1. Introduction

During the last few years several new results on packing problems were obtained using a blend of tools from semidefinite optimization, polynomial optimization, and harmonic analysis. Schrijver [19] used semidefinite optimization and the Terwilliger algebra to obtain new upper bounds for binary codes, Bachoc and Vallentin [2] used semidefinite optimization and spherical harmonics for spherical codes, and Cohn and Elkies [5] used linear optimization and Fourier analysis for sphere packings leading to the breakthrough result of Cohn and Kumar [6], who proved that the Leech lattice in dimension 24 gives the best lattice sphere packing in its dimension. De Laat, Oliveira and Vallentin [13] generalized the approach of Cohn and Elkies to provide upper bounds for maximal densities of packings of spheres having different radii. The most recent extension is by Oliveira and Vallentin [17], providing new upper bounds for the density of packings of congruent copies of a given convex body.

Typical in all this work is the use of semidefinite optimization and harmonic analysis which gives newcomers to the field — often overwhelmed with technical details — a hard time. Also typical is that the computational challenge grows dramatically if one goes from compact spaces, like binary Hamming space or the sphere, to non-compact spaces like the Euclidean space.

Our goal in this paper is to provide an introduction to this topic in an attempt to paint the big picture without losing essential detail. The paper is however not meant as a survey on results about geometric packing problems — this task would easily fill books! For a first orientation we refer the interested reader to the now classical book by Conway and Sloane [7].

2. Some history

The sphere packing problem asks: How much of three-dimensional space can be filled with pairwise nonoverlapping translates of unit spheres? It was considered by Johannes Kepler (1571–1630) in his work *Strena seu de Nive Sexangula* (On the Six-Cornered Snowflake) from 1611, which was his New Year’s gift to his friend and supporter Johann Matthäus Wacker von Wackenfels (1550–1619). He explains the formation of snowflakes into crystals having sixfold symmetry by drawing an analogy to dense sphere packings which possess the same kind of symmetry. The general acceptance of atomism was yet to come, so this explanation was a remarkable achievement. Kepler’s work is the first scientific writing about crystal formation; in it he claims (essentially without any justification) that a specific periodic structure, the face-centered cubic lattice, describes the densest sphere packing having density $\pi/\sqrt{18} = 0.74\ldots$. This claim is now called Kepler’s conjecture.

In 1998 Thomas Hales proved Kepler’s conjecture; his proof makes heavy use of computers and in 2009 he, together with his student Samuel P. Ferguson, was rewarded the Fulkerson Prize for his work.
The sphere packing problem, and more generally the problem of packing copies of a given body, was also considered by David Hilbert. He mentions it as part of his 18th problem:

18. Building up of Space from Congruent Polyhedra

(...) I point out the following question, related to the preceding one, and important to number theory and perhaps sometimes useful to physics and chemistry: How can one arrange most densely in space an infinite number of equal solids of given form, e.g., spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

The problem of packing congruent copies of regular tetrahedra, mentioned by Hilbert, goes back to Aristotle’s (384–322 BC) refutation of a theory of Plato (428–348 BC), presented in the *Timaeus*, that claimed that each of the four elements had a specific shape, namely one of the Platonic solids, and that the properties of each element derived from its shape. So, for instance, earth, the most stable and plastic element, is cubic in shape, and fire, the acutest and most penetrating, has the shape of a tetrahedron.

Aristotle presents several arguments against this theory in his treatise *De Caelo*. In one of his arguments (cf. *De Caelo*, Book III, Chapter VIII), he claims that it is irrational to assign geometrical shapes to the four elements, since not all of space can be thus filled. Indeed, says Aristotle, only the cube and the pyramid (i.e., the regular tetrahedron) can fill space. So Aristotle’s argument uses the idea of the impossibility of a vacuum, together with the fact that only two of the solids (corresponding to earth and fire) can fill the whole of space, to refute Plato’s theory.

Aristotle’s claim that one can tile space with tetrahedra was picked up by many of his commentators. Simplicius of Cilicia (c. 490–c. 560), one of the main commentators of Aristotle in late Antiquity, even states that, as eight cubes are sufficient to fill the space around a given point, so are twelve regular tetrahedra (cf. page 42 in the translation by Mueller [20]).

In the Middle Ages, Aristotle’s Arabic commentator, Averroës (1126–1198), restates the claim that twelve pyramids fill the space around a point and gives an argument for it. Three planes meet at the vertex of a cube, forming a so-called “solid angle” composed of three right angles. Eight cubes fill the space around a point in three-dimensional space, and these eight solid angles add up to a total of $8 \times 3$ right angles. Now, a solid angle of a tetrahedron is composed of three angles of $60^\circ$ each, totaling two right angles. Since one needs $8 \times 3$ right angles to fill the space around a point (as can be seen from the cubes), and since $8 \times 3 = 12 \times 2$, it follows that twelve tetrahedra fill the space around a point.

Averroës’ commentary introduced the problem to the medieval schoolmen. Roger Bacon (c. 1214–1294) defended Averroës’ position against the claim that not twelve, but twenty tetrahedra are needed to fill the space around a point. Thomas Bradwardine (c. 1290–1349) disproved Averroës’ claim with a very simple argument: If indeed it would be possible to place twelve regular tetrahedra around a point in such a way that no empty space results, then in addition to the five Platonic solids, one would have another one, what is impossible. According to him, those who argue that twenty tetrahedra can be placed around a point have therefore a stronger position, since one can obtain twenty pyramids by joining the bases of a regular icosahedron to its center. Bradwardine observes that it is still necessary to check whether the pyramids so obtained are regular or not, but he leaves the question open (these pyramids are, as can be shown using the construction of the icosahedron given in the thirteenth book of Euclid’s Elements, not regular).
The question was finally settled, it is believed, by Johannes Müller von Königsberg (1436–1476), known as Regiomontanus, who proved that it is impossible to tile space with regular tetrahedra. Of Regiomontanus’ manuscript only the title, describing the contents of the work, has been preserved, but there is no doubt he had all the tools at his disposal to settle the problem. Francesco Maurolico (1494–1575) computed the angle between two faces of a regular tetrahedron. This angle, equal to \( \arccos\left(\frac{1}{3}\right) \approx 70.52877^\circ \), is greater than 60° and smaller than 72°, and hence it follows that one cannot tile space with tetrahedra. Maurolico’s work has been recently rediscovered (see Addabbo [1]). For more on the fascinating history of the tetrahedra packing problem, including all the details presented here, see the historical survey by Struik [21] and the survey by Lagarias and Zong [14].

If one cannot tile space with regular tetrahedra, how much of space can be filled with them? Even today, the problem is far from being solved. In 2006, Conway and Torquato [8] found surprisingly dense packings of tetrahedra. This sparked renewed interest in the problem and a race for the best construction (cf. Lagarias and Zong [14] and Ziegler [23]). The current record is held by Chen, Engel, and Glotzer [4], who found in 2010 a packing with density \( \approx 0.8563 \), a much larger fraction of space than that which can be covered by spheres. This prompted the quest for upper bounds; the current record rests with Gravel, Elser, and Kallus [10], who proved an upper bound of \( 1 - 2.6 \cdot 10^{-25} \). They are themselves convinced that the bound can be greatly improved:

In fact, we conjecture that the optimal packing density corresponds to a value of \( \delta \) [the fraction of empty space] many orders of magnitude larger than the one presented here. We propose as a challenge the task of finding an upper bound with a significantly larger value of \( \delta \) (e.g., \( \delta > 0.01 \)) and the development of practical computational methods for establishing informative upper bounds.

