COMPUTING UPPER BOUNDS FOR THE PACKING DENSITY OF CONGRUENT COPIES OF A CONVEX BODY I

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Abstract. In this paper we prove a theorem that provides an upper bound for the density of packings of congruent copies of a given convex body in \( \mathbb{R}^n \); this theorem is a generalization of the linear programming bound for sphere packings. We illustrate its use by computing an upper bound for the maximum density of packings of regular pentagons in the plane. Our computational approach is numerical and uses a combination of semidefinite programming, sums of squares, and the harmonic analysis of the Euclidean motion group. We show how, with some extra work, the bounds so obtained can be made rigorous.

1. Introduction

How much of Euclidean space can be filled with pairwise nonoverlapping congruent (i.e., rotated and translated) copies of a given convex body \( \mathcal{K} \)?

A union of congruent copies of \( \mathcal{K} \) with pairwise disjoint interiors is a packing of congruent copies of \( \mathcal{K} \), or just a packing of \( \mathcal{K} \) for short; below, packings are always packings of congruent copies of the body. The density of a packing is the fraction of Euclidean space it covers. Rewritten, the question of the previous paragraph is: What is the maximum density of a packing of congruent copies of \( \mathcal{K} \)? We call this the body packing problem.

Theorem 1, the main theorem of this paper, provides a way to compute upper bounds to the density of any packing of a given convex body \( \mathcal{K} \). We then illustrate the use of this theorem by applying computational methods to obtain bounds for packings of regular pentagons in the Euclidean plane — the case when \( \mathcal{K} \subseteq \mathbb{R}^2 \) is a regular pentagon.

Before presenting our main theorem and its application, let us first discuss some of the most interesting cases of the body packing problem.

Perhaps the most well-known case occurs when \( \mathcal{K} \) is a unit sphere. We then have the classical sphere packing problem. It is easy to find out which sphere packings are optimal (i.e., attain the maximum packing density) in dimensions 1 and 2. In dimension 3, it was conjectured by the German mathematician and astronomer Johannes Kepler (1571–1630) \[21\] that a certain packing covering \( \pi/(3\sqrt{2}) = 0.74048\ldots \) of
space is optimal. The Kepler conjecture has been proven by Hales [19], who makes massive use of computers in his proof.

In all other dimensions only upper and lower bounds are known. In dimensions 4, . . . , 36, the best known upper bounds come from the linear programming bound of Cohn and Elkies [12]; their bound was recently improved in dimensions 4, 5, 6, 7, and 9 by de Laat, Oliveira, and Vallentin [23], who also provided upper bounds for binary sphere packings, that is, for packings of spheres of two different sizes.

Another case of the body packing problem that has attracted attention happens when \( K \) is a regular tetrahedron in \( \mathbb{R}^3 \). We called the sphere packing problem “classical”, but this adjective most properly applies to the problem of packing tetrahedra, as it was considered by Aristotle (384 BC–322 BC).

In his treatise \textit{De Caelo} (On the Heavens), Aristotle attacks the Platonic theory of assigning geometrical figures to the elements, stating (cf. \textit{De Caelo}, Book III, Chapter VIII, in translation by Guthrie [3]):

This attempt to assign geometrical figures to the simple bodies is on all counts irrational. In the first place, the whole of space will not be filled up. Among surfaces it is agreed that there are three figures which fill the place that contains them — the triangle, the square, and the hexagon: among solids only two, the pyramid and the cube. But they need more than these, since they hold that the elements are more.

Here, the “pyramid” is the regular tetrahedron. Aristotle then thought it to be possible to tile the space with regular tetrahedra. Only much latter, Johannes Müller von Königsberg (1436–1476), commonly known as Regiomontanus, a pioneer of trigonometry, would prove that it is actually not possible to do so — it is amusing to observe that this in fact makes Aristotle’s argument stronger.

