathcal{K}$ and $y+\mathcal{K}$ is empty. Since the packing of a lattice packing coincides in each fundamental domain, we just have to check whether the solids do not intersect in the fundamental domain spanned by the basis vectors $b_1, \dots, b_n$. For the following lemma, we consider solids which are *proper*, which means, their interior is not empty.

Lemma 4.2. *Let $\mathcal{K}$ be a proper convex body, $D = \frac{1}{2}(\mathcal{K} - \mathcal{K})$ its centrally symmetrization, and Λ a lattice. Then Λ is a packing lattice of $\mathcal{K}$ if and only if $(2D)^\circ \cap \Lambda = \{0\}$.*

Proof. In [42, Proposition 30.4], Gruber provide the following proof of Lemma 4.2

$$\begin{aligned}
&\Lambda \text{ is a packing lattice of } D \\
&\iff D^\circ \cap \left(\frac{1}{2}D^\circ + x\right) = \emptyset \quad \text{for all } x \in \Lambda \setminus \{0\} \\
&\iff x \notin D^\circ - D^\circ \qquad\qquad \text{for all } x \in \Lambda \setminus \{0\}
\end{aligned}$$

Since D is centrally-symmetric, we get $D - D = 2D$. This implies

$$\Lambda \text{ is a packing lattice of } D \iff (2D)^\circ \cap \Lambda = \{0\}$$

By applying the following result of Minkowski [61]

$$\Lambda \text{ is a packing lattice of } \mathcal{K} \iff \Lambda \text{ is a packing lattice of } D,$$

the claim follows. □

The equality $\mathcal{K} = \frac{1}{2}(\mathcal{K} - \mathcal{K})$ for convex bodies $\mathcal{K}$, which are centrally-symmetric with respect to the origin, leads to the following corollary.

Corollary 4.3. *Let Λ be a lattice and $\mathcal{K}$ be a centrally-symmetric proper convex body. Then 2Λ is a packing lattice of $\mathcal{K}$ if and only if $\mathcal{K}^\circ \cap \Lambda = \{0\}$.*

Due to Corollary 4.3, we can check whether a given lattice 2Λ is a packing lattice for a solid $\mathcal{K}$ by checking whether zero is the only common point of the interior of the solid and the lattice Λ. For this, we calculate the shortest nonzero vector of Λ. Then, the intersection consists just of the zero point, if and only if, the shortest vector of Λ lies not in $\mathcal{K}^\circ$.

The *shortest vector problem* is a famous problem in number theory and has been studied by mathematicians for more than a century. We consider the case for calculating a shortest vector concerning the ℓ_n^p norm in dimension n. For more information about the general problem, see for example [77].

To calculate the shortest vector concerning the ℓ_n^p norm in a lattice, the following lemma inspired by the work of Dieter [29], gives a necessary condition.

Lemma 4.4. *Let $b_1, \ldots, b_n \in \mathbb{R}^n$ be a basis of a lattice Λ and let $\mu \in \mathbb{R}$ and $p \in \mathbb{R}$. A lattice point $v = \sum_{i=1}^n \alpha_i b_i$ with $\alpha \in \mathbb{Z}^n$ and $\|v\|_p \leq \mu$, has to satisfy*

$$|\alpha_i| \leq \mu \sqrt{n} \sqrt{G_{ii}^{-1}} \quad \text{for all } i \in \{1, \ldots, n\},$$

where G is the Gram matrix of Λ given by $G_{ij} = \langle b_i, b_j \rangle$.

Before proving this lemma, we define the dual lattice. The *dual lattice* $\Lambda^\#$ of $\Lambda \subset \mathbb{R}^n$ is defined by

$$\Lambda^\# = \{x \in \mathbb{R}^n : \langle x, v \rangle \in \mathbb{Z} \ \text{ for all } v \in \Lambda\}.$$

The vectors $b_1^\#, \ldots, b_n^\# \in \Lambda^\#$ satisfying

$$\langle b_i, b_j^\# \rangle = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{otherwise.} \end{cases}$$

for $i, j \in [n]$ build a basis of the n-dimensional lattice $\Lambda^\#$. Furthermore, the dual of the dual of a lattice is equal to the lattice, that is $(\Lambda^\#)^\# = \Lambda$. The Gram matrix $G^\#$ concerning the dual basis vectors $b^\#$ is the inverse matrix of G.

Proof of Lemma 4.4. Let $v = \sum_{i=1}^n \alpha_i b_i$ be a lattice point in Λ. Then, we get the value α_i by the inner product $\langle v, b_i^\# \rangle$. Thus, each α_i is bounded above by

$$|\alpha_i| = \left|\langle v, b_i^\# \rangle\right| = \left|\sum_{j=1}^n v_j b_{ij}^\#\right| \leq \sum_{j=1}^n \left|v_j b_{ij}^\#\right|.$$

The *Hölder inequality* [44, p. 24, Theorem 12] states

$$\sum_{i=1}^n |x_i y_i| \leq \|x\|_p \|y\|_q,$$

for $x, y \in \mathbb{R}^n$ and $1 < p, q < \infty$ with $1/p + 1/q = 1$. Thus, by applying the *Hölder inequality* we obtain

$$\sum_{j=1}^{n} \left| v_j b_{ij}^{\#} \right| \leq \|v\|_p \, \|b_i^{\#}\|_q \leq \mu \, \|b_i^{\#}\|_q,$$

for q satisfying $1/p + 1/q = 1$. Moreover, we can use the property

$$\|x\|_q \leq \|x\|_1 \leq \sqrt{n} \, \|x\|_2 \, ,$$

for $q \geq 1$. The square of the ℓ_n^2 norm of the dual basis vectors $b_1^{\#}, \ldots, b_n^{\#}$ is given in the Gram matrix, because $G_{ii}^{-1} = \langle b_i^{\#}, b_i^{\#} \rangle = \|b_i^{\#}\|_2^2$ and therefore, $|\alpha_i| \leq \mu \sqrt{n} \sqrt{G_{ii}^{-1}}$. □

To check whether a lattice Λ is a packing lattice for B_3^p, we compute all lattice points satisfying the necessary condition given in Lemma 4.4 for $n = 3$, and then, we take the one with the smallest ℓ_3^p norm. A lattice Λ is a packing lattice of B_3^p if and only if the ℓ_3^p norm of the shortest vector in Λ is at least two.

4.3 Locally optimal lattice packings

Since we could not solve the optimization problem (4.8) – (4.11) for finding an optimal lattice packing by using SOS relaxations, as explained in Section 4.1, we calculate locally optimal lattice packings. To do so, we determine packing lattices by using Newton's method and check whether these solutions satisfy the KKT conditions as well as the second order condition. If so, the obtained solution is locally optimal. First, we formulate the KKT conditions and the second order condition explicitly for the considered optimization problem (4.8) – (4.11). Then, we describe the approach for computing locally optimal lattice packings using these conditions. Furthermore, for each of the four regimes of p, we provide the best obtained locally optimal packing lattice. In this section, we consider superballs defined by arbitrary $p \geq 1$, thus $p_u(x)$ is not a polynomial unless p is an even integer.

4.3.1 Sufficient condition

Our goal is to check whether a feasible solution x^* of the problem (4.8) – (4.11) is locally optimal. In order to apply the sufficient condition of local optimality given in Theorem 2.7, we have to determine the objective function $f(x)$ and the constraint functions $h_i(x)$ and $g_i(x)$ used in this theorem.

The objective function $f(x)$ is defined by the polynomial $p_0(x) = d(x)^2$ in (4.7). The problem (4.8) – (4.11) contains the equality condition

$$p_u(x) = 0 \quad \text{for all } u \in \mathcal{U}_B^i,$$

for $i \in \{1, 2, 3\}$ depending on the considered case of Theorem 1.3. Thus, the functions p_u for $u \in \mathcal{U}_B^i$ correspond to the desired functions $h_i(u)$. For the first two cases of Minkowski's theorem, the optimization problem also contains strict inequality conditions

$$p_u(x) > 0 \quad \text{for all } u \in \widetilde{\mathcal{U}}_B^i,$$

for $i \in \{1,2\}$. To be able to apply the KKT conditions to our problem, we have to transform the strict inequality conditions into non-strict inequality conditions. The functions $p_u(x)$ for $u \in \widetilde{\mathcal{U}}_B^i$ with $i \in \{1,2\}$, which define these inequality conditions, correspond to the remaining functions g_j for $j \in [n]$, which we need to apply Theorem (2.7). Note that for $i = 3$, there exist no inequality conditions.

The sufficient condition requires that the objective function $f(x)$ and the constraint functions $h_i(x)$ and $g_j(x)$, which are $p_u(x)$ for $u \in \mathcal{U}_B^i \cup \widetilde{\mathcal{U}}_B^i$, are twice-differentiable at x^*. The objective function satisfies this condition. The functions $p_u(x)$ for $u \in \mathcal{U}_B^i \cup \widetilde{\mathcal{U}}_B^i$ are of the form

$$\left|\gamma_1^\mathsf{T}\, x\right|^p + \left|\gamma_2^\mathsf{T}\, x\right|^p + \left|\gamma_3^\mathsf{T}\, x\right|^p, \tag{4.16}$$

with $\gamma_1, \gamma_2, \gamma_3 \in \{-1, 0, +1\}^9$. Since we know the considered solution x^* before checking the second order condition, we can determine the function

$$\left(\operatorname{sign}\left(\gamma_1^\mathsf{T}\, x^*\right)\, \gamma_1^\mathsf{T}\, x\right)^p + \left(\operatorname{sign}\left(\gamma_2^\mathsf{T}\, x^*\right)\, \gamma_2^\mathsf{T}\, x\right)^p + \left(\operatorname{sign}\left(\gamma_3^\mathsf{T}\, x^*\right)\, \gamma_3^\mathsf{T}\, x\right)^p, \tag{4.17}$$

which is equal to (4.16) for x being close to x^*. This function is twice-differentiable at x^* for $p \geq 1$ unless there exist no $p_u(x^*)$ with summand 0^p for $p < 2$.