3. Mathematical Modeling

How can one model mathematically the problem of packing spheres or regular tetrahedra in \( \mathbb{R}^3 \)? Packing problems are optimization problems and can be seen as infinite analogues of a well-known problem in combinatorial optimization, namely the problem of finding a maximum-weight independent set in a graph. To see this, let us first consider two kinds of packing problems.

**Problem 1** (Translational body packings). Given convex bodies \( K_1, \ldots, K_N \subseteq \mathbb{R}^n \), how much of \( \mathbb{R}^n \) can be filled with pairwise nonoverlapping translated copies of \( K_1, \ldots, K_N \)?

The sphere packing problem is then obtained by taking \( N = 1 \) and letting \( K_1 \) be the unit ball.

**Problem 2** (Congruent body packings). Given a convex body \( K \subseteq \mathbb{R}^n \), how much of \( \mathbb{R}^n \) can be filled with pairwise nonoverlapping congruent (i.e., translated and rotated) copies of \( K \)?

Here letting \( K \) be the unit ball gives the sphere packing problem, and letting \( K \) be the regular tetrahedron gives the tetrahedra packing problem. In a sense, Problem [2] is a limiting case of Problem [1]. Given a convex body \( K \) one tries to pack translatable copies of infinitely many rotations \( AK \) of \( K \), where \( A \in SO(n) \) and \( SO(n) \) is the special orthogonal group of \( \mathbb{R}^n \) (i.e., the group of all orthogonal \( n \times n \) matrices with determinant 1).

We call a union of nonoverlapping (congruent or translated) copies of some bodies a *packing* of these bodies. In a packing bodies are allowed to touch on their
boundaries but not to intersect in their interiors. The fraction of space covered by a packing is its density, so our goal is to find the maximum density of packings. Here we are using an informal definition of density; later in Section 6 we will give a precise definition.

Let $G = (V, E)$ be a graph, finite or infinite. An independent set is a set $I \subseteq V$ that does not contain adjacent vertices. Packings of bodies can be seen as independent sets in some specially defined graphs called packing graphs. Given convex bodies $K_1, \ldots, K_N \subseteq \mathbb{R}^n$, the translational packing graph of $K_1, \ldots, K_N$ is the graph $G$ whose vertex set is $\{1, \ldots, N\} \times \mathbb{R}^n$. The vertices of $G$ correspond to possible choices of bodies in the packing: vertex $(i, x)$ corresponds to placing the body $x + K_i$ in the packing. This interpretation defines the adjacency relation of $G$: vertices $(i, x)$ and $(j, y)$ are adjacent if the corresponding bodies overlap, i.e., if

$$(x + K_i) \cap (y + K_j) \neq \emptyset,$$

where $A^\circ$ is the interior of set $A$. So independent sets of $G$ correspond to packings of translated copies of $K_1, \ldots, K_N$ and vice versa.

A similar idea can be used regarding packings of congruent copies of a given convex body $K$. Given such a body, we consider its congruent packing graph, which is the graph $G$ whose vertex set is $\text{SO}(n) \times \mathbb{R}^n$. The elements of $\text{SO}(n)$ correspond to the possible rotations of $K$, so that a vertex $(A, x)$ of $G$ corresponds to placing the body $x + AK$ in the packing. Again, this gives the adjacency relation of $G$: vertices $(A, x)$ and $(B, y)$ are adjacent if

$$(x + AK) \cap (y + BK) \neq \emptyset.$$

With this, independent sets of $G$ correspond to packings of congruent copies of $K$ and vice versa.

Packings therefore correspond to independent sets of the packing graph. If we measure the weight of an independent set by the density of the associated packing, then Problems 1 and 2 ask us to find maximum-weight independent sets in the corresponding packing graphs.

Does this modeling help? Finding a maximum cardinality independent set in a finite graph is a well-known NP-hard problem, figuring in Karp’s list of 21 problems. Many techniques have been developed in combinatorial optimization to deal with hard problems: the basic approach is that one tries to develop efficient methods to find lower and upper bounds. In the case of the maximum-cardinality independent set problem, lower bounds are constructive and come from heuristics that try to find independent sets of large size. Analogously, for packing problems one has the adaptive shrinking cell scheme of Torquato and Jiao [22], which can successfully generate dense packings.

As for upper bounds, Lovász [16] introduced a graph parameter, the theta number, that provides an upper bound for the maximum cardinality of independent sets of a finite graph; Lovász’s theta number can moreover be computed efficiently using semidefinite optimization. The most successful approaches to obtain upper bounds for the maximum densities of packings all use extensions of the theta number. The theta number can be quite naturally extended to graphs having compact vertex sets, as we show in Section 4; still, this extension cannot be applied to the packing graphs we described above, because they have noncompact vertex sets. These graphs can be compactified, however, as we discuss in Section 6 and then the extension of the theta number can be applied.
4. The Lovász theta number and an extension

The **independence number** of a graph $G = (V, E)$ (finite or infinite) is the graph parameter

\[
\alpha(G) = \max \{|I| : I \text{ is independent}\}.
\]

Given a nonnegative weight function $w: V \to \mathbb{R}_+$, one may also define the **weighted independence number** of $G$ as

\[
\alpha_w(G) = \max \{w(I) : I \text{ is independent}\},
\]

where $w(I) = \sum_{x \in I} w(x)$. Weights will be useful in packing problems because, when we want to pack different kinds of bodies, like spheres having different radii, the weight function allows us to distinguish between big and small bodies.

The theta number introduced by Lovász [16] provides an upper bound to the independence number of a graph. It was later strengthened and extended to the weighted case by Grötschel, Lovász, and Schrijver [11]. There are many equivalent ways of defining their graph parameter; the one most convenient for us is the following. Given a finite graph $G = (V, E)$ and a weight function $w: V \to \mathbb{R}_+$, we define

\[
\vartheta'_w(G) = \min M
\]

\[
\begin{align*}
K(x, x) &\leq M \quad \text{for all } x \in V, \\
K(x, y) &\leq 0 \quad \text{for all } \{x, y\} \not\in E \text{ with } x \neq y, \\
K &\in \mathbb{R}^{V \times V} \text{ is symmetric,} \\
K - (w^{1/2})(w^{1/2})^T &\text{ is positive semidefinite,}
\end{align*}
\]

where $w^{1/2} \in \mathbb{R}^V$ is such that $w^{1/2}(x) = w(x)^{1/2}$.

**Theorem 1.** Let $G = (V, E)$ be a finite graph and $w: V \to \mathbb{R}_+$ be a weight function. Then $\alpha_w(G) \leq \vartheta'_w(G)$.

**Proof.** Let $I \subseteq V$ be an independent set such that $w(I) > 0$ (if there is no such independent set, then $\alpha_w(G) = 0$, and the theorem follows trivially) and let $M$ and $K$ be a feasible solution of (I).