Regiomontanus’ manuscript, titled \textit{De quinque corporibus aequilateris quae vulgo regularis nuncupantur: quae videlicet eorum locum impleant corporalem et quae non, contra commentatorem Aristotelis Averroës¹} is lost. The Italian mathematician and astronomer Francesco Maurolico (1494–1575) mentions Regiomontanus’ work on a manuscript of very similar title [27]. Considering Regiomontanus’ manuscript as lost, he sets out to obtain the same results. He observes (cf. §2, ibid.) that the angles between the faces of a solid are of importance in determining whether the solid tiles space or not. Nowadays one may easily check that the angle between two faces of a regular tetrahedron is \( \arccos \frac{1}{3} \approx 70.52877^\circ \), thus a little less than \( \frac{360^\circ}{5} = 72^\circ \), and one sees that it is therefore impossible to tile \( \mathbb{R}^3 \) with regular tetrahedra. Maurolico himself did a similar computation (cf. §73, ibid.):

\[
\begin{align*}
(...) & \quad \text{Nunc exponam hosce angulos cum suis chordis hic inferius:} \\
& \quad \text{Pyramidis angulus – gradus 70. minutæ 31. secundæ 43\frac{1}{2}. chorda} \\
& \quad 1154701² \\
& \text{More on the history of the tetrahedra packing problem can be found in the paper by Lagarias and Zong [24].}
\end{align*}
\]

¹On the five equilateral bodies, that are usually called regular, and which of them fill their natural space, and which do not, in contradiction to the commentator of Aristotle, Averroës.

²Below I show these angles with their chords:

Angle of the pyramid – 70 degrees. 31 minutes. 43\frac{1}{2} seconds. chord 1154701.
In 2006, Conway and Torquato [15] found surprisingly dense packings of tetrahedra. This sparked renewed interest in the problem and a race for the best construction (cf. Lagarias and Zong [24] and Ziegler [33]). The current record is held by Chen, Engel, and Glotzer [10], who found 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: We know tetrahedra do not tile space, so the maximum packing density is strictly less than 1. The current record rests with Gravel, Elser, and Kallus [18], who proved an upper bound of \( 1 - \frac{2\sqrt{2}}{10^{25}} \).

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.

Our paper can be seen as a step in the search for good upper bounds for the maximum density of tetrahedra packings. Its main theorem is a generalization of the linear programming bound of Cohn and Elkies [12] for the sphere packing density, which provides the best known upper bounds in small and high dimensions (cf. Cohn and Zhao [13]). To specify a sphere packing it suffices to give the centers of the spheres in the packing; this is the reason why the Cohn-Elkies bound is a linear programming bound. In our case, to specify a packing of congruent copies of a body, we need also to consider different rotations of the body, and so linear programming is replaced by semidefinite programming.

We apply the theorem to packings of pentagons in the plane because the specific structure of the Euclidean plane simplifies computations and because such packings are interesting in themselves (see e.g. Kuperberg and Kuperberg [22], Casselman [9], and Atkinson, Jiao, and Torquato [2]), obtaining an upper bound of 0.98103 for the density of any such packing, whereas the best known construction is a packing consisting of pentagons placed in two opposite orientations achieving a density of \( (5 - \sqrt{5})/3 = 0.9213 \ldots \) (cf. Kuperberg and Kuperberg, ibid.). Using more refined computational tools, it is conceivable that our upper bound could be improved. Our main goal however was to show how the theorem can be applied and that it gives bounds well-below the trivial bound of 1. Our long-term goal is to apply the theorem to obtain upper bounds for packings in \( \mathbb{R}^3 \), in particular tetrahedra packings.

1.1. The main theorem. We defined the density of a packing informally, as the fraction of space it covers. There are different ways to formalize this definition, and questions arise as to whether every packing has a density and so on. We postpone such discussion to [2] when we shall prove the main theorem.