KKT conditions

The sufficient condition given in Theorem 2.7 requires that the KKT conditions (2.12) – (2.16) are satisfied. Thus, we have to determine Lagrange multipliers. For each equality condition, we consider one Lagrange multiplier μ_u. Furthermore, for each inequality condition, we need one Lagrange multiplier ν_u. Thus, we need Lagrange multipliers

$$\begin{aligned} \mu &= \{\mu_1, \ldots, \mu_m\} && \text{for } m = \left|\mathcal{U}_B^i\right|, \\ \nu &= \{\nu_1, \ldots, \nu_n\} && \text{for } n = \left|\widetilde{\mathcal{U}}_B^i\right|. \end{aligned}$$

Based on the objective function, the constraint functions and the Lagrange multipliers, the corresponding Lagrange function is

$$\mathcal{L}(x, \mu, \nu) = p_0(x) + \sum_{u \in \mathcal{U}_B^i} \mu_u p_u(x) + \sum_{u \in \widetilde{\mathcal{U}}_B^i} \nu_u p_u(x). \tag{4.18}$$

Furthermore, the KKT conditions for the considered optimization problem (4.8) – (4.11) are

$$\nabla_x \mathcal{L}(x^*, \mu^*, \nu^*) = 0 \tag{4.19}$$

$$p_u(x^*) > 0 \quad \text{for all } u \in \widetilde{\mathcal{U}}_B^i \tag{4.20}$$

$$p_u(x^*) = 0 \quad \text{for all } u \in \mathcal{U}_B^i \tag{4.21}$$

$$\nu_u^* \geq 0 \quad \text{for all } u \in \widetilde{\mathcal{U}}_B^i \tag{4.22}$$

$$\nu_u^* p_u(x^*) = 0 \quad \text{for all } u \in \widetilde{\mathcal{U}}_B^i \tag{4.23}$$

with Lagrange multipliers $\mu^* = \{\mu_1^*, \ldots, \mu_m^*\}$ and $\nu^* = \{\nu_1^*, \ldots, \nu_n^*\}$.

The conditions (4.20) and (4.21) are the constraint conditions of the considered optimization problem to ensure the feasibility of x^*. Since we are interested in solutions satisfying the inequality constraints strictly, we use in (4.20) strict inequality conditions. Thus, the condition (4.23) can just be satisfied if $\nu_u^* = 0$ for $u \in \widetilde{\mathcal{U}}_B^i$. Consequently, we set ν_u^* equal to 0 for all $u \in \widetilde{\mathcal{U}}_B^i$, and thus, the conditions in (4.22) and (4.23) are satisfied. Hence, a feasible solution x^* of the considered problem satisfies the KKT conditions, if there exists Lagrange multipliers $\mu^* = \{\mu_1^*, \dots, \mu_m^*\}$, such that $\nabla_x \mathcal{L}(x^*, \mu^*, 0) = 0$.

Second order condition

Due to Theorem 2.7, the second order condition is satisfied if and only if for all $y \neq 0$ with

$$y^\mathsf{T} g_u(x^*) = 0 \text{ for all } u \in \widetilde{\mathcal{U}}_B^i \text{ where } \nu_u^* > 0 \tag{4.24}$$

$$y^\mathsf{T} \nabla_x\, p_u(x^*) \geq 0 \text{ for all } u \in \widetilde{\mathcal{U}}_B^i \text{ where } p_u(x^*) = 0,\ \nu_u^* = 0 \tag{4.25}$$

$$y^\mathsf{T} \nabla_x\, p_u(x^*) = 0 \text{ for all } u \in \mathcal{U}_B^i, \tag{4.26}$$

the second derivative of the Lagrange function satisfies the following condition

$$y^\mathsf{T} \left(\nabla_x^2\, \mathcal{L}(x^*, \mu^*, \nu^*) \right) y > 0. \tag{4.27}$$

Since ν^* is equal to zero, condition (4.24) is satisfied. Furthermore, for a feasible solution x of the considered optimization problem (4.8) – (4.11), the value $p_u(x)$ is strictly positive for all $\in \widetilde{\mathcal{U}}_B^i$, therefore, condition (4.25) holds, too. Thus, condition (4.26) is left to check. For this, we define

$$Y = \left\{ y \in \mathbb{R}^9 : y \neq 0,\ y^\mathsf{T}\, \nabla_x p_u(x^*) = 0 \text{ for all } u \in \mathcal{U}_B^i \right\}.$$

To check the second order condition (4.27), we just have to check the condition

$$y^\mathsf{T} \left(\nabla_x^2\, \mathcal{L}(x^*, \mu^*, \nu^*) \right) y > 0 \quad \text{ for all } y \in Y.$$

Let I be the vector subspace generated by the polynomials $(\nabla p_u(x^*))^\mathsf{T}\, y$ for $u \in \mathcal{U}_B^i$ and $y^\mathsf{T} = (y_1, \dots, y_n)$. Furthermore, let $\tilde{y}$ consists of the standard monomials corresponding to the basis of I and let M be a symmetric matrix such that

$$y \left(\nabla_x^2 \mathcal{L}(x^*, \mu^*, \nu^*) \right) y = \tilde{y} M \tilde{y}^\mathsf{T} \bmod I. \tag{4.28}$$

Then, the second order condition (4.27) is satisfied if and only if M is positive definite, which means the eigenvalues of M are strictly positive. Since for $i \in \{1, 2\}$ the set $\mathcal{U}_B^i$ has cardinality six, the matrix M has dimension three. For $i = 3$ the set $\mathcal{U}_B^i$ has cardinality seven, and thus, the matrix M has dimension two. In Section 4.3.6, we determine $\tilde{y}$ and M explicitly for a certain solution (x^*, μ^*).

4.3.2 Computations via Newton's method

We have determined the KKT conditions and the second order condition explicitly for the considered problem. The next task is to compute locally optimal lattices. Since we have to

determine solutions $(x^*, \mu^*) \in \mathbb{R}^{9+k}$ for $k = |\mathcal{U}_B^i|$ and $i \in [3]$, such that

$$\nabla_x \mathcal{L}(x^*, \mu^*, 0) = 0 \tag{4.29}$$

$$p_u(x^*) = 0 \qquad \text{for } u \in \mathcal{U}_B^i, \tag{4.30}$$

we have to calculate the roots of these functions to obtain locally optimal solutions. To do so, we apply *Newton's method*: This is an iterative approach to find roots of a given strictly convex, differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ close to a given point s, which is an initial guess for the desired root r. For this we approximate f around a point a by using the *Taylor approximation*

$$f(a + x) = \left(f(a) + \nabla f(a)^\mathsf{T} x + \frac{1}{2} x^\mathsf{T} \nabla^2 f(a) x \right) + \alpha,$$

where α represents higher order terms. In each *Newton step*, we use this approximation in order to find the minimizer. This can be done by setting the gradient of

$$q(x) = f(a) + \nabla f(a)^\mathsf{T} x + \frac{1}{2} x^\mathsf{T} \nabla^2 f(a) x$$

equal to zero. The Newton's method starts with an initial guess s_1 and in each iteration the considered point s_j will be updated to s_{j+1} by

$$s_{j+1} = s_j - \frac{\nabla_x f(s_j)}{\nabla_x^2 f(s_j)}.$$

In such a way, Newton's method determines a sequence of points converging to r. The procedure terminates by reaching a desired accuracy. We refer interested reader to [56, Chapter XVIII] of Akilov and Kantorovich. This book also includes the first thorough analysis of the convergence behavior of the Newton's method.

To compute locally optimal lattice packings, we have to find the roots of $\nabla_x \mathcal{L}(x, \mu, 0)$ and of $p_u(x)$ for $u \in \mathcal{U}_B^i$. For this, we apply Newton's method, with an initial guess $s = (x, \mu)$, where $x \in \mathbb{R}^9$ is a random point and we set $\mu \in \{0\}^k$ with $k = |\mathcal{U}_B^i|$. For the computation of locally optimal lattice packings, we used Sage, which provides a method for applying the Newton's method to a given vector function f and a given initial guess s. In our case, we use $f^\mathsf{T} = [\mathcal{L}(x, \mu, 0), p_{u_1}(x), \ldots, p_{u_k}(x)]$, where $k = |\mathcal{U}_B^i|$. If the computation was successful, we check whether the obtained root $[x^*, \mu^*]$ is indeed a locally optimal solution.

First, we have to check whether x^* defines a feasible lattice packing. To do so, we define the vectors

$$b_1^\mathsf{T} = \left(x_1^*, x_2^*, x_3^*\right), \quad b_2^\mathsf{T} = \left(x_4^*, x_5^*, x_6^*\right), \quad b_3^\mathsf{T} = \left(x_7^*, x_8^*, x_9^*\right).$$

Furthermore, let Λ be the lattice defined by the basis vectors b_1, b_2, and b_3. Due to Corollary 4.3, 2Λ is a packing lattice for B_3^p if and only if the shortest vector in Λ has ℓ_3^p norm one. Thus, we check this condition by computing the shortest vector. For this, we can apply Lemma 4.4.

Next, we have to check whether x^* is a feasible solution of the optimization problem (4.8) – (4.11). Since x^* is a root of f, the equality conditions are satisfied. Thus, the inequality conditions $p_u(x^*) > 0$ for all $u \in \tilde{U}_B^i$ are remain to check.

Since we would like to compute locally optimal solutions, we have to check whether (x^*, μ^*) satisfies the second order condition. In case the solution (x^*, μ^*) satisfies these conditions, x^* defines a locally optimal lattice packing. Since the given optimization problem is not convex, the locally optimal solution is not necessary globally optimal. Thus, we apply the above approach to many random starting points s, which are in our approach 10,000, to obtain many locally optimal solutions. Then, we take the best solution over all obtained locally optimal solutions, which is hopefully equal to a globally optimal solution. We run this procedure for each of the three cases of Theorem 1.3 and take the one with a densest lattice packing. In the following sections, we provide the obtained locally optimal lattice packings.

In [53, 54], Jiao, Stillinger, and Torquato divide the range of $p \in [1, \infty)$ into four regimes:

$$[1, \log_2 3], [\log_2 3, 2], [2, 2.3018\ldots], [2.3018\ldots, \infty)\,.$$

For each of these regimes, they give a family of lattices defining a lattice packing. Analogously, we divide the range of $p \in [1, \infty)$ in a similar way, and for each of these regimes we compute lattice packings, for which we numerically prove local optimality. Due to the pattern of the obtained lattices, we define the second regime in such a way, that it does not include the value $\log_2 3$. Thus, we consider the following partitioning:

$$[1, \log_2 3], (\log_2 3, 2], [2, 2.3018\ldots], [2.3018\ldots, \infty)\,.$$

4.3.3 First regime

For the first regime $[1, \log_2 3]$, we obtained locally optimal lattice packings for each of the three cases of Theorem 1.3. The lattice L_3, which is defined as

$$L_3 = \mathbb{Z}\, 2b_1 \oplus \mathbb{Z}\, 2b_2 \oplus \mathbb{Z}\, 2b_3,$$

with

$$b_1 = (-x, y, z)\,,\ b_2 = (z, -x, y)\,,\ b_3 = (y, z, -x)\,,$$

where $x, y, z \in \mathbb{R}_{>0}$ with $z \geq x \geq y$ such that

$$\begin{aligned} z &= 3^{-1/p} + x - y,\\ x^p + y^p + z^p &= 1,\\ (x-y)^p + (3^{-1/p} + x)^p + (3^{-1/p} - y)^p &= 1, \end{aligned}$$

is the best locally optimal lattice we computed. In this packing, each solid has fourteen contacting neighbors. For $p = 1$, the lattice L_3 coincides with an optimal packing lattice for octahedra found by Minkowski [61]. This lattice is defined by the basis vectors

$$b_1^\mathsf{T} = 2\,(-1/3, 1/6, 1/2)\,,\ b_2^\mathsf{T} = 2\,(1/2, -1/3, 1/6)\,,\ b_3^\mathsf{T} = 2\,(1/6, 1/2, -1/3)$$

and has density $18/19 = 0.947368421\ldots$.