Consider the sum

\[
\sum_{x,y \in I} w(x)^{1/2} w(y)^{1/2} K(x, y).
\]

This sum is at least

\[
\sum_{x,y \in I} w(x)^{1/2} w(y)^{1/2} w(x)^{1/2} w(y)^{1/2} = w(I)^2
\]

because $K - (w^{1/2})(w^{1/2})^T$ is positive semidefinite.

The same sum is also at most

\[
\sum_{x \in I} w(x) K(x, x) \leq M w(I)
\]

because $K(x, x) \leq M$ and $K(x, y) \leq 0$ for distinct $x, y \in I$. Combining both inequalities proves the theorem. \(\square\)

Notice that the formulation we use for $\vartheta'_w(G)$ is a **dual formulation**, since any feasible solution gives an upper bound for the independence number.

So $\vartheta'_w(G)$ provides an upper bound for $\alpha_w(G)$ when $G$ is finite. When more generally $V$ is a separable and compact measure space satisfying a mild technical condition, graph parameter $\vartheta'_w$ can be extended in a natural way so as to provide an upper bound for the weighted independence number.

This extension relies on a basic notion from functional analysis, that of kernel. Let $V$ be a separable and compact topological space and $\mu$ be a finite Borel measure over $V$. A kernel is a complex-valued function $K \in L^2(V \times V)$. 

A kernel $K$ can be seen as a generalization of a matrix. Like a matrix, a kernel defines an operator on $L^2(V)$ by

$$(Kf)(x) = \int_V K(x, y) f(y) \, d\mu(y).$$

Kernel $K$ is Hermitian if $K(x, y) = \overline{K(y, x)}$ for all $x, y \in V$. Hermitian kernels are the analogues of Hermitian matrices, and an analogue of the spectral decomposition theorem, known as the Hilbert-Schmidt theorem, holds, as we describe now.

A function $f \in L^2(V)$, $f \neq 0$, is an eigenfunction of $K$ if $Kf = \lambda f$ for some number $\lambda$, which is the associated eigenvalue of $f$. We say $\lambda$ is an eigenvalue of $K$ if it is the associated eigenvalue of some eigenfunction of $K$. The Hilbert-Schmidt theorem states that, for a Hermitian kernel $K$, there is a complete orthonormal system $\varphi_1, \varphi_2, \ldots$ of $L^2(V)$ consisting of eigenfunctions of $K$ such that

$$K(x, y) = \sum_{i=1}^{\infty} \lambda_i \varphi_i(x) \overline{\varphi_i(y)}$$

with $L^2$ convergence, where the real number $\lambda_i$ is the associated eigenvalue of $\varphi_i$. Then the $\lambda_i$ with their multiplicities are all the eigenvalues of $K$.

A Hermitian kernel $K$ is positive if all its eigenvalues are nonnegative; this is the analogue of a positive semidefinite matrix. An equivalent definition is as follows: $K$ is positive if for every $\rho \in L^2(V)$ we have

$$\int_V \int_V K(x, y) \rho(x) \overline{\rho(y)} \, d\mu(x) \, d\mu(y) \geq 0.$$

Using kernels, one may extend the definition of $\vartheta_w$ also to graphs defined over separable and compact measure spaces, simply by replacing the matrices in (1) by continuous kernels. In other words we define

$$\vartheta_w'(G) = \inf M \quad \begin{align*}
K(x, x) &\leq M \quad \text{for all } x \in V, \\
K(x, y) &\leq 0 \quad \text{for all } \{x, y\} \notin E \text{ with } x \neq y, \\
K : V \times V &\rightarrow \mathbb{R} \text{ is continuous and Hermitian}, \\
K - W &\text{ is positive},
\end{align*}$$

(2)

where $W \in L^2(V \times V)$ is the kernel such that $W(x, y) = w(x)^{1/2} w(y)^{1/2}$.

One then has the theorem:

**Theorem 2.** Let $G = (V, E)$ be a graph where $V$ is a separable and compact measure space in which any open set has nonzero measure. Let $w : V \rightarrow \mathbb{R}_+$ be a continuous weight function. Then $\alpha_w(G) \leq \vartheta_w'(G)$.

**Proof.** Since $V$ is compact and since we assume that every open subset of $V$ has nonzero measure, we may use the following observation of Bochner [3]: a continuous kernel $K$ is positive if and only if for any choice of $N$ and points $x_1, \ldots, x_N \in V$ we have that the matrix

$$(K(x_i, x_j))_{i,j=1}^{N}$$

is positive semidefinite.

Using this characterization of continuous and positive kernels, we may mimic the proof of Theorem 1 and obtain the desired result. This is why we require $K$ to be continuous in the definition of $\vartheta_w'$ and also why we require $w$ to be a continuous function: because we want to apply Bochner’s characterization to $K - W$. \qed

As was the case with Theorem 1 any feasible solution of (2) gives an upper bound for the weighted independence number. This is actually quite useful in the
infinite setting, because then it is often harder to obtain optimal solutions. Notice that it might also be that \( \alpha_w(G) = \infty \). In this case, the theorem still holds, since \( \vartheta_w(G) \) will be infeasible, and therefore \( \vartheta_w(G) = \infty \).

5. Exploiting symmetry with harmonic analysis

If \( G \) is a finite graph, then computing \( \vartheta_w(G) \) is solving a semidefinite program whose value can be found with the help of a computer, i.e., it can be approximated up to arbitrary precision in polynomial time. This is a theoretical assertion however; in practice, for moderately big graphs (say with thousands of vertices), if one cannot exploit any special structure of the graph, then computing the theta number is often impossible with today’s methods and computers.

If the graph \( G \) is infinite, we are dealing with an infinite-dimensional semidefinite program. If one then desires to use computational optimization methods, at some point the transition from infinite to finite has to be made. One way to make this transition is to use finer and finer grids to discretize the infinite graph and solve the corresponding finite semidefinite programs, obtaining bounds for the infinite problem. For coarse grids, however, this approach performs poorly, and for fine grids it becomes soon computationally infeasible. Moreover, with this approach one looses the entire geometrical structure of the packing graphs.

The alternative is to use harmonic analysis. Instead of computing \( \vartheta_w \) in the “time domain”, we could formulate the optimization problem in the “Fourier domain”. This has a twofold advantage. First, the Fourier domain can be discretized essentially by truncation and in doing so we do not lose too much, since it is to be expected that most of the information in a well-structured problem (like a packing problem) is to be concentrated in the beginning of the spectrum. Second, the translation group \( \mathbb{R}^n \) acts on the translational packing graph and the group of Euclidean motions \( \text{SO}(n) \times \mathbb{R}^n \) acts on the congruent packing graph; using harmonic analysis we can exploit the symmetry of this situation. On the down side, a very explicit understanding of the harmonic analysis of these two groups is needed, what in the case of the motion group can be cumbersome.

To make things concrete, let us demonstrate the basic strategy using the cyclic group \( \mathbb{Z}_n \). This group is finite, so that discretization is unnecessary, and Abelian, so that harmonic analysis becomes simple. Nevertheless, this simple example already carries many essential features, and ought to be kept in mind by the reader when the more complicated cases are treated later.