Let \( \text{SO}(n) \) be the group of rotations of \( \mathbb{R}^n \), that is,

\[
\text{SO}(n) = \{ A \in \mathbb{R}^{n \times n} : A^T A = I \text{ and } \det A = 1 \}.
\]

The set \( \mathcal{M}(n) = \mathbb{R}^n \times \text{SO}(n) \) is a group with identity element \((0, I)\), multiplication defined as

\[
(x, A)(y, B) = (x + Ay, AB),
\]
and inversion given by 
\[(x, A)^{-1} = (-A^{-1}x, A^{-1}).\]

The group \(M(n)\), the semidirect product \(\mathbb{R}^n \rtimes \text{SO}(n)\), is the *Euclidean motion group* of \(\mathbb{R}^n\); it is a noncompact (but locally compact), noncommutative group. When we integrate functions over \(M(n)\), we always use the measure \(dx\) for \(\mathbb{R}^n\) with the Haar measure \(dA\) for \(\text{SO}(n)\), normalized so that \(\text{SO}(n)\) has total measure 1.

A bounded complex-valued function \(f \in L^\infty(M(n))\) is said to be of **positive type** if 
\[f(x, A) = f((x, A)^{-1}) \quad \text{for all } (x, A) \in M(n)\]
and for all \(\rho \in L^1(M(n))\) we have
\[\int_{M(n)} \int_{M(n)} f((y, B)^{-1}(x, A)) \rho(y, A) \rho(y, B) d(y, B) d(x, A) \geq 0.\]

With this we have all we need for presenting the main theorem.

**Theorem 1.** Let \(K \subseteq \mathbb{R}^n\) be a convex body and let \(f \in L^1(M(n))\) be a bounded real-valued function such that:

(i) \(f\) is continuous and of positive type;
(ii) \(f(x, A) \leq 0\) whenever \(K^c \cap (x + AK^c) = \emptyset\), where \(K^c\) is the interior of \(K\);
(iii) \(\lambda = \int_{M(n)} f(x, A) d(x, A) > 0\).

Then the density of any packing of congruent copies of \(K\) is at most 
\[\frac{f(0, I)}{\lambda} \text{vol } K,\]
where \(\text{vol } K\) is the volume of \(K\).

This theorem is a generalization of a theorem of Cohn and Elkies [12] that provides upper bounds for the maximum density of sphere packings, and more generally also for translational packings of convex bodies.

It can also be seen as an extension of the Lovász theta number [26], a parameter originally defined for finite graphs, to the infinite packing graph for the body \(K\). Our proof of Theorem 1 in [2] relies on this connection and will make it clear.

Finally, applying Theorem 1 to find upper bounds for the densities of packings of a given body \(K \subseteq \mathbb{R}^n\) means finding a good function \(f\) satisfying the conditions required in the theorem. In §3 to find such a function for the case of pentagon packings, we use a computational approach that relies on semidefinite programming (see §2) and the harmonic analysis of the Euclidean motion group of the plane (see §4). Here is a place where we see that it is simpler to deal with pentagon packings than with tetrahedra packings, since the formulas describing the harmonic analysis of \(M(2)\) are much simpler, specially from a computational perspective, than those describing the harmonic analysis of \(M(3)\).

2. Proving the main theorem

2.1. Packing density and periodic packings. To give a proof of Theorem 1 we need to present some technical considerations regarding the density of a packing. Here we follow Appendix A of Cohn and Elkies [12].
Let $K \subseteq \mathbb{R}^n$ be a convex body and $\mathcal{P}$ be a packing of congruent copies of $K$. We say that the density of $\mathcal{P}$ is $\Delta$ if for all $p \in \mathbb{R}^n$ we have

$$\Delta = \lim_{r \to \infty} \frac{\text{vol}(B(p,r) \cap \mathcal{P})}{\text{vol} B(p,r)},$$

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

$$\limsup_{r \to \infty} \sup_{p \in \mathbb{R}^n} \frac{\text{vol}(B(p,r) \cap \mathcal{P})}{\text{vol} B(p,r)}.$$