On the left-hand side in Figure 4.2 a part of the L_3 lattice packing for superballs with $p = 1.2$ is given. For the sake of clarity, in the figure one superball with just six of its fourteen contacting neighbors is pictured. Furthermore, on the right-hand side in Figure

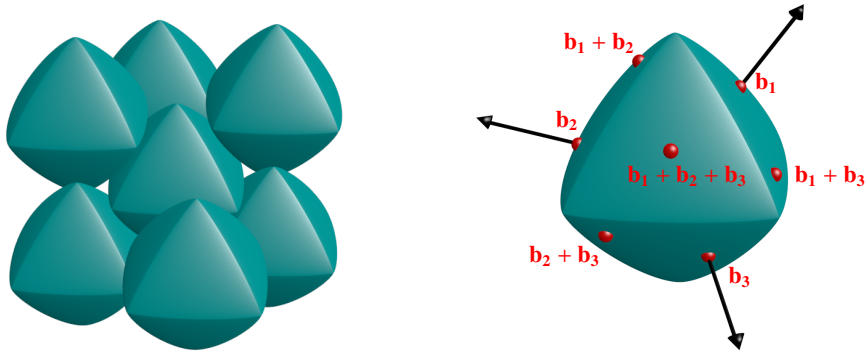


Figure 4.2: Left: A part of the L_3 lattice packing for $B_3^{1.2}$. Right: Seven of fourteen contact points in the L_3 lattice packing for $B_3^{1.2}$. The contact points are labeled in red.

4.2 the superball $B_3^{1.2}$ with seven of its fourteen contact points is shown. The contacting neighbors on the left-hand side correspond to the contact points $\pm b_1$, $\pm b_2$, and $\pm b_3$ shown on the right-hand side.

In our computations, we numerically proved local optimality of L_3. For this, we checked the KKT conditions and the second order condition by a computer program. In [53, 54], Jiao, Stillinger, and Torquato publish a lattice O_1 for the lattice packing of superballs in the first regime. This lattice is defined by

$$O_1 = \mathbb{Z}\, 2b_1 \oplus \mathbb{Z}\, 2b_2 \oplus \mathbb{Z}\, 2b_3,$$

with

$$b_1 = \left(3^{-1/p}, 3^{-1/p}, 3^{-1/p}\right),\ b_2 = (-q, s, -q)\,,\ b_3^{\mathsf{T}} = (q, -q, -s)\,,$$

where

$$\begin{aligned} &2q^p + s^p = 1,\\ &(s - q - 3^{-1/p})^p + (s + q - 3^{-1/p})^p = 2/3. \end{aligned}$$

The O_1 lattice satisfies none of the three cases of Theorem 1.3, because each solid has just eight contacting neighbors in the packing for $p \in (1, \log_2 3)$. In 1953, Swinnerton-Dyer proved that the number of contact points in any locally optimal lattice packing in dimension d is at least $d(d+1)$ [73]. For $d = 2, 3$, this was already proven by Minkowski in 1904 [61]. Since we are considering three-dimensional packings, any locally optimal lattice packing has to have at least twelve contact points. Thus, the O_1 lattice is not even locally optimal.

In case $p \in \{1, \log_2 3\}$, the density of the L_3 lattice packing is equal to the density of the O_1 lattice packing. For $p \in \{1.05, 1.1, \ldots, 1.55\}$, the lattice L_3 defines a lattice packing with a higher density than the O_1 lattice.

In [63], Ni, Gantapara, de Graaf, van Roij, and Dijkstra state that they found better lattice packings for the first regime than the O_1 lattice packing. They give one example for

$p = 1.4$: The basis vectors of their lattice are

$$b_1 = \begin{pmatrix} 0.912492 \\ 0.912403 \\ -0.912165 \end{pmatrix}, \; b_2 = \begin{pmatrix} -0.271668 \\ 1.80916 \\ -0.288051 \end{pmatrix}, \; b_3 = \begin{pmatrix} 0.28834 \\ -0.272001 \\ -1.80882 \end{pmatrix}.$$

The packing density they claim is equal to the density of the L_3 lattice packing. If b_1, b_2, and b_3 generate a packing lattice Λ for $B_3^{1.4}$, then there is no lattice point in $1/2\Lambda$ with $\ell_3^{1.4}$ norm less than one. Thus, we have to check whether there is no lattice point in Λ with $\ell_3^{1.4}$ norm less than 2. If we consider the lattice point $2b_1 - b_2 - b_3$, we obtain

$$\| 2b_1 - b_2 - b_3 \|_{1.4} = \left\| (1.808312, 0.287647, 0.272541)^{\mathsf{T}} \right\|_{1.4} = 1.994\ldots.$$

Since the $\ell_3^{1.4}$ norm of this lattice point is less than two, the vectors b_1, b_2, and b_3 do not generate a packing lattice for $B_3^{1.4}$. This means, their provided vectors does not define a feasible lattice packing. Thus, they claim that they found better lattice packings for the first regime than the O_1 lattice packing, but the only example they state is wrong.

For the first regime, the densities of the O_1 and L_3 lattice packing are given in Table 4.1 and in Figure 4.3. The numerical upper bounds, which are displayed in the table as well as in the figure, are obtained by using the approach described in Section 3.3. As mentioned before, the L_3 lattice gives the best lattice packing over all three cases for the considered values of p in the first regime. In this regime, the upper bounds obtained by using the insphere method, explained in Section 1.1.4, are equal to one. Thus, these upper bounds are not given in Table 4.1 or in Figure 4.3.

p	O_1 packing density	L_3 packing density	Upper bound
1.05	0.92482...	0.92713...	0.93832...
1.1	0.90461...	0.90913...	0.9166...
1.15	0.88686...	0.89305...	0.89843...
1.2	0.87121...	0.87861...	0.8823...
1.25	0.85738...	0.86558...	0.86798...
1.3	0.84516...	0.85375...	0.8553...
1.35	0.83435...	0.84290...	0.84415...
1.4	0.82497...	0.83284...	0.8341...
1.45	0.81674...	0.82330...	0.82517...
1.5	0.80948...	0.81395...	0.8169...
1.55	0.80240...	0.80417...	0.80961...
$\log_2 3$	0.79594...	0.79594...	0.80495...

Table 4.1: Lower bounds given by the O_1 and L_3 lattice packing density. For $p > 1$, numerical upper bounds obtained by the approach explained in Section 3.3.

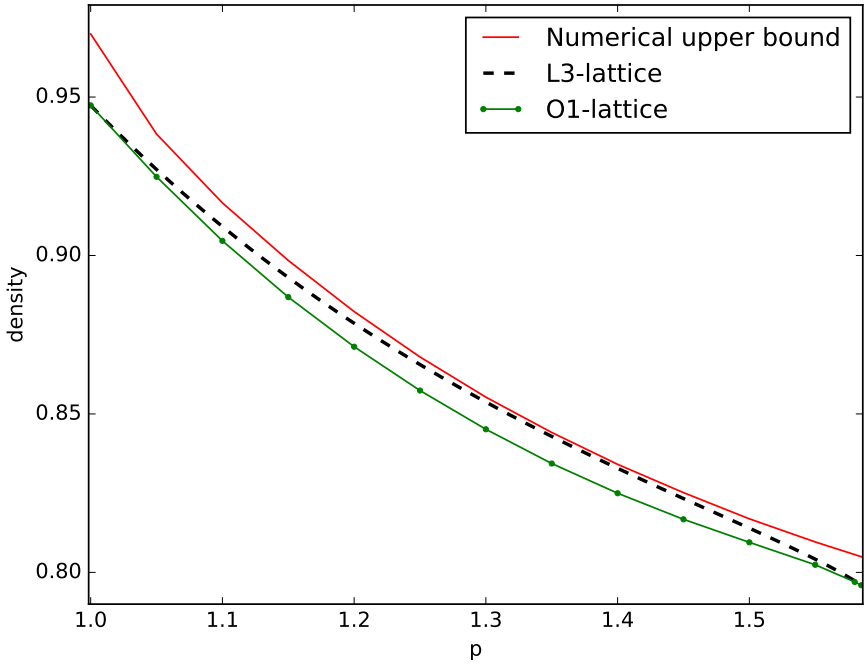


Figure 4.3: O_1 and L_3 lattice packing density, and numerical upper bounds obtained by the approach explained in Section 3.3

4.3.4 Second regime

For $p \in \{1.59, 1.6, \ldots, 2\}$, we searched for locally optimal solutions by using 10,000 random starting vectors $x \in \mathbb{R}^9$ defining a lattice $\Lambda \subset \mathbb{R}^3$. For Case 2 and 3, our computations did not find any solution satisfying the KKT conditions (4.19) – (4.23). This leads to the following conjecture.

Conjecture 4.5. *For $p \in (\log_2 3]$, there exists no locally optimal solution satisfying Case 2 or 3 of Theorem 1.3.*

For Case 1, we found locally optimal solutions. We proved the local optimality of these lattices by checking the KKT conditions as well as the second order condition numerically. Since we did not find any pattern in these lattices, we are not able to describe them as a family of lattices depending on p like the L_3 lattice. In the appendix, we give the basis vectors of the best obtained lattices for $p \in \{1.59, 1.99\}$ and for $p \in \{1.6, 1.65, \ldots, 1.95\}$.

In [53], Jiao, Stillinger, and Torquato provide a family of lattices called O_0 defined as

$$O_0 = \mathbb{Z}\, 2b_1 \oplus \mathbb{Z}\, 2b_2 \oplus \mathbb{Z}\, 2b_3,$$

with

$$b_1 = (1,0,0)\,,\ b_2 = (0,1,0)\,,\ b_3 = \left(\frac{1}{2}, \frac{1}{2}, \left(1 - 2^{1-p}\right)^{1/p}\right).$$

They state that each solid in this lattice has twelve contacting neighbors. Furthermore, they define the regime in which O_0 would be the densest packing by $[\log_2 3, 2]$. Thus, the difference to the regime we consider is that they include the value $\log_2 3$. For $p = \log_2 3$, we do not obtain any locally optimal solution from our calculations for Case 1. Therefore, in this regime we consider $p > \log_2 3$. For $p = \log_2 3$ the basis vectors of the O_0 lattice are

$$2b_1^{\mathsf{T}} = (2,0,0),\ 2b_2^{\mathsf{T}} = (0,2,0),\ 2b_3^{\mathsf{T}} = (1,1,1).$$

For the considered values of p, the basis vectors of the L_3 lattice are

$$2\tilde{b}_1^{\mathsf{T}} = (-1,1,1),\ 2\tilde{b}_2^{\mathsf{T}} = (1-1,1),\ 2\tilde{b}_3^{\mathsf{T}} = (1,1,-1)$$

Since $\tilde{b}_1 = -b_1 + b_3$, $\tilde{b}_2 = -b_2 + b_3$, and $\tilde{b}_3 = b_1 + b_2 - b_3$, the O_0 and L_3 lattice coincides for $p = \log_2 3$. Hence, for $p = \log_2 3$ the O_0 lattice satisfies Case 3 and, thus, the solids in this packing have fourteen contacting neighbors. A part of the packing and some of the contact points are shown in Figure 4.4. The contacting neighbors on the left-hand side correspond to the contact points on the right-hand side, except for the contact point $b_1 + b_2 + b_3$. For that point, we do not show the contacting neighbors, since it would be in front of the centered superball.