Let \( \Sigma \subseteq \mathbb{Z}_n \) with \( 0 \not\in \Sigma \) be closed under taking negatives, i.e., \( \Sigma = -\Sigma \). Then we define the Cayley graph

\[
\text{Cayley}(\mathbb{Z}_n, \Sigma) = (\mathbb{Z}_n, \{ \{ x, y \} : x - y \in \Sigma \}),
\]

which is an undirected graph whose vertices are the elements of \( \mathbb{Z}_n \) and where \( \Sigma \) defines the neighborhood of the neutral element 0; this neighborhood is then transported to every vertex by group translations. Since \( \Sigma = -\Sigma \), the definition is consistent, and since \( 0 \not\in \Sigma \), the Cayley graph does not have loops. For example, the \( n \)-cycle can be represented as a Cayley graph:

\[
C_n = \text{Cayley}(\mathbb{Z}_n, \Sigma) \quad \text{with} \quad \Sigma = \{ 1, -1 \}.
\]

The goal in this section is to show that the computation of the theta number \( \vartheta_w(\text{Cayley}(\mathbb{Z}_n, \Sigma)) \) with unit weights \( e = (1, \ldots, 1) \) reduces from a semidefinite program to a linear program if one works in the Fourier domain.

For this we need the characters of \( \mathbb{Z}_n \), which are group homomorphisms \( \chi : \mathbb{Z}_n \to \mathbb{T} \), where \( \mathbb{T} \) is the unit circle in the complex plane. So every character \( \chi \) satisfies

\[
\chi(x + y) = \chi(x)\chi(y)
\]
for all \( x, y \in \mathbb{Z}_n \).

The characters themselves form a group with the operation of pointwise multiplication \((\chi \psi)(x) = \chi(x)\psi(x)\); this is the dual group \( \hat{\mathbb{Z}}_n \) of \( \mathbb{Z}_n \). The trivial character \( e \) of \( \mathbb{Z}_n \) defined by \( e(x) = 1 \) for all \( x \in \mathbb{Z}_n \) is the unit element. Moreover, if \( \chi \) is a character, then its inverse is its complex conjugate \( \overline{\chi} \) that is such that \( \overline{\chi}(x) = \overline{\chi(x)} \) for all \( x \in \mathbb{Z}_n \). We often view characters as vectors in the vector space \( \mathbb{C}^{\mathbb{Z}_n} \).

**Lemma 1.** Let \( \chi \) and \( \psi \) be characters of \( \mathbb{Z}_n \). Then the following orthogonality relation holds:

\[
\chi^* \psi = \sum_{x \in \mathbb{Z}_n} \overline{\chi(x)} \psi(x) = \begin{cases} |\mathbb{Z}_n| & \text{if } \chi = \psi, \\ 0 & \text{otherwise.} \end{cases}
\]

**Proof.** If \( \chi = \psi \), then,

\[
\chi^* \chi = \sum_{x \in \mathbb{Z}_n} \overline{\chi(x)} \chi(x) = \sum_{x \in \mathbb{Z}_n} 1 = |\mathbb{Z}_n|
\]

holds. If \( \chi \neq \psi \), then there is \( y \in \mathbb{Z}_n \), so that \( (\overline{\chi})\psi)(y) \neq 1 \). Furthermore, we have

\[
(\overline{\chi})\psi)(y)\chi^* \psi = (\overline{\chi})\psi)(y) \sum_{x \in \mathbb{Z}_n} \overline{\chi(x)} \psi(x) = \sum_{x \in \mathbb{Z}_n} \overline{\chi(x + y)} \psi(x + y)
\]

so \( \chi^* \psi \) has to be zero. \( \square \)

As a corollary we can explicitly give all characters of \( \mathbb{Z}_n \) and see that they form an orthogonal basis of \( \mathbb{C}^{\mathbb{Z}_n} \). It follows that the dual group \( \hat{\mathbb{Z}}_n \) is isomorphic to \( \mathbb{Z}_n \).

**Corollary 1.** Every element \( u \in \mathbb{Z}_n \) defines a character of \( \mathbb{Z}_n \) by

\[
\chi_u(x) = e^{2\pi i ux/n}.
\]

The map \( u \mapsto \chi_u \) is a group isomorphism between \( \mathbb{Z}_n \) and its dual group \( \hat{\mathbb{Z}}_n \).

**Proof.** One immediately verifies that the map \( u \mapsto \chi_u \) is well-defined, that it is an injective group homomorphism, and that \( \chi_u \) is a character of \( \mathbb{Z}_n \). By the orthogonality relation we see that the number of different characters of \( \mathbb{Z}_n \) is at most the dimension of the space \( \mathbb{C}^{\mathbb{Z}_n} \), hence \( |\mathbb{Z}_n| \) equals \( |\hat{\mathbb{Z}}_n| \) and the map is a bijection. \( \square \)

Given a function \( f: \mathbb{Z}_n \to \mathbb{C} \), the function \( \hat{f}: \hat{\mathbb{Z}}_n \to \mathbb{C} \) such that

\[
\hat{f}(\chi) = \frac{1}{|\mathbb{Z}_n|} \sum_{x \in \mathbb{Z}_n} f(x) \chi^{-1}(x)
\]

is the discrete Fourier transform of \( f \); the coefficients \( \hat{f}(\chi) \) are called the Fourier coefficients of \( f \). We have then the Fourier inversion formula:

\[
f(x) = \sum_{\chi \in \mathbb{Z}_n} \hat{f}(\chi) \chi(x).
\]

We say that \( f: \mathbb{Z}_n \to \mathbb{C} \) is of positive type if \( f(x) = \overline{f(-x)} \) for all \( x \in \mathbb{Z}_n \) and for all \( \rho: \mathbb{Z}_n \to \mathbb{C} \) we have

\[
\sum_{x, y \in \mathbb{Z}_n} f(x - y) \rho(x) \rho(y) \geq 0.
\]

So \( f \) is of positive type if and only if the matrix \( K(x, y) = f(x - y) \) is positive semidefinite. With this we have the following characterization for the theta number of \( \text{Cayley}(\mathbb{Z}_n, \Sigma) \).
Theorem 3. We have that
\[ d_e'(\text{Cayley}(\mathbb{Z}_n, \Sigma)) = \min f(0) \]
\[ f(x) \leq 0 \quad \text{for all } x \notin \Sigma \cup \{0\}, \]
\[ \sum_{x \in \mathbb{Z}_n} f(x) \geq |\mathbb{Z}_n|, \]
\[ f: \mathbb{Z}_n \to \mathbb{R} \text{ is of positive type.} \]

Alternatively, expressing \( f \) in the Fourier domain we obtain:
\[ d_e'(\text{Cayley}(\mathbb{Z}_n, \Sigma)) = \min \sum_{\chi \in \hat{\mathbb{Z}}_n} \hat{f}(\chi) \]
\[ \sum_{\chi \in \hat{\mathbb{Z}}_n} \hat{f}(\chi) \chi(x) \leq 0 \quad \text{for all } x \notin \Sigma \cup \{0\}, \]
\[ \hat{f}(\psi) \geq 1, \]
\[ \hat{f}(\chi) \geq 0 \text{ and } \hat{f}(\chi) = \hat{f}(\chi^{-1}) \text{ for all } \chi \in \hat{\mathbb{Z}}_n. \]

Proof. Functions \( f: \mathbb{Z}_n \to \mathbb{C} \) correspond to \( \mathbb{Z}_n \)-invariant matrices \( K: \mathbb{Z}_n \times \mathbb{Z}_n \to \mathbb{C} \), which are matrices such that \( K(x+z, y+z) = K(x, y) \) for all \( x, y, z \in \mathbb{Z}_n \).