We say that a packing $\mathcal{P}$ is periodic if there is a lattice $L \subseteq \mathbb{R}^n$ that leaves $\mathcal{P}$ invariant, i.e., which is such that $\mathcal{P} = x + \mathcal{P}$ for all $x \in L$; here, $L$ is the periodicity lattice of $\mathcal{P}$. In other words, an invariant packing consists of some congruent copies of $K$ arranged 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 have well-defined densities. Moreover, it is not hard to prove that given any packing $\mathcal{P}$, one may define a sequence of periodic packings whose fundamental cells have volumes approaching infinity and whose densities converge to the upper density of $\mathcal{P}$. So in computing bounds for the packing density of a given body, one may restrict oneself to periodic packings. This restriction is particularly interesting because it allows us to compactify the problem, as we will see later on.

2.2. A generalization of the Lovász theta number. Let $G = (V,E)$ be an undirected graph without loops, finite or infinite. A set $I \subseteq V$ is independent if no two vertices in $I$ are adjacent. The independence number of $G$, denoted by $\alpha(G)$, is the maximum cardinality of an independent set of $G$.

Packings of a given body $K \subseteq \mathbb{R}^n$ correspond to the independent sets of the packing graph of $K$. This is the graph whose vertices are the elements of $M(n)$. Here, vertex $(x,A) \in M(n)$ corresponds to the congruent copy $x + AK$ of $K$. Two vertices are adjacent when the corresponding copies of $K$ cannot both be in the packing at the same time, i.e., when they intersect in their interiors. In other words, distinct vertices $(x,A)$ and $(y,B)$ are adjacent if

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

Clearly, an independent set of the packing graph corresponds to a packing and vice versa. The packing graph however has infinite independent sets, and so its independence number is also infinite.

If we consider periodic packings we may manage to work with graphs that, though infinite, have a compact vertex set and also a finite independence number. Given a lattice $L \subseteq \mathbb{R}^n$, write $M(n)/L = (\mathbb{R}^n/L) \times \text{SO}(n)$. Note that this is a compact set. Here, we assume that the fundamental cell of $L$ is big enough so that there exists a nonempty periodic packing with periodicity lattice $L$.

Consider the graph $G_L$ whose vertex set is $M(n)/L$ and in which two distinct vertices $(x,A)$ and $(y,B)$ are adjacent if there is $v \in L$ such that

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

\[A\] A lattice is a discrete subgroup of $(\mathbb{R}^n, +)$.

\[4\] Like all the graphs considered in this paper.
In this setting, a vertex \((x, A) \in M(n)/L\) now represents all bodies \(v + x + AK\) for \(v \in L\), and we put an edge between two distinct vertices if any of the corresponding bodies overlap.

So, independent sets of \(G_L\) correspond to periodic packings with periodicity lattice \(L\) and vice versa. Moreover, \(G_L\) has finite independence number, and we actually have that the maximum density of a periodic packing with periodicity lattice \(L\) is equal to

\[
\frac{\alpha(G_L)}{\text{vol}(\mathbb{R}^n/L)} \text{ vol} K.
\]

In view of the fact that we may restrict ourselves to periodic packings, as seen in the previous section, if we manage to find an upper bound for \(\alpha(G_L)\) for every \(L\), then we obtain an upper bound for the maximum density of any packing of \(K\).

Computing the independence number of a finite graph is an NP-hard problem, figuring in the list of combinatorial problems proven to be NP-hard by Karp [20]. Lovász [26] introduced a graph parameter, the theta number, that provides an upper bound for the independence number of a finite graph and that can be computed in polynomial time. In Theorem 2 we present a generalization of the theta number to graphs defined over certain measure spaces, like the graph \(G_L\).

To present our theorem we need first a few definitions and facts from functional analysis. For background we refer the reader to the book by Conway [14].