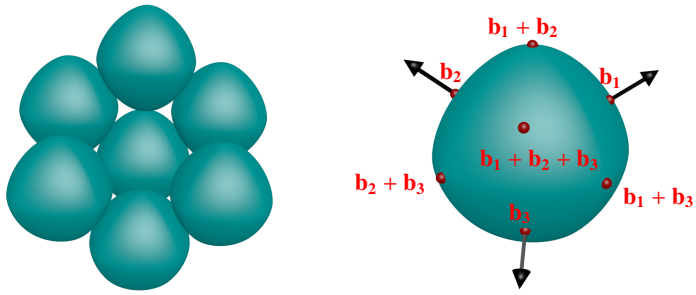


Figure 4.4: Left: A part of a lattice packing for $B_3^{\log_2 3}$ satisfying Case 3 of Theorem 1.3. Right: Seven of twelve contact points of the packing, which is partially pictured on the left-hand side. The contact points are labeled in red.

For $p \in (\log_2 3, 2]$, the O_0 lattice satisfies Case 1. To see this, one has to define the basis vectors by $\tilde{b}_1 = b_1$, $\tilde{b}_2 = b_1 - b_3$, and $\tilde{b}_3 = b_1 + b_2 - b_3$. For $p = \log_2 3$, the lattice point $-\tilde{b}_1 + \tilde{b}_2 + \tilde{b}_3 = -2\left(0, 0, \left((1-2)^{1-p}\right)^{1/p}\right)^{\mathsf{T}}$ is equal to $(0,0,1)^{\mathsf{T}}$. Since this is a point on the boundary of the superball, Case 1 is not satisfied.

In [63], Ni, Gantapara, de Graaf, van Roij, and Dijkstra assert that they found better lattice packings than the O_0 lattice packing for the second regime. They give an example for $p = 1.7$, where they obtained a lattice packing density of 0.7661. Unfortunately, they do not publish the basis vectors defining the corresponding packing lattice. The density of their lattice packing is equal to the best density we computed. However, we determined

better lattice packings than the O_0 lattice packings, except for $p \in \{1.59, 1.6, 2\}$. In these three cases, the lattice packing density we obtained is equal to the density of the O_0 lattice packing. For the second regime, the densities of the O_0 lattice and the best densities we computed, are listed in Table 4.2. The upper bound given in Table 4.2 is for $p \leq 1.8$ obtained by a numerical solution of the approach described in Section 3.3. For $1.85 \leq p < 2$, the upper bound is given by applying the insphere method. Furthermore, for $p = 2$, where the superball is a round ball, the optimal density is known [43]. In this case, the density of the O_0 lattice is

$$\frac{\operatorname{vol} B_3^2}{8(1-2^{1-p})^{1/p}} = \frac{4/3\,\pi}{8/\sqrt{2}} = \frac{\pi}{3\sqrt{2}},$$

which is equal to the optimal density of $\pi/\sqrt{18}$. Furthermore, by our calculations, we obtained the optimal lattice packing density, too.

p	O_0 packing density	New packing density	Upper bound
1.59	0.79418...	0.79418...	0.80432...
1.6	0.79084...	0.79084...	0.80308...
1.65	0.77656...	0.77663...	0.79744...
1.7	0.76567...	0.76610...	0.79262...
1.75	0.75742...	0.75854...	0.78859...
1.8	0.75126...	0.75303...	0.78535...
1.85	0.74677...	0.7488...	0.77942^*...
1.9	0.74364...	0.74550...	0.76574^*...
1.95	0.74161...	0.74277...	0.75278^*...
2	$\pi/\sqrt{18} \approx 0.74048$	$\pi/\sqrt{18}$	$\pi/\sqrt{18}^*$

Table 4.2: O_0 lattice packing density and the new packing density given by the * lattices. Numerical upper bounds for $p \leq 1.8$ obtained by the approach of Section 3.3 are displayed. For $p \in \{1.85, 1.9, 1.95\}$, upper bounds via insphere method, explained in Section 1.1.4, are shown. For $p = 2$, the optimal density is listed. The upper bounds with a star are rigorous bounds.

In Figure 4.5, lower and upper bounds, which are also displayed in Table 4.2, are shown. The * lattices denote the best obtained packing lattices for this regime. One can see that at the beginning and at the end of the regime both lower bounds are equal. The largest improvement of the lower bounds by the * lattices is between $p = 1.8$ and $p = 1.9$. Furthermore, the difference between the new lower bounds and the upper bounds obtained by the calculations of Section 3.3 becomes larger the closer p gets to two. For $p = 2$, our upper bound coincides with the upper bound provided by Cohn and Elkies [19].

Note that in the best computed lattice packing in the previous regime, each solid has fourteen contacting neighbors. However, in this regime, our computer program did not find any locally optimal solution satisfying Case 3 of Theorem 1.3. This means, we did not find

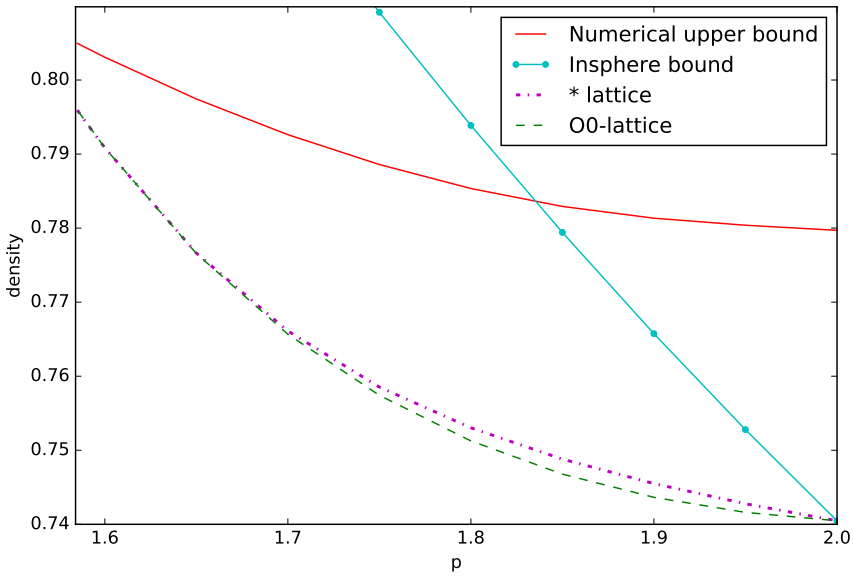


Figure 4.5: Density of the O_0 lattice packing and the new lattice packings defined by the * lattices. Numerical upper bounds obtained from the approach of Section 3.3. Rigorous upper bounds via insphere method, explained in Section 1.1.4.

any locally optimal solution with fourteen contacting neighbors. For $p = 2$, it is known that the maximal number of round balls which can simultaneously touch a ball without pairwise intersection is equal to twelve. This number is called the *kissing number*. For three-dimensional superballs with $p \notin \{1, 2, \infty\}$, we do not know the kissing number.

4.3.5 Third regime

For $p \in \{2, 2.05, \ldots, 2.3\}$ and for $p = 2.3018$, we computed locally optimal lattice packings. The best obtained lattice packings are equal to the lattice packings found by Jiao, Stillinger, and Torquato [53] for this regime. The family of these lattices is defined by

$$C_0 = \mathbb{Z}\, 2b_1 \oplus \mathbb{Z}\, 2b_2 \oplus \mathbb{Z}\, 2b_3$$

with

$$b_1 = \left(2^{-\frac{1}{p}}, 2^{-\frac{1}{p}}, 0\right), \quad b_2 = (0, 0, 1), \quad b_3 = \left(-s, \left(s + 2^{-\frac{1}{p}}\right), \frac{1}{2}\right),$$

where s is the smallest positive root of the equation

$$\left(s + 2^{-\frac{1}{p}}\right)^p + s^p + 2^{-p} - 1 = 0\,.$$

It has density

$$\frac{\operatorname{vol} B_3^p}{2^{3-\frac{1}{p}}\left(2s+2^{-\frac{1}{p}}\right)}.$$

The C_0 lattice packing has twelve contact points

$$\pm b_1,\ \pm b_2,\ \pm b_3,\ \pm(b_1-b_3),\ \pm(b_2-b_3),\ \pm(b_1+b_2-b_3).$$

We define the basis vectors

$$\tilde{b}_1 = b_1 - b_3,\quad \tilde{b}_2 = b_2,\quad \tilde{b}_3 = b_1 + b_2 - b_3,$$

generating the same lattice. Using the new basis vectors, one can easily check that Case 1 of Theorem 1.3 is satisfied. On the left-hand side in Figure 4.6, a round ball B_3^2 is pictured with nine of its twelve contact points in the C_0 lattice packing. There are three contact points in front of the ball, and six contact points around the ball uniformly distributed. Furthermore, there are three contact points behind the ball. In the center of the figure a superball with $p = 2.3018$ is shown from the same perspective with the corresponding nine contact points. For this solid, there are also three further contact points behind the ball. Furthermore, on the right-hand side, we also displayed these contact points for the superball with $p = 6$. From this picture, one can see how the contact points are distributed over the surface of the superball for p tend to infinity.

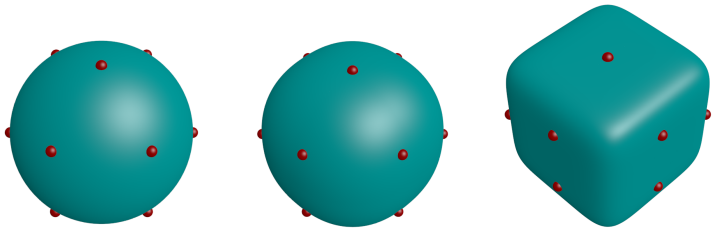


Figure 4.6: Contact points in the C_0 lattice packing for $p = 2$, $p = 2.3018$, and $p = 6$. The contact points are pictured in red.

For $p = 2$, the C_0 lattice packing is equal to the packing shown in Figure 1.3. In this case, the value of s is $\left(1-\frac{1}{\sqrt{2}}\right)/2$, and by calculating the packing density

$$\frac{\operatorname{vol} B_3^2}{2^{2.5}\,(2s+2^{-1/2})} = \frac{4/3\,\pi}{2^{2.5}\,(1+2^{-1/2}+2^{-1/2})} = \frac{\pi}{3\sqrt{2}},$$

we obtain the optimal packing density $\pi/\sqrt{18}$.