In solving problem (1) for computing \( d_e' \) we may restrict ourselves to \( \mathbb{Z}_n \)-invariant matrices. This can be seen via a symmetrization argument: If \((M, K)\) is an optimal solution of (1), then so is \((M, K)\) with
\[ K(x, y) = \frac{1}{|\mathbb{Z}_n|} \sum_{z \in \mathbb{Z}_n} K(x+z, y+z), \]
which is \( \mathbb{Z}_n \)-invariant.

So we can translate problem (1) into (3). The objective function and the constraint on non-edges translate easily. The positive-semidefiniteness constraint requires a bit more work.

First, observe that to require \( K \) to be real and symmetric is to require \( f \) to be real and such that \( f(x) = f(-x) \) for all \( x \in \mathbb{Z}_n \). We claim that each character \( \chi \) of \( \mathbb{Z}_n \) gives an eigenvector of \( K \) with eigenvalue \( |\mathbb{Z}_n| \hat{f}(\chi) \). Indeed, using the inversion formula we have
\[ (K \chi)(x) = \sum_{y \in \mathbb{Z}_n} K(x, y) \chi(y) = \sum_{y \in \mathbb{Z}_n} f(x-y) \chi(y) \]
\[ = \sum_{y \in \mathbb{Z}_n} \sum_{\psi \in \hat{\mathbb{Z}}_n} \hat{f}(\psi) \psi(x-y) \chi(y) \]
\[ = \sum_{\psi \in \hat{\mathbb{Z}}_n} \hat{f}(\psi) \sum_{y \in \mathbb{Z}_n} \psi(y) \chi(x-y) \]
\[ = \sum_{\psi \in \hat{\mathbb{Z}}_n} \hat{f}(\psi) \chi(x) \sum_{y \in \mathbb{Z}_n} \psi(y) \chi(y) \]
\[ = |\mathbb{Z}_n| \hat{f}(\chi) \chi(x), \]
as claimed.

This immediately implies that \( K \) is positive semidefinite — or, equivalently, \( f \) is of positive type — if and only if \( \hat{f}(\chi) \geq 0 \) for all characters \( \chi \). Now, since \( \hat{f}(e) = |\mathbb{Z}_n|^{-1} \sum_{x \in \mathbb{Z}_n} f(x) \), and since \( e \) is an eigenvalue of \( K \), then \( K - ee^T \) is positive semidefinite if and only if \( \sum_{x \in \mathbb{Z}_n} f(x) \geq |\mathbb{Z}_n| \) and \( f \) is of positive type.

So we see that (1) can be translated into (3). Using the inversion formula and noting that \( f \) is real-valued if and only if \( \hat{f}(\chi) = \hat{f}(\chi^{-1}) \) for all \( \chi \), one immediately obtains (4). \( \square \)

Cayley graphs on the cyclic group are not particularly exciting. Everything in this section, however, can be straightforwardly applied to any finite Abelian group. If, for instance, one considers the group \( \mathbb{Z}_2^n \), then it becomes possible to model
6. Upper bounds for congruent and translational body packings

The packing graphs described above have noncompact vertex sets, but we said they can be compactified so that the theta number can be applied. Let us now see how that can be done.

First we need a definition of packing density. Given a packing \( P \), we say that its density is \( \Delta \) if for every \( p \in \mathbb{R}^n \) we have
\[
\Delta = \lim_{r \to \infty} \frac{\text{vol}(B(p, r) \cap P)}{\text{vol} B(p, r)},
\]
where \( B(p, r) \) is the ball of radius \( r \) centered at \( p \). Not every packing has a density, but every packing has an upper density given by
\[
\limsup_{r \to \infty} \sup_{p \in \mathbb{R}^n} \frac{\text{vol}(B(p, r) \cap P)}{\text{vol} B(p, r)}.
\]

We say that a packing \( P \) is periodic if there is a lattice \( L \subseteq \mathbb{R}^n \) that leaves \( P \) invariant, that is, \( P = x + P \) for every \( x \in L \). Lattice \( L \) is the periodicity lattice of \( P \). In other words, \( P \) consists of some bodies placed inside the fundamental cell of \( L \), and this arrangement repeats itself at each copy of the fundamental cell translated by vectors of the lattice.

Periodic packings always have a density. Moreover, given any packing \( P \), one may define a sequence of periodic packings whose fundamental cells have volumes approaching infinity and whose densities converge to the upper density of \( P \). So, when computing bounds for the maximum density of packings, we may restrict ourselves to periodic packings.

This is the key observation that allows us to compactify the packing graphs. For let \( K_1, \ldots, K_N \subseteq \mathbb{R}^n \) be some given convex bodies. We have defined the translational packing graph of \( K_1, \ldots, K_N \). Given a lattice \( L \subseteq \mathbb{R}^n \), we may define a periodic version of the packing graph. This is the graph \( G_L \), whose vertex set is \( V = \{1, \ldots, N\} \times (\mathbb{R}^n/L) \). Now, vertex \((i, x)\) of \( G_L \) corresponds not only to one body, but to many: it corresponds to all the bodies \( x + v + K_i \), for \( v \in L \). Vertices \((i, x)\) and \((j, y)\) are then adjacent if for some \( v \in L \) we have
\[
(x + v + K_i)^o \cap (y + K_j)^o \neq \emptyset.
\]

Then an independent set of \( G_L \) corresponds to a periodic packing of translations of \( K_1, \ldots, K_N \) with periodicity lattice \( L \), and vice versa.

Graph \( G_L \) has a compact vertex set and each one of its independent sets is finite. If we consider the weight function \( w: V \to \mathbb{R}_+ \) such that \( w(i, x) = \text{vol} K_i \), then the maximum density of a periodic packing with periodicity lattice \( L \) is given by
\[
\frac{\alpha_w(G_L)}{\text{vol}(\mathbb{R}^n/L)}.
\]
So one strategy to find an upper bound for the maximum density of a packing is to find an upper bound for \( \alpha_w(G_L) \) for every \( L \).

Notice \( V \) is actually a separable and compact measure space that satisfies the hypothesis of Theorem 2. So \( \vartheta_w(G_L) \) provides an upper bound for \( \alpha_w(G_L) \). Let us see how one may obtain a feasible solution of (2) for every graph \( G_L \).

Let \( f: \mathbb{R}^n \to \mathbb{C} \) be a rapidly decreasing function. This is an infinitely differentiable function with the following property: any derivative, multiplied by any polynomial, is a bounded function.