For $p = 2.3018$, a superball with six of its twelve contacting neighbors in the C_0 lattice packing is pictured on the left-hand side in Figure 4.7. On the right-hand side nine of twelve contact points of a superball with $p = 2.3018$ are shown. The remaining three contact points $-b_2$, $-(b_2 + b_3)$, and $-(b_1 + b_2 - b_3)$ lie behind the solid. The contacting

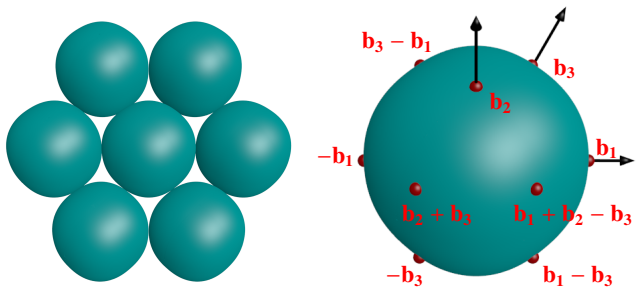


Figure 4.7: Left: A part of the C_0 lattice packing for $p = 2.3018$. Right: Nine of twelve contact points in the C_0 lattice packing for $p = 2.3018$. The contact points are labeled in red.

neighbors on the left-hand side correspond to the contact points $\pm b_1$, $\pm b_3$, and $\pm(b_1 - b_3)$ on the right-hand side.

For the considered values of p, lower bounds given by the C_0 lattice packing are listed in Table 4.3. Furthermore, we compare these lower bounds with the best known upper bounds. For $p \leq 2.1$, we display the upper bounds obtained by using the insphere method. Furthermore, the remaining upper bounds are obtained by numerical results of the approach described in Section 3.3. In Figure 4.8, the computed lower and upper bounds of the third regime are shown.

Lemma 4.6. *The C_0 lattice satisfies the KKT conditions (4.19) – (4.23) for $p \in \mathbb{R}_{>0}$.*

Proof. Let B be a 3×3 matrix with columns equal to the basis vectors $\tilde{b}_1$, $\tilde{b}_2$, and $\tilde{b}_3$. By computing the ℓ_3^p norm of the elements of $\mathcal{U}_B^1$ and $\widetilde{\mathcal{U}}_B^1$, one can easily check that the conditions (4.20) and (4.21) are satisfied. Since we set $\nu^* = (0, 0, 0)$, the conditions (4.22) and (4.23) are satisfied, too. The next task is to check condition (4.19). To do so, we have to find suitable Lagrange multipliers $\mu_1^*, \ldots, \mu_6^*$, such that for $f = \mathcal{L}(x^*, \mu^*, \nu^*)$ the equality

$$\nabla_x \mathcal{L}(x^*, \mu^*, \nu^*) = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_9} \right)^\mathsf{T} = 0$$

holds. Since $|\mathcal{U}_B^1| = 6$, we have to consider six functions p_u:

$$p_1(x) = |x_1|^p + |x_2|^p + |x_3|^p - 1 \tag{4.31}$$
$$p_2(x) = |x_4|^p + |x_5|^p + |x_6|^p - 1 \tag{4.32}$$
$$p_3(x) = |x_7|^p + |x_8|^p + |x_9|^p - 1 \tag{4.33}$$
$$p_4(x) = |x_1 - x_4|^p + |x_2 - x_5|^p + |x_3 - x_6|^p - 1 \tag{4.34}$$
$$p_5(x) = |x_1 - x_7|^p + |x_2 - x_8|^p + |x_3 - x_9|^p - 1 \tag{4.35}$$
$$p_6(x) = |x_4 - x_7|^p + |x_5 - x_8|^p + |x_6 - x_9|^p - 1 \tag{4.36}$$

Furthermore, we have to calculate the partial derivative of the Lagrange function for each variable x_i. Since we are considering the basis vectors $\tilde{b}_1, \tilde{b}_2, \tilde{b}_3$ of a lattice 2Λ, the basis

vectors of Λ have to satisfy the conditions of the optimization problem. Thus, the considered solution is

$$x^* = \left(2^{-1/p} + s, -s, -0.5, 2^{-1/p}, 2^{-1/p}, 0, 2^{-1/p} + s, -s, 0.5\right).$$

Since we have to calculate the derivative of $p_i(x)$ for $i \in [6]$, we express these functions as in (4.17) by using the considered solution x^* in order to get rid of the absolute values. Then, we start with the partial derivative of x_1:

$$\begin{aligned}\frac{\partial f}{\partial x_1} &= \frac{\partial p_0}{\partial x_1} + \mu_1^* p x_1^{*p-1} + \mu_4^* p \left(x_1^* - x_4^*\right)^{p-1} + \mu_5^* p \left(x_1^* - x_7^*\right)^{p-1} \\ &= \frac{\partial p}{\partial x_1} + \mu_1^* p \left(2^{-1/p} + s\right)^{p-1} + \mu_4^* p s^{p-1}\end{aligned}$$

Thus, we have to find Lagrange multipliers such that

$$-\frac{\partial p_0}{\partial x_1} = \mu_1^* p \left(2^{-1/p} + s\right)^{p-1} + \mu_4^* p s^{p-1}$$

Similarly, we compute the remaining partial derivatives of $\mathcal{L}$ and set them equal to zero:

$$\begin{aligned}
-\frac{\partial p_0}{\partial x_2} &= -\mu_4^* p \left(2^{-1/p} + s\right)^{p-1} - \mu_1^*\ p\ s^{p-1} \\
-\frac{\partial p_0}{\partial x_3} &= -\mu_1^* p 2^{1-p} - \mu_4^*\ p\ 2^{1-p} - \mu_5^*\ p \\
-\frac{\partial p_0}{\partial x_4} &= \mu_2^* p 2^{(1-p)/p} - \mu_4^*\ p\ s^{p-1} - \mu_6^*\ p\ s^{p-1} \\
-\frac{\partial p_0}{\partial x_5} &= \mu_2^* p 2^{(1-p)/p} + \mu_4^* p \left(2^{-1/p} + s\right)^{p-1} + \mu_6^* p \left(2^{-1/p} + s\right)^{p-1} \\
-\frac{\partial p_0}{\partial x_6} &= \mu_4^* p 2^{1-p} - \mu_6^* p 2^{1-p} \\
-\frac{\partial p_0}{\partial x_7} &= \mu_3^* p \left(2^{-1/p} + s\right)^{p-1} + \mu_6^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_8} &= -\mu_6^* p \left(2^{-1/p} + s\right)^{p-1} - \mu_3^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_9} &= \mu_3^* p 2^{1-p} + \mu_6^* p 2^{1-p} + \mu_5^* p
\end{aligned}$$

We use the following equalities of the partial derivatives of the objective function $p_0(x^*)$:

$$\frac{\partial p_0}{\partial x_1} = -\frac{\partial p_0}{\partial x_2}, \quad \frac{\partial p_0}{\partial x_6} = 0, \quad \frac{\partial p_0}{\partial x_3} = -\frac{\partial p_0}{\partial x_9}, \quad \frac{\partial p_0}{\partial x_7} = -\frac{\partial p_0}{\partial x_8}, \quad \frac{\partial p_0}{\partial x_5} = 2\frac{\partial p_0}{\partial x_1} + \frac{\partial p_0}{\partial x_4}.$$

Consequently, we obtain the following equations

$$\begin{aligned}
\mu_1^* p\left(2^{-1/p}+s\right)^{p-1} + \mu_4^* p s^{p-1} &= \mu_4^* p\left(2^{-1/p}+s\right)^{p-1} + \mu_1^* p s^{p-1} \\
\mu_4^* p 2^{1-p} - \mu_6^* p 2^{1-p} &= 0 \\
\mu_1^* p 2^{1-p} + \mu_4^* p 2^{1-p} + \mu_5^*\, p &= \mu_3^* p 2^{1-p} + \mu_6^* p 2^{1-p} + \mu_5^* p \\
\mu_3^* p\left(2^{-1/p}+s\right)^{p-1} + \mu_6^* p s^{p-1} &= \mu_6^* p\left(2^{-1/p}+s\right)^{p-1} + \mu_3^* p s^{p-1} \\
\mu_2^* p 2^{(1-p)/p} + \left(\mu_4^*+\mu_6^*\right) p\left(2^{-1/p}+s\right)^{p-1} &= 2\mu_1^* p\left(2^{-1/p}+s\right)^{p-1} + \left(\mu_4^*-\mu_6^*\right) p s^{p-1} + \\
&\qquad \mu_2^* p 2^{(1-p)/p}
\end{aligned}$$

From these equalities we deduce $\mu_1^* = \mu_3^* = \mu_4^* = \mu_6^*$. Then, we define $\alpha = \mu_1^* = \mu_3^* = \mu_4^* = \mu_6^*$, $\beta = \mu_2^*$, and $\delta = \mu_5^*$. Now, the following equalities are left

$$\begin{aligned}
-\frac{\partial p}{\partial x_1} &= ((2^{-1/p}+s)^{p-1} + s^{p-1}) p\alpha \\
\frac{\partial p}{\partial x_3} &= 2\alpha p s^{p-1} - 2^{(1-p)/p} p\beta \\
\frac{\partial p}{\partial x_3} &= 2^{2-p} p\alpha + p\delta
\end{aligned}$$

By using the Lagrange multipliers

$$\mu^* = (\alpha, \beta, \alpha, \alpha, \gamma, \alpha) \text{ and } \nu^* = (0,0,0),$$

with

$$\begin{aligned}
\alpha &= -\frac{\partial p}{\partial x_1} \Big/ \left(\left(\left(2^{-1/p}+s\right)^{p-1} + s^{p-1}\right) p\right) \\
\beta &= \left(2\alpha p s^{p-1} - \frac{\partial p}{\partial x_3}\right) \frac{2^{(p-1)/p}}{p} \\
\delta &= \left(\frac{\partial p}{\partial x_3} - 2^{2-p} p\alpha\right) \frac{1}{p}
\end{aligned}$$

condition (4.19) is satisfied. Since p and s are strictly positive, the denominators in the formula of α, β, and δ are not equal to zero. □

Since our program is based on Minkowski's theorem for convex bodies, we restrict p to be at least one. Although the considered KKT conditions just make sense for $p \geq 1$, the lattice C_0 satisfies them even for $p > 0$.

To check local optimality of the C_0 lattice, we still have to check the second order condition given in (4.27). To do so, we have to compute a matrix M and a vector $\tilde{y}$ suitable for the equation (4.28). Then, the second order condition is satisfied if and only if the eigenvalues of M are strictly positive. For $p \in \{2, 2.05, \ldots, 2.3\}$ and for $p = 2.3018$, we checked this condition numerically. Thus, we have a numerical proof that the C_0 lattice is locally optimal for the considered values of p. The corresponding densities are listed in Table 4.3.

p	C_0 packing density	Upper bound
2	$\pi/\sqrt{18} \approx 0.74048$	$\pi/\sqrt{18}^*$
2.05	$0.74359\ldots$	$0.75867^*\ldots$
2.1	$0.74673\ldots$	$0.77623^*\ldots$
2.15	$0.74991\ldots$	$0.78107\ldots$
2.2	$0.75311\ldots$	$0.78134\ldots$
2.25	$0.75633\ldots$	$0.78423\ldots$
2.3	$0.75954\ldots$	$0.78255\ldots$
2.3018	$0.75968\ldots$	$0.78305\ldots$

Table 4.3: Lattice packing density by the C_0 lattice. For $p = 2$, optimal packing density [43]. For $p < 2.15$, upper bounds via insphere method. For $p \geq 2.15$ numerical upper bounds computed by the approach of Section 3.3. Upper bounds with a star are rigorous bounds.

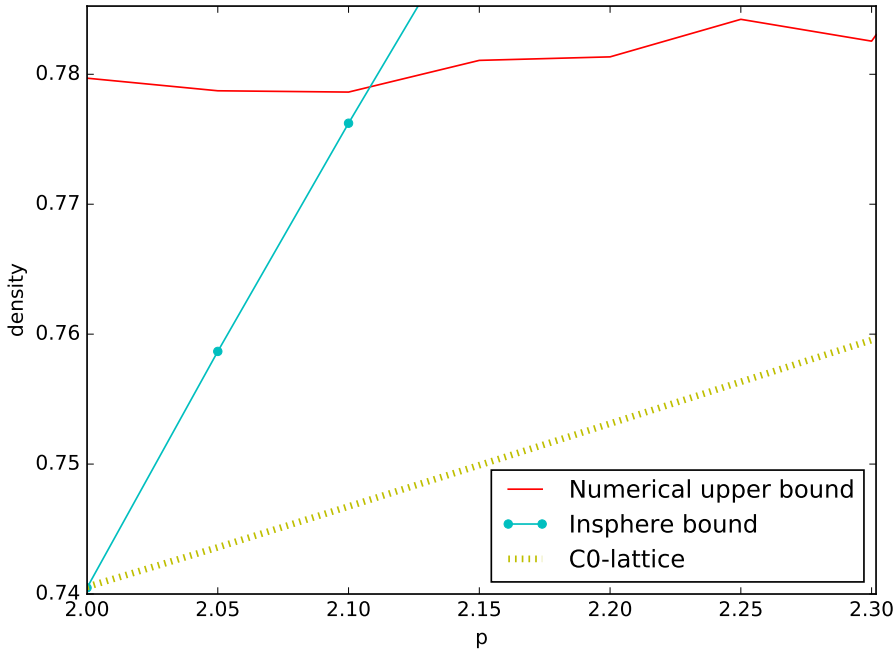


Figure 4.8: Lower bounds given by the C_0 lattice packing. Numerical upper bounds obtained by the approach from Section 3.3. Rigorous upper bounds via insphere method.

4.3.6 Fourth regime

For $p \in \{2.4, 2.5, \dots, 6\}$ and for $p \in \{2.3018, 2.31, 6.5, 7, 7.5, 8\}$, we computed locally optimal lattice packings. For Case 2 and 3, our computer program did not find any locally optimal solution. For Case 1, the best obtained locally optimal lattice is equal to the C_1 lattice given by Jiao, Stillinger, and Torquato [53]. This lattice is defined as

$$C_1 = \mathbb{Z}\, 2b_1 \oplus \mathbb{Z}\, 2b_2 \oplus \mathbb{Z}\, 2b_3$$

with

$$b_1 = \left(2^{-\frac{1}{p}}, 2^{-\frac{1}{p}}, 0\right),\ b_2 = \left(2^{-\frac{1}{p}}, 0, 2^{-\frac{1}{p}}\right),\ b_3 = \left(s + 2^{-\frac{1}{p}}, -s, -s\right),$$

where s is the smallest positive root of the equation

$$(s + 2^{-\frac{1}{p}})^p + 2s^p - 1 = 0.$$

It has density

$$\frac{\operatorname{vol} B_3^p}{2^{3-\frac{2}{p}}\left(3s + 2^{-\frac{1}{p}}\right)}.$$

In this lattice packing each solid has twelve contacting neighbors. For superballs with $p = 2, p = 2.3018$, and for $p = 6$, seven of the twelve contact points in the corresponding C_1 lattice packing are shown in Figure 4.9. These pictures are from the same perspective as in Figure 4.6.

To make the difference between the C_0 and C_1 lattice packing more clear, we show in Figure 4.10 the contact points of B_3^6 for both lattice packings. For the C_0 lattice packing these contact points are displayed on the left-hand side, and for the C_1 lattice packing they are pictured in the center. In the C_1 lattice packing there are more contact points on the *round edges* of the solid than in the C_0 lattice packing. Furthermore, we obtain the picture on the right-hand side in Figure 4.10 by rotating the picture, which is placed in the center. In the picture on the right-hand side, it is easier to see the relation between the contact points and the contacting neighbors in Figure 4.1.

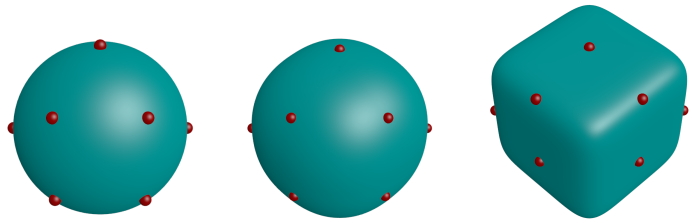


Figure 4.9: Seven of twelve contact points in the C_1 lattice packing for B_3^p with $p = 2$, $p = 2.3018$, and $p = 6$. The contact points are pictured in red.

To prove local optimality of the C_1 lattice, we have to check the KKT conditions.

Lemma 4.7. *The C_1 lattice satisfies the KKT conditions (4.19) – (4.23) for $p \in \mathbb{R}_{>0}$.*

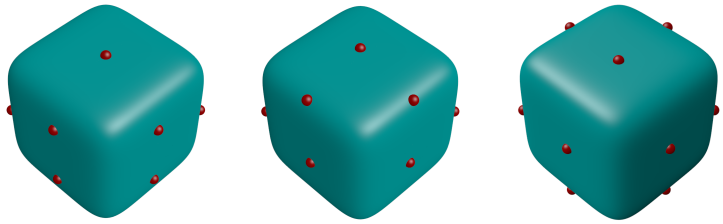


Figure 4.10: Contact points for B_3^6 in the C_0 lattice packing (left-hand side) and in the C_1 lattice packing (center and right-hand side). The superball on the left-hand side and the superball in the center are pictured from the same perspective. The contact points are shown in red.

Proof. The KKT conditions (4.19) – (4.23) are satisfied, if and only if, there exist Lagrange multipliers $\mu_1^*, \dots, \mu_6^*$ and $\nu_1^*, \dots, \nu_3^*$, such that

$$\nabla_x \mathcal{L}(x^*, \mu^*, \nu^*) = \left(\frac{\partial \mathcal{L}}{\partial x_1}, \dots, \frac{\partial \mathcal{L}}{\partial x_9} \right)^\mathsf{T} = 0.$$

Analogously to the proof of the KKT conditions (4.19) – (4.23) for the C_0 lattice, we compute the partial derivatives of $\mathcal{L}(x^*, \mu^*, \nu^*)$ to obtain the following conditions on the Lagrange multipliers:

$$\begin{aligned}
-\frac{\partial p_0}{\partial x_1} &= \mu_1^* p 2^{(1-p)/p} - \mu_5^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_2} &= \mu_1^* p 2^{(1-p)/p} + \mu_4^* p 2^{(1-p)/p} + \mu_5^* p \left(2^{-1/p} + s\right)^{p-1} \\
-\frac{\partial p_0}{\partial x_3} &= -\mu_4^* p 2^{(1-p)/p} + \mu_5^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_4} &= \mu_2^* p 2^{(1-p)/p} - \mu_6^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_5} &= -\mu_4^* p 2^{(1-p)/p} + \mu_6^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_6} &= \mu_2^* p 2^{(1-p)/p} + \mu_4^* p 2^{(1-p)/p} + \mu_6^* p \left(2^{-1/p} + s\right)^{p-1} \\
-\frac{\partial p_0}{\partial x_7} &= \mu_3^* p \left(2^{-1/p} + s\right)^{p-1} + \mu_5^* p s^{p-1} + \mu_6^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_8} &= -\mu_3^* p s^{p-1} - \mu_5^* p \left(2^{-1/p} + s\right)^{p-1} - \mu_6^* p s^{p-1} \\
-\frac{\partial p_0}{\partial x_9} &= -\mu_3^* p s^{p-1} - \mu_5^* p s^{p-1} - \mu_6^* p \left(2^{-1/p} + s\right)^{p-1}
\end{aligned}$$

Furthermore, the following partial derivatives of the objective function $p(x^*)$ coincide:

$$\frac{\partial p_0}{\partial x_1} = \frac{\partial p_0}{\partial x_4}, \quad \frac{\partial p_0}{\partial x_3} = \frac{\partial p_0}{\partial x_5}, \quad \frac{\partial p_0}{\partial x_2} = \frac{\partial p_0}{\partial x_6}, \quad \frac{\partial p_0}{\partial x_7} = -\frac{\partial p_0}{\partial x_8}, \quad \frac{\partial p_0}{\partial x_8} = \frac{\partial p_0}{\partial x_9}.$$

Consequently, we obtain the following equations

$$\begin{aligned}
\mu_1^* p 2^{(1-p)/p} - \mu_5^* p s^{p-1} &= \mu_2^* p 2^{(1-p)/p} - \mu_6^* p s^{p-1} \\
-\mu_4^* p 2^{(1-p)/p} + \mu_5^* p s^{p-1} &= -\mu_4^* p 2^{(1-p)/p} + \mu_6^* p s^{p-1} \\
\left(\mu_1^* + \mu_4^*\right) p 2^{(1-p)/p} + \mu_5^* p \left(2^{-1/p} + s\right)^{p-1} &= \left(\mu_2^* + \mu_4^*\right) p 2^{(1-p)/p} + \mu_6^* p \left(2^{-1/p} + s\right)^{p-1} \\
\mu_3^* p \left(2^{-1/p} + s\right)^{p-1} + \left(\mu_5^* + \mu_6^*\right) p s^{p-1} &= \left(\mu_3^* + \mu_6^*\right) p s^{p-1} + \mu_5^* p \left(2^{-1/p} + s\right)^{p-1} \\
\left(\mu_3^* + \mu_6^*\right) p s^{p-1} + \mu_5^* p \left(2^{-1/p} + s\right)^{p-1} &= \left(\mu_3^* + \mu_5^*\right) p s^{p-1} + \mu_6^* p \left(2^{-1/p} + s\right)^{p-1}
\end{aligned}$$

From these equalities we deduce $\mu_1^* = \mu_2^* = \mu_4^*$ and $\mu_3^* = \mu_5^* = \mu_6^*$. Furthermore, we define $\alpha = \mu_1^* = \mu_2^* = \mu_4^*$ and $\beta = \mu_3^* = \mu_5^* = \mu_6^*$. Now, the following equalities are left

$$\begin{aligned}
-\frac{\partial p_0}{\partial x_1} &= \alpha p 2^{(1-p)/p} - \beta p s^{p-1} \\
-\frac{\partial p_0}{\partial x_7} &= \beta \left(\left(2^{-1/p} + s\right)^{p-1} + 2 p s^{p-1} \right)
\end{aligned}$$

By using the Lagrange multipliers

$$\mu^* = (\alpha, \alpha, \beta, \alpha, \beta, \beta) \text{ and } \nu^* = (0, 0, 0),$$

where

$$\alpha = \frac{2^{\frac{p-1}{p}}}{p} \left(p s^{p-1} \beta - \frac{\partial p_0}{\partial x_1} \right)$$

and

$$\beta = \frac{\partial p_0}{\partial x_7} \frac{1}{2 p s^{p-1} + p (2^{-1/p} + s)^{p-1}}$$

this condition is satisfied. Since p and s are strictly positive, the denominators in the formula of α and β are not equal to zero. □

Analogously to the third regime, the considered lattice satisfies the KKT conditions even for all positive values of p and not just for $p \geq 1$.