---

1A lattice is a discrete subgroup of \((\mathbb{R}^n, +)\).
The Fourier transform of $f$ computed at $u \in \mathbb{R}^n$ is
\[
\hat{f}(u) = \int_{\mathbb{R}^n} f(x)e^{-2\pi i u \cdot x} \, dx,
\]
where $u \cdot x = u_1x_1 + \cdots + u_nx_n$. Since $f$ is rapidly decreasing, the inversion formula holds, giving
\[
f(x) = \int_{\mathbb{R}^n} \hat{f}(u)e^{2\pi i u \cdot x} \, du.
\]

Consider now a matrix-valued function $f: \mathbb{R}^n \to \mathbb{C}^{N \times N}$, where $f(x) = (f_{ij}(x))_{i,j=1}^N$ and each function $f_{ij}$ is rapidly decreasing. For $u \in \mathbb{R}^n$ we write
\[
\hat{f}(u) = (\hat{f}_{ij}(u))_{i,j=1}^N.
\]
So the Fourier transform of $f$ is also a matrix-valued function.

We say $f$ is of positive type if $\hat{f}(x) = f(-x)^*$ for every $x \in \mathbb{R}^n$ and for every $L^\infty$ function $\rho: \mathbb{R}^n \to \mathbb{C}^N$ we have
\[
\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \rho(y)^* f(x-y)\rho(x) \, dxdy \geq 0.
\]
One may prove that $f$ is of positive type if and only if $\hat{f}(u)$ is positive semidefinite for every $u \in \mathbb{R}^n$.

With this we have the following theorem:

**Theorem 4.** Let $K_1, \ldots, K_N \subseteq \mathbb{R}^n$ be convex bodies. Suppose $f: \mathbb{R}^n \to \mathbb{C}^{N \times N}$ is such that each $f_{ij}$ is rapidly decreasing and that it satisfies the following conditions:

(i) $f_{ij}(x) \leq 0$ whenever $(x + K_i)^o \cap K_j^o = \emptyset$;

(ii) $\hat{f}(0) - (\text{vol } K_i)^{1/2}(\text{vol } K_j)^{1/2})_{i,j=1}^N$ is positive semidefinite;

(iii) $f$ is of positive type.

Then the maximum density of a packing of translated copies of $K_1, \ldots, K_N$ is at most $\max\{f_{ii}(0) : i = 1, \ldots, N\}$.

**Proof.** Let $w: V \to \mathbb{R}_+$ be the weight function such that $w(i,x) = \text{vol } K_i$ for all $(i,x) \in V$. The proof of the theorem consists in deriving from $f$, for every lattice $L \subseteq \mathbb{R}^n$, a kernel $K_L \in L^2(V \times V)$, where $V = \{1, \ldots, N\} \times (\mathbb{R}^n/L)$, and a number $M_L$ that together give a feasible solution of (2), thus obtaining an upper bound for $\alpha_w(G_L)$.

For a given lattice $L$, we let
\[
K_L((i,x), (j,y)) = \text{vol}(\mathbb{R}^n/L) \sum_{v \in L} f_{ij}(x-y+v).
\]
The above sum is well-defined since each $f_{ij}$ is rapidly decreasing. Moreover, this also implies that $K_L$ is continuous.

Given two distinct, nonadjacent vertices $(i,x)$ and $(j,y)$ of $G_L$, we have that for all $v \in L$,
\[
(x + v + K_i)^o \cap (y + K_j)^o = \emptyset \iff (x - y + v + K_i)^o \cap K_j^o = \emptyset.
\]
This means that $f_{ij}(x-y+v) \leq 0$ for all $v \in L$. But then $K_L((i,x), (j,y)) \leq 0$, as we wanted.

Now we show that $K_L - W$ is a positive kernel. This is implied by conditions (ii) and (iii) of the theorem, and can be proven directly with a bit of work by combining the definition of a positive kernel with that of a function of positive type. We take however another road and exhibit a complete list of eigenfunctions and eigenvalues of $K_L - W$.

Let $L' = \{ v \in \mathbb{R}^n : u \cdot v \in \mathbb{Z} \text{ for all } u \in L \}$ be the dual lattice of $L$ and consider the matrix $W' \in \mathbb{R}^{N \times N}$ with $W'_{ij} = (\text{vol } K_i)^{1/2}(\text{vol } K_j)^{1/2}$. Since $f$ is of positive
type, for each \( u \in \mathbb{R}^n \) we have that \( \hat{f}(u) \) is positive semidefinite. Moreover, from condition (ii) we have that \( \hat{f}(0) - W' \) is positive semidefinite. So the matrices

\[
\hat{f}(u) - \delta_u W',
\]

where \( \delta_u \) equals 1 if \( u = 0 \) and 0 otherwise, are positive semidefinite.

For \( u \in L^* \), let \( a_{1,u}, \ldots, a_{N,u} \) be an orthonormal basis of \( \mathbb{R}^N \) consisting of eigenvectors of \( \hat{f}(u) - \delta_u W' \), with associated eigenvalues \( \lambda_{1,u}, \ldots, \lambda_{N,u} \), which are all nonnegative.

Also for \( u \in L^* \), let \( \chi_u(x) = e^{2\pi i u \cdot x} \). Then \( (\text{vol}(\mathbb{R}^n/L))^{1/2} \chi_u \), \( u \in L^* \), forms a complete orthonormal system of \( L^2(\mathbb{R}^n/L) \), and so

\[
(\text{vol}(\mathbb{R}^n/L))^{1/2} a_{k,u} \otimes \chi_u
\]

for \( k = 1, \ldots, N \) and \( u \in L^* \) forms a complete orthonormal system of \( L^2(V) \). We claim that each such function is an eigenfunction of \( K_L - W \).

Indeed, let \((i, x) \in V \) be given. Notice that

\[
[W(a_{k,u} \otimes \chi_u)((i, x), (j, y))] = \int_V W((i, x), (j, y))(a_{k,u} \otimes \chi_u)(j, y) d(j, y)
\]

\[
= \sum_{j=1}^{N} W'_{ij}(a_{k,u})_j \int_{\mathbb{R}^n/L} e^{2\pi i u \cdot y} dy
\]

\[
= \sum_{j=1}^{N} W'_{ij}(a_{k,u})_j \text{vol}(\mathbb{R}^n/L) \delta_u
\]

\[
= \text{vol}(\mathbb{R}^n/L)(W' a_{k,u})_j \delta_u.
\]

Similarly we have

\[
[K_L(a_{k,u} \otimes \chi_u)((i, x), (j, y))] = \int_V K_L((i, x), (j, y))(a_{k,u} \otimes \chi_u)(j, y) d(j, y)
\]

\[
= \text{vol}(\mathbb{R}^n/L) \sum_{j=1}^{N} \int_{\mathbb{R}^n/L} \int_{\mathbb{R}^n/L} f_{ij}(x - y + v)(a_{k,u})_j e^{2\pi i u \cdot y} dy
dy
\]

\[
= \text{vol}(\mathbb{R}^n/L) \sum_{j=1}^{N} (a_{k,u})_j \int_{\mathbb{R}^n} f_{ij}(x - y) e^{2\pi i u \cdot y} dy
dy
\]

\[
= \text{vol}(\mathbb{R}^n/L) \sum_{j=1}^{N} (a_{k,u})_j \int_{\mathbb{R}^n} f_{ij}(y) e^{2\pi i u \cdot (x - y)} dy
dy
\]

\[
= \text{vol}(\mathbb{R}^n/L) \sum_{j=1}^{N} \hat{f}_{ij}(u)(a_{k,u})_j e^{2\pi i u \cdot x}
\]

\[
= \text{vol}(\mathbb{R}^n/L)(\hat{f}(u)a_{k,u})_j e^{2\pi i u \cdot x}.
\]

Putting it all together we have

\[
[(K_L - W)(a_{k,u} \otimes \chi_u)](i, x) = \text{vol}(\mathbb{R}^n/L)(\hat{f}(u)a_{k,u} - \delta_u W'(a_{k,u})) e^{2\pi i u \cdot x}
\]

\[
= \text{vol}(\mathbb{R}^n/L)\lambda_{k,u}(a_{k,u}) e^{2\pi i u \cdot x}
\]

\[
= \text{vol}(\mathbb{R}^n/L)\lambda_{k,u}(a_{k,u} \otimes \chi_u)(i, x).
\]

So we see that all the functions \( a_{k,u} \otimes \chi_u \) are eigenfunctions of \( K_L - W \) with nonnegative associated eigenvalues, and it follows that \( K_L - W \) is a positive kernel.

Finally, we need to provide the bound \( M_L \) on the diagonal elements of \( K_L \). To do that, we assume that the minimum vector of \( L \) is large enough so that \((v + K_{\lambda})^2 \cap K_{\lambda}^c = \emptyset \) for all nonzero \( v \in L \); this is no loss of generality, since we care only
Theorem 5. Let $M(\mathbb{R}^n)$ be a convex body. Suppose $f : M(\mathbb{R}^n) \to \mathbb{R}$ is rapidly decreasing and that it satisfies the following conditions:

(i) $f(A, x) \leq 0$ whenever $(x + A\mathcal{K}) \cap \mathcal{K} = \emptyset$;
(ii) $\int_{M(\mathbb{R}^n)} f(A, x) d(A, x) \geq \text{vol} \mathcal{K}$;
(iii) $f$ is of positive type.

Then the maximum density of a packing of congruent copies of $K$ is at most $f(I, 0)$.

The proof of Theorem 5 is slightly more technical than the proof of Theorem 4, but otherwise it follows the same pattern.
Notice that the congruent packing graph is a Cayley graph whose vertex set is the Euclidean motion group. So Theorem 5 is also an analogue of Theorem 3. It is, however, more distant from Theorem 3 than Theorem 4 is, since \( \mathbb{R}^n \) is Abelian, but \( M(n) \) is not. This means that when one does harmonic analysis over \( M(n) \), using the characters is not enough: one also needs to consider higher-dimensional irreducible representations, most of them are even infinite-dimensional.

Though it is clear that Theorem 5 can be restated in the Fourier domain just like Theorem 3 could, it now becomes harder to carry out this procedure explicitly — already for \( n = 2 \) or \( 3 \), the formulas involved are significantly more complicated than the ones for \( \mathbb{R}^n \). Using the formulas effectively in a computational approach remains the main obstacle in applying Theorem 5.

7. A COMPUTATIONAL APPROACH

Theorem 4 and Theorem 5 might be mathematically pleasing per se but the real challenge is to determine explicit functions giving good bounds. So far this has been done only for a few cases. When \( N = 1 \), Theorem 4 becomes a theorem of Cohn and Elkies [5]. The Cohn-Elkies bound provides the basic framework for proving the best known upper bounds for the maximum density of sphere packings in dimensions 4, . . . , 36. It is also conjectured to provide tight bounds in dimensions 8 and 24 and there is strong numerical evidence to support this conjecture. De Laat, Oliveira, and Vallentin [13] have proposed a strengthening of the Cohn-Elkies bound and computed better upper bounds for the maximum density of sphere packings in dimensions 4, 5, 6, 7, and 9.

Here we want to give an idea of how to set up a semidefinite program for finding good functions. Let \( B_n \) be the unit ball in \( \mathbb{R}^n \). To find bounds for the density of a sphere-packing, we want to find a function \( f : \mathbb{R}^n \to \mathbb{R} \) with \( f(0) \) as large as possible such that

1. \( f(x) \leq 0 \) whenever \( (x + B_n)^o \cap B_n^o = \emptyset \);
2. \( \hat{f}(0) - \text{vol} B_n \geq 0 \);
3. \( f \) is of positive type, which means that \( \hat{f}(u) \) is nonnegative for all \( u \in \mathbb{R}^n \).

Without loss of generality we can assume that the function \( f \) is even and radial, i.e., \( f(x) \) depends only on the norm of \( x \), so it is essentially an even univariate function. Another good thing is that the Fourier transform of a radial function is radial again. Functions whose Fourier transform have the form

\[
\hat{f}(u) = p(\|u\|)e^{-\pi \|u\|^2},
\]

where \( p \) is an even and univariate polynomial, are dense in the space of rapidly decreasing even and radial functions. Then by the Fourier inversion formula we can compute \( f \) explicitly, monomial by monomial, through

\[
\int_{\mathbb{R}^n} \|u\|^{2k} e^{-\pi \|u\|^2} e^{2\pi i u \cdot x} \, du = k! \pi^{-k} e^{-\pi \|x\|^2} L_k^{n/2-1}(\pi \|x\|^2),
\]

where \( L_k^{n/2-1} \) is the Laguerre polynomial of degree \( k \) with parameter \( n/2 - 1 \). These are orthogonal polynomials on the half open interval \([0, \infty)\) with respect to the measure \( x^{n/2-1}e^{-x} \, dx \).

We specify function \( f \) via the polynomial \( p \). To do so, we fix \( d > 0 \) and work with polynomials of degree up to \( 2d \), that is, we work with polynomials of the form

\[
p(t) = \sum_{k=0}^{d} a_{2k} t^{2k},
\]

Working with finite \( d \) is our way of discretizing the Fourier domain, a necessary step as we observed in Section 5.
Now constraints on $f$ become constraints on $p$, which can be modeled as sum-of-squares constraints (see, e.g., the expository papers of Lasserre and Parrilo in SIAG/OPT Views-and-News 15 (2004)). So we can set up a semidefinite programming problem to find a function $f$ satisfying the required constraints:

$$
\max \sum_{k=0}^{d} a_k! \pi^{-k} L_k^{n/2-1}(0)
$$

$$p(t) = \sum_{k=0}^{d} a_k t^k,$$

$$\sum_{k=0}^{d} a_k! \pi^{-k} L_k^{n/2-1}(\pi w^2)
+ v_2^T(w) R v_d(w) + (w^2 - 2^2) v_{d-2}^T(w) S v_{d-2}(w) = 0,$$

$$p(0) - \text{vol } B_n \geq 0,$$

$$p(t) = v_3^T(t) Q v_d(t),$$

$Q$, $R$, $S$ are positive semidefinite matrices,

where $v_d(z) = (1, z, \ldots, z^d)$ is the vector of all monomials up to degree $d$.

From a numerical perspective this formulation is a catastrophe — a fact well known to specialists in the field — since the monomial basis is used. Even though the resulting semidefinite program is small, say when we use $d = 10$, it is impossible to get a solution from standard numerical solvers. On the other hand there are many equivalent ways to implement this program by using different choices of polynomial bases. Here we have two choices: one for the vectors $v_d$ and one for testing the polynomial identities. With quite some experimentation we found that the basis

$$P_k(t) = \mu_k^{-1} L_k^{n/2-1}(2\pi t),$$

where $\mu_k$ is the absolute value of the coefficient of $L_k^{n/2-1}(2\pi t)$ with largest absolute value, performs well.