To prove local optimality, we have to check the second order condition (4.27). For this, we have to compute a matrix M and a vector $\tilde{y}$ suitable for the equation (4.28). We first compute $\tilde{y}$ and then we compute the matrix M. By evaluating $\nabla p_u(x^*)$, we see that a vector $y \in \mathbb{R}^9$ satisfies the condition $y^\mathsf{T} \nabla p_u(x^*) = 0$ for all $u \in \mathcal{U}_B^1$ if the entries of the vector

$$\begin{pmatrix}
y_1 - y_6 + (a-1)\, y_8 + (a-1)\, y_9 \\
y_2 + y_6 + (1-a)\, y_8 + (1-a)\, y_9 \\
y_3 - \left(1 + \frac{1}{a}\right) y_6 + \left(\frac{1}{a} + a - 1\right) y_9 \\
y_4 + y_6 \\
y_5 + \left(1 + \frac{1}{a}\right) y_6 - (1-a)\, y_8 - \frac{1}{a} x_9 \\
y_7 - a y_8 + a y_9
\end{pmatrix}$$

with $a = \left(\frac{s}{2^{-1/p}+s}\right)^{p-1}$ are equal to zero. Since we can express all elements of y by the monomials y_6, y_8, and y_9, we obtain $\tilde{y} = (x_6, x_8, x_9)$.

Let $T \in \mathbb{R}^{3\times 9}$ be the basis change matrix, such that $\tilde{y} = Ty$. Then we get the matrix M satisfying the equation (4.28), by computing

$$M = T\left(\nabla_x^2 \mathcal{L}(x^*, \mu^*, \nu^*)\right) T^{-1},$$

which is equal to

$$M = 4v^2 M_1 + p(p-1)(M_2 + \beta M_3),$$

with $q = \left(\frac{s}{v+s}\right)^{p-1}$ and

$$M_1 = 3s^2 \begin{pmatrix} \left(2+\frac{1}{q}\right)^2 & \left(2+\frac{1}{q}\right)(q-1) & \left(q-\frac{1}{q}\right)\left(2+\frac{1}{q}\right) \\ \left(2+\frac{1}{q}\right)(q-1) & (q-1)^2 & (q-1)\left(q-\frac{1}{q}\right) \\ \left(q-\frac{1}{q}\right)\left(2+\frac{1}{q}\right) & (q-1)\left(q-\frac{1}{q}\right) & \left(q-\frac{1}{q}\right)^2 \end{pmatrix}$$
$$+sv \begin{pmatrix} 2\left(2+\frac{5}{q}+\frac{2}{q^2}\right) & 2q-1-\frac{1}{q} & 2q+7-\frac{5}{q}-\frac{4}{q^2} \\ 2q-1-\frac{1}{q} & 2\left(2-q-q^2\right) & \frac{1}{q}-1+2q-2q^2 \\ 2q+7-\frac{5}{q}-\frac{4}{q^2} & \frac{1}{q}-1+2q-2q^2 & 6q-2q^2-8+\frac{4}{q^2} \end{pmatrix}$$
$$+v^2 \begin{pmatrix} \frac{2}{q}+\frac{1}{q^2} & 0 & 2-\frac{1}{q}-\frac{1}{q^2} \\ 0 & 1-q^2 & q-q^2 \\ 2-\frac{1}{q}-\frac{1}{q^2} & q-q^2 & 2q-q^2-2+\frac{1}{q^2} \end{pmatrix},$$

$$M_2 = \frac{\alpha}{v^2} \begin{pmatrix} \frac{1}{q^2}+2 & q-1 & q-\frac{1}{q^2}+\frac{1}{q}-1 \\ q-1 & (q-1)^2 & (q-1)^2 \\ q-\frac{1}{q^2}+\frac{1}{q}-1 & (q-1)^2 & q^2-2q+2+\frac{1}{q^2}-\frac{2}{q} \end{pmatrix},$$

$$M_3 = (v+s)^{p-2} \begin{pmatrix} 2 & q & q-2 \\ q & 2q^2 & q(2q-1) \\ q-2 & q(2q-1) & 2\left(q^2-q+1\right) \end{pmatrix}$$
$$+2s^{p-2} \begin{pmatrix} 2\left(2+\frac{2}{q}+\frac{1}{q^2}\right) & 2q & 2\left(q-\frac{1}{q}-\frac{1}{q^2}\right) \\ 2q & 2\left(q^2+1\right) & 2q^2 \\ 2\left(q-\frac{1}{q}-\frac{1}{q^2}\right) & 2q^2 & 2\left(q^2+\frac{1}{q^2}\right) \end{pmatrix}.$$

For $p \in \{2.3018, 2.31\}$ and for $p \in \{2.3, 2.4, \ldots, 8\}$, we numerically proved that the matrix M is positive definite. For this, we checked whether their eigenvalues are strictly positive. For some values of p, the eigenvalues of M are displayed in Table 4.4.

p	Eigenvalues of M		
2.3	88.9...	0.16182...	0.32707...
2.5	175.2...	0.17046...	0.38883...
3	1477.7...	0.33113...	0.83038...
3.5	16976.4...	0.54260...	1.32512...
4	216469.6...	0.68213...	1.61308...
6	14694858160.5...	0.76898...	1.71202...
8	4463545021899008.0...	0.88388...	1.57882...

Table 4.4: Eigenvalues of M for some values of p.

From the positive definiteness, we can conclude the local optimality of C_1 for the considered values of p.

Furthermore, we computed the C_1 lattice packing density for $p \in \{2.4, 2.5, \ldots, 6\}$ and for $p \in \{2.3018, 2.31, 6.5, 7, 7.5, 8\}$. Some of these results are listed in Table 4.5. The computed lower bounds as well as the numerical upper bounds are pictured in Figure 4.11. The upper bound obtained via insphere method is equal to one for this regime. Thus, these upper bounds are not displayed in Table 4.5 or in Figure 4.11.

p	C_1 packing density	Upper bound
2.3018	0.7596...	0.7830...
3	0.8095...	0.8236*...
4	0.8698...	0.8742*...
5	0.9080...	0.9224*...
6	0.9318...	0.9338*...
7	0.9474...	0.9504...
8	0.9582...	0.9619...

Table 4.5: Lower bounds given by the C_1 lattice packing density and numerical upper bounds obtained by the approach from Section 3.3. The upper bounds with a star are rigorous.

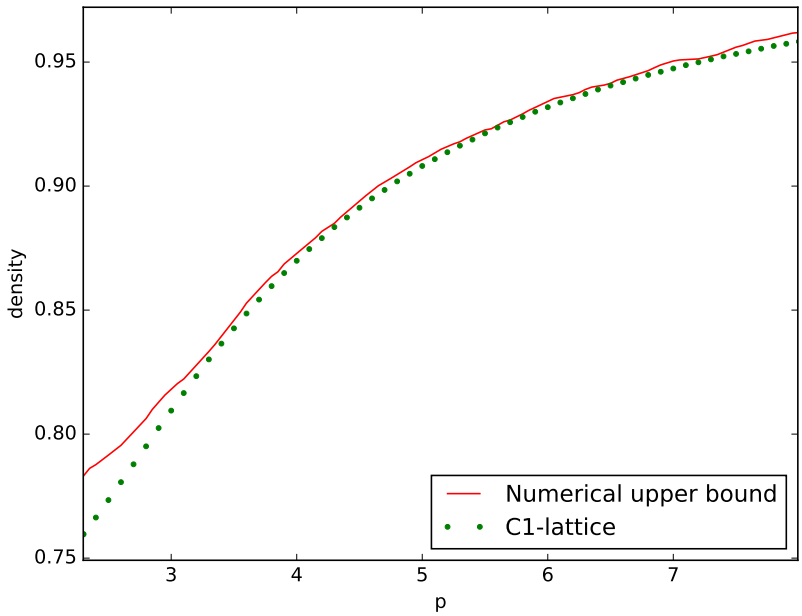


Figure 4.11: Density of the C_1 lattice packings. Numerical upper bounds obtained from the approach in Section 3.3.

4.4 Summary and outlook

For each of the four regimes, we computed feasible packing lattices by using Newton's method. For each of these lattices, we proved local optimality. This proof is divided into two parts: first we have to check the KKT conditions, and then, we have to ensure that the second order condition is satisfied. In Figure 4.6, we display the best obtained locally optimal lattices for each regime, as well as information which parts of these proofs are numerically and which are rigorous. For the best obtained packing lattices in the second regime, we did not find any pattern. For $p \in (1,2) \setminus [\log_2 3, 1.6]$, we improved the best known lattice packing density provided by Jiao, Stillinger, and Torquato [53].

The L_3 lattice is the best obtained packing lattice for the considered values of $p \in [1, \log_2 3]$ and thus, it gives a better lattice packing density than the O_1 lattice found by Jiao, Stillinger, and Torquato [53]. One can probably show that this holds for all values of p in the first regime.

Conjecture 4.8. *The L_3 lattice packing density is higher than the O_1 lattice packing density for all $p \in [1, \log_2 3]$.*

Furthermore, we proved local optimality of the best obtained lattices numerically. For the C_0 and C_1 lattice we also give a rigorous proof of the KKT conditions, but checking

Regime of p	Best obtained packing lattice	Proof of KKT conditions	Proof of second order condition
$[1, \log_2 3]$	L_3	numerical	numerical
$(\log_2 3, 2]$	*	numerical	numerical
$[2, 2.3018\ldots]$	C_0	rigorous	numerical
$[2.3018\ldots, 8]$	C_1	rigorous	numerical

Table 4.6: Locally optimal lattice packings for superballs with $p \in [1, 8]$.

the second order condition seems to be more complicated. For the L_3 lattice it should be easier since the matrix which we have to check for positive definiteness is a symmetric two dimensional matrix, not as in the other cases in which it is three dimensional. Thus, one would have to prove that the entries and the determinant are strictly positive.

Conjecture 4.9. *L_3, C_0, and C_1 are indeed locally optimal packing lattices for superballs with p in the corresponding regime.*

The best obtained lattice packing density is close to our upper bound, especially in the first and last regime. If we can improve the upper bound, for example by increasing the considered degree d or by determining better sample methods, we might be able to prove optimality of the best obtained lattice packing for some values of p. Maybe there is a better way to check the nonpositivity condition in the bounded part than using sample points.

Conjecture 4.10. *L_3 is optimal for the first regime and C_1 for the last regime.*

Assume we are able to improve the upper bound for some values of p in the first and last regime in such a way that they coincide with our lower bound. Then, we would not just have proven optimality for these packing lattices, we also would have obtained the optimal translative packing density. The lower bounds for the lattice packing densities are remarkably close to the upper bounds for the translative packing densities, especially in the first and last regime. Thus, it seems that for at least some values of p the optimal lattice packing density coincides with the optimal translative packing density. Even for $p = 2$, where the difference between the lower and upper bound reach their maximum, it is proven that the best optimal lattice packing density coincides with the optimal translative packing density.

Problem 4.11. *For which superballs is the optimal lattice packing density equal to the optimal translative packing density?*

In our calculations we did not find any locally optimal packing lattice for the second, third, and forth regime satisfying Case 2 or Case 3 of Theorem 1.3. Furthermore, our computer program did not even find any packing lattice satisfying the KKT conditions for these two cases unless $p \leq \log_2 3$. Thus, this leads to the question, whether there exists any locally optimal solution for these two cases by considering $p > \log_2 3$.

Conjecture 4.12. *For $p > \log_2 3$, there exist no locally optimal packing lattice satisfying Case 2 or 3 of Theorem 1.3.*

If we find a way to solve the optimization problem (4.8) – (4.11) in practice, we could determine optimal lattice packings for three-dimensional superballs with $p \geq 1$. Since for larger values of i and j, the SOS relaxation of (4.8) – (4.11) is too large for current SDP solvers, one has probably to find a way to use symmetries for simplifying the program.

Problem 4.13. *Determining optimal lattice packings for superballs.*

Appendix

For $p \in \{1.6, 1.65, \ldots, 1.95\}$ and for $p \in \{1.59, 1.99\}$, the basis vectors of the best obtained lattice packings are displayed in the following tables. Each matrix represents a lattice in the form that its columns contain the corresponding basis vectors.

p	Basis matrices
1.59	$\begin{pmatrix} 0.499926470 & 0.50004973 & 0.99999959 \\ -0.500073118 & 0.49992647 & -0.00012326 \\ 0.503293851 & 0.50331714 & 0.00002329 \end{pmatrix}$
1.6	$\begin{pmatrix} 0.00144215 & 0.50057269 & -0.49940825 \\ 0.99998095 & 0.49940851 & 0.50085062 \\ -0.00027473 & 0.50978394 & 0.50950921 \end{pmatrix}$
1.65	$\begin{pmatrix} 0.9979212 & 0.51754606 & 0.48675064 \\ 0.0061634 & -0.5425021 & -0.53633836 \\ 0.03077145 & -0.48025521 & 0.51766348 \end{pmatrix}$, $\begin{pmatrix} 0.03079542 & 0.51754606 & -0.48037515 \\ 0.99791869 & 0.48025521 & 0.51102666 \\ 0.00616374 & 0.5425021 & 0.5486655 \end{pmatrix}$
1.7	$\begin{pmatrix} -0.43562497 & -0.52902864 & -0.98867247 \\ 0.57701813 & 0.59729026 & 0.0202829 \\ 0.55171075 & -0.43701488 & 0.09367698 \end{pmatrix}$

Table 4.7: Locally optimal lattices

p	Basis matrices
1.75	$\begin{pmatrix} 0.42758357 & 0.59733183 & 0.97168858 \\ -0.61032918 & -0.57021722 & 0.04019376 \\ -0.55107367 & 0.42092518 & -0.17086613 \end{pmatrix}$, $\begin{pmatrix} 0.37435675 & -0.16974826 & -0.59733183 \\ 0.61041098 & -0.04011196 & 0.57021722 \\ -0.59179131 & -0.97199885 & -0.42092518 \end{pmatrix}$, $\begin{pmatrix} 0.38020754 & 0.97199885 & 0.55107367 \\ -0.54410501 & -0.16974826 & 0.42758357 \\ 0.65052294 & 0.04011196 & 0.61032918 \end{pmatrix}$
1.8	$\begin{pmatrix} -0.05881466 & 0.5790554 & 0.63758048 \\ -0.2373794 & 0.38728256 & -0.56758784 \\ -0.95402774 & -0.63746795 & -0.40256933 \end{pmatrix}$, $\begin{pmatrix} -0.33020844 & -0.56758784 & -0.9548704 \\ 0.55145841 & -0.40256933 & 0.23489862 \\ -0.69639514 & -0.63758048 & -0.05852508 \end{pmatrix}$, $\begin{pmatrix} 0.9548704 & 0.38728256 & 0.62466196 \\ 0.23489862 & 0.63746795 & -0.3165598 \\ -0.05852508 & 0.5790554 & 0.63787006 \end{pmatrix}$
1.85	$\begin{pmatrix} -0.58601804 & 0.0725444 & -0.65924243 \\ 0.35956556 & 0.94126075 & 0.64870975 \\ 0.67038117 & 0.28514582 & -0.2693437 \end{pmatrix}$, $\begin{pmatrix} 0.29255099 & -0.64870975 & -0.28914419 \\ -0.55448952 & -0.2693437 & -0.93972488 \\ 0.73178683 & 0.65924243 & 0.07322439 \end{pmatrix}$, $\begin{pmatrix} -0.58169518 & -0.28914418 & 0.35956557 \\ 0.38523536 & 0.93972488 & 0.67038117 \\ 0.65856244 & -0.07322439 & 0.58601804 \end{pmatrix}$

Table 4.8: Locally optimal lattices

p	Basis matrices
1.9	$\begin{pmatrix} -0.08288738 & 0.67623115 & 0.59207566 \\ 0.32536621 & -0.2306987 & 0.6978566 \\ -0.93086763 & -0.6666684 & -0.33576866 \end{pmatrix}$, $\begin{pmatrix} 0.26419923 & 0.59509897 & 0.93086763 \\ 0.75911852 & 0.67496304 & 0.08288738 \\ 0.55606491 & -0.37249039 & 0.32536621 \end{pmatrix}$, $\begin{pmatrix} 0.59207566 & -0.08415549 & 0.67496304 \\ 0.6978566 & 0.9285553 & 0.37249039 \\ -0.33576866 & 0.33089973 & 0.59509897 \end{pmatrix}$
1.95	$\begin{pmatrix} 0.09275833 & 0.78084097 & 0.69012658 \\ 0.36647539 & -0.2420198 & 0.6806764 \\ 0.91953165 & 0.55732048 & 0.19795805 \end{pmatrix}$, $\begin{pmatrix} -0.72157359 & -0.35936243 & 0.19795805 \\ -0.314201 & -0.9226962 & -0.6806764 \\ -0.59736824 & 0.0907144 & -0.69012658 \end{pmatrix}$
1.99	$\begin{pmatrix} -0.55836637 & -0.38359316 & 0.35495499 \\ 0.22729804 & 0.91723813 & 0.61935069 \\ 0.79531069 & 0.09575527 & 0.69677868 \end{pmatrix}$

Table 4.9: Locally optimal lattices

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Publication list

In preparation

- *Local optimal lattice packing for three-dimensional superballs.* Maria Dostert, Cristóbal Guzmán, Frank Vallentin

Research article

- *New upper bounds for the density of translative packings of three-dimensional convex bodies with tetrahedral symmetry.* Maria Dostert, Cristóbal Guzmán, Fernando Mário de Oliveira, Frank Vallentin, 30 pages, accepted in Discrete & Computational Geometry 2017, http://arxiv.org/abs/1510.02331

- *A Complexity Analysis and an Algorithmic Approach to Student Sectioning in Existing Timetables* Maria Dostert, Andreas Politz, Heinz Schmitz, April 2015, 9 pages, Journal of Scheduling, Springer, http://link.springer.com/article/10.1007%2Fs10951-015-0424-2

Surveys

- *Das Problem der Kugelpackung (in German).* Maria Dostert, Stefan Krupp, Jan Rolfes, Snapshot of modern mathematics from Oberwolfach, April 2016, 12 pages, https://imaginary.org/snapshot/das-problem-der-kugelpackung

Extended Abstracts

- *New upper bounds for the density of translative packings of superballs.* Maria Dostert, page 58-60, February 2016, Oberwolfach Report 3/2016

- *Die parametrisierte Komplexität des Student Sectioning Problems (in German).* Maria Dostert, March 2013, page 15-18, GI-Edition Lecture Notes in Informatics http://subs.emis.de/LNI/Seminar/Seminar12/S-12.pdf

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Ich versichere, dass ich die von mir vorgelegte Dissertation selbständig angefertigt, die benutzten Quellen und Hilfsmittel vollständig angegeben und die Stellen der Arbeit - einschließlich Tabellen, Karten und Abbildungen -, die anderen Werken im Wortlaut oder dem Sinn nach entnommen sind, in jedem Einzelfall als Entlehnung kenntlich gemacht habe; dass diese Dissertation noch keiner anderen Fakultät oder Universität zur Prüfung vorgelegen hat; dass sie - abgesehen von unten angegebenen Teilpublikationen - noch nicht veröffentlicht worden ist sowie, dass ich eine solche Veröffentlichung vor Abschluss des Promotionsverfahrens nicht vornehmen werde. Die Bestimmungen der Promotionsordnung sind mir bekannt. Die von mir vorgelegte Dissertation ist von Prof. Dr. Frank Vallentin betreut worden.

Maria Margarethe Dostert

Teilpublikationen:

- *New upper bounds for the density of translative packings of three-dimensional convex bodies with tetrahedral symmetry.* Maria Dostert, Cristóbal Guzmán, Fernando Mário de Oliveira, Frank Vallentin, 30 pages, Discrete & Computational Geometry 2017, http://arxiv.org/abs/1510.02331
- *Das Problem der Kugelpackung (in German).* Maria Dostert, Stefan Krupp, Jan Rolfes, Snapshot of modern mathematics from Oberwolfach, April 2016, 12 pages, https://imaginary.org/snapshot/das-problem-der-kugelpackung
- *New upper bounds for the density of translative packings of superballs.* Maria Dostert, page 58-60, February 2016, Oberwolfach Report 3/2016

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