We believe that the problem of finding a good basis deserves further investigation. Currently almost nothing (to the best of our knowledge only the papers by Löfberg and Parrilo [15] and Roh and Vandenberghe [18] address this issue) is known about it although it is a crucial factor for solving polynomial optimization problems in practice.

Another use of Theorem 4 is to provide bounds for binary sphere packings. These are packings of balls of two different sizes, i.e., we have $N = 2$ and $K_1, K_2$ are balls. Binary sphere packings occur naturally in applications such as material science and chemistry. De Laat, Oliveira, and Vallentin [13] used Theorem 4 to compute upper bounds for the maximum densities of binary sphere packings in dimensions 2, . . . , 5.

Recently, Oliveira and Vallentin [17] used Theorem 5 to compute upper bounds for the densities of pentagon packings. Here yet a new challenge arises: The Fourier transform is no longer matrix-valued but takes infinite-dimensional Hilbert-Schmidt kernels as values. Oliveira and Vallentin determined a first upper bound (0.98 in comparison to the best known lower bound of 0.92) and the numerical result obtained gives hope that the theorem will also be useful in the case of tetrahedra packings to meet the challenge of Gravel, Elser and Kallus.

8. Conclusion

It is natural to consider optimization methods when dealing with geometric packing problems, and we tried to show how well-known methods from combinatorial optimization, namely the Lovász theta number and its variants, can be extended so as to provide upper bounds for the packing density. Such extensions provide a uniform framework to deal with geometric packing problems.

For finite graphs, only in very specific cases does the Lovász theta number provide tight bounds. The same happens for geometric packing graphs: only in very few
cases are the bounds coming from extensions of the theta number tight; in most cases, such bounds are but a first step in solving the problem.

The link made with combinatorial optimization techniques not only allows us to provide a unified framework and to have access to well-known optimization tools, it also points out to ways in which such bounds can be strengthened. The obvious approach is to extend ideas like the Lasserre hierarchy to geometric packing problems. Such higher-order bounds can incorporate more sophisticated constraints like those coming from the local interaction of more than two vertices; in other words, we then deal with \( k \)-point correlation functions and not only with 2-point correlation functions.

Schrijver [19] considered 3-point correlation functions for binary codes and Bachoc and Vallentin [2] used 3-point correlation functions for packings of spherical caps on the unit sphere. De Laat and Vallentin [12] recently showed that this approach has the (theoretical) potential to solve all geometric packing problems. However, the price to pay is that the size of the optimization problems involved grows fast.

The success of such techniques will depend on several factors, among which:

(i) how to analyze the optimization problem without using a computer, for instance to find asymptotic results, (ii) how to automatize the use of harmonic analysis, and (iii) how to solve semidefinite programs involving sums-of-squares constraints in an efficient and numerically stable manner.

\[ \text{References} \]

[1] C. Addabbo, Il libellus de impletione loci di Francesco Maurolico, to appear in Quaderni del Dipartimento di Matematica, Sezione Didattica e Storia, 2013, 59pp.
[2] C. Bachoc and F. Vallentin, New upper bounds for kissing numbers from semidefinite programming, J. Amer. Math. Soc. 21 (2008) 909–924.
[3] S. Bochner, Hilbert distances and positive definite functions, Ann. of Math. 42 (1941) 647–656.
[4] E.R. Chen, M. Engel, and S.C. Glotzer, Dense crystalline dimer packings of regular tetrahedra, Discrete & Computational Geometry 44 (2010) 253–280.
[5] H. Cohn and N.D. Elkies, New upper bounds on sphere packings I, Ann. of Math. 157 (2003) 689–714.
[6] H. Cohn and A. Kumar, Optimality and uniqueness of the Leech lattice among lattices, Ann. of Math. 170 (2009) 1003–1050.
[7] J.H. Conway and N.J.A. Sloane, Sphere Packings, Lattices and Groups, Springer-Verlag, New York, 1988.
[8] J.H. Conway and S. Torquato, Packing, tiling, and covering with tetrahedra, Proc. Natl. Acad. Sci. USA 103 (2006) 10612–10617.
[9] P. Delsarte, An algebraic approach to the association schemes of coding theory, Philips Research Reports Supplements 1973 No. 10, Philips Research Laboratories, Eindhoven, 1973.
[10] S. Gravel, V. Elser, and Y. Kallus, Upper bound on the packing density of regular tetrahedra and octahedra, Discrete & Computational Geometry 46 (2011) 799–818.
[11] M. Grötschel, L. Lovász, and A. Schrijver, The ellipsoid method and its consequences in combinatorial optimization, Combinatorica 1 (1981) 169–197.
[12] D. de Laat and F. Vallentin, A semidefinite programming hierarchy for packing problems in discrete geometry, arXiv:1311.3789, 2013, 21pp.
[13] D. de Laat, F.M. de Oliveira Filho, and F. Vallentin, Upper bounds for packings of spheres of several radii, to appear in Forum of Mathematics, Sigma, arXiv:1206.2608, 2012, 31pp.
[14] J.C. Lagarias and C. Zong, Mysteries in packing regular tetrahedra, Notices of the A.M.S 59 (2012) 1540–1549.
[15] J. Löfberg and P.A. Parrilo, From coefficients to samples: A new approach to SOS optimization, in: Proceedings of the 43rd IEEE Conference on Decision and Control, 2004, pp. 3154–3159.
[16] L. Lovász, On the Shannon capacity of a graph, IEEE Transactions on Information Theory IT-25 (1979) 1–7.
[17] F.M. de Oliveira Filho and F. Vallentin, Computing upper bounds for the packing density of congruent copies of convex bodies I, arXiv:1308.4893, 2013, 28pp.

[18] T. Roh and L. Vandenberghe, Discrete transforms, semidefinite programming, and sum-of-squares representations of nonnegative polynomials, *SIAM J. Optim.* 16 (2006) 939–964.

[19] A. Schrijver, New code upper bounds from the Terwilliger algebra and semidefinite programming, *IEEE Transactions on Information Theory* 51 (2005) 2859–2866.

[20] Simplicius, *On Aristotle On the Heavens* 3.7–4.6 (translated by I. Mueller), Gerald Duckworth & Co. Ltd., London, 2009.

[21] D.J. Struik, Het probleem “de impletione loci”, *Nieuw Archief voor Wiskunde II* 15 (1926) 121–137.

[22] S. Torquato and Y. Jiao, Dense packings of the Platonic and Archimedean solids, *Nature* 460 (2009) 876–879.

[23] G.M. Ziegler, Three Mathematics Competitions, in: *An Invitation to Mathematics: From Competitions to Research* (D. Schleicher and M. Lackmann, eds.), Springer-Verlag, Berlin, 2011, pp. 195–206.

F.M. de Oliveira Filho, Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão 1010, 05508-090 São Paulo/SP, Brazil

E-mail address: fmario@gmail.com

F. Vallentin, Mathematisches Institut, Universität zu Köln, Wevertal 86–90, 50931 Köln, Germany

E-mail address: frank.vallentin@uni-koeln.de