Let \(V\) be a separable and compact topological space and \(\mu\) be a finite Borel measure on \(V\) which is such that every nonempty open subset of \(V\) has nonzero measure. There are many examples of such a space. For instance, any finite set \(V\) with the counting measure provides such an example, as does \(M(n)/L\) with its natural measure.

A Hilbert-Schmidt kernel, or simply a kernel, is a square-integrable function \(K: V \times V \to \mathbb{C}\). A kernel defines an operator \(T_K: L^2(V) \to L^2(V)\) as follows: for \(f \in L^2(V)\) and \(x \in V\) we have

\[
\langle T_K f \rangle(x) = \int_V K(x, y) f(y) \, d\mu(y).
\]

An eigenfunction of \(K\) is a nonzero function \(f \in L^2(V)\) such that \(T_K f = \lambda f\) for some \(\lambda \in \mathbb{C}\). We say that \(\lambda\) is the eigenvalue associated with \(f\).

A kernel \(K\) is Hermitian if \(K(x, y) = \overline{K(y, x)}\) for all \(x, y \in V\); a Hermitian kernel defines a self-adjoint operator \(T_K\). We say that \(K\) is positive if it is Hermitian and for all \(\rho \in L^2(V)\) we have

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

This is equivalent to \(\langle T_K \rho, \rho \rangle \geq 0\) for all \(\rho \in L^2(V)\), where

\[
\langle f, g \rangle = \int_V f(x) \overline{g(x)} \, d\mu(x)
\]

is the standard inner product between \(f, g \in L^2(V)\). Further still, a Hermitian kernel is positive if and only if all its eigenvalues are nonnegative.

**Theorem 2.** Let \(G = (V, E)\) be a graph, where \(V\) is a separable and compact topological space having a finite Borel measure \(\mu\) such that every nonempty open
set of $V$ has nonzero measure. Suppose that kernel $K: V \times V \to \mathbb{R}$ satisfies the following conditions:

(i) $K$ is continuous;
(ii) $K(x, y) \leq 0$ whenever $x \neq y$ are nonadjacent;
(iii) $K - J$ is positive, where $J$ is the constant 1 kernel.

Then, for any number $B$ such that $B \geq K(x, x)$ for all $x \in V$, we have $\alpha(G) \leq B$.

Notice that any kernel $K$ satisfying the conditions of the theorem provides an upper bound for $\alpha(G)$. For a finite graph, the optimal bound given by the theorem is exactly the theta prime number of the graph $G$, a strengthening of the theta number introduced independently by McEliece, Rodemich, and Rumsey [28] and Schrijver [29].

Such generalizations of the theta number have been considered before by Bachoc, Nebe, Oliveira, and Vallentin [6], where it is proved that the linear programming bound of Delsarte, Goethals, and Seidel [16] for the sizes of spherical codes comes from such a generalization.

To prove the theorem we need the following alternative characterization of continuous and positive kernels: A continuous kernel $K: V \times V \to \mathbb{C}$ is positive if and only if for all $m$ and any choice $x_1, \ldots, x_m$ of points in $V$ the matrix $(K(x_i, x_j))_{i,j=1}^m$ is positive semidefinite (cf. Lemma 1 in Bochner [7]). In fact, here is where the hypothesis on $V$ is used: To prove this, one needs to use the fact that $V$ is compact, separable, and that the measure $\mu$ is finite and nonzero on nonempty open sets.

Proof of Theorem 2. Let $I \subseteq V$ be a nonempty finite independent set. Since $K - J$ is a continuous and positive kernel, we have that

$$\sum_{x,y \in I} K(x,y) \geq \sum_{x,y \in I} J(x,y) = |I|^2.$$  

Since $K$ satisfies condition (ii), if $B$ is an upper bound on the diagonal entries of $K$ we have that

$$|I|B \geq \sum_{x \in I} K(x,x) \geq \sum_{x,y \in I} K(x,y) \geq |I|^2,$$

and then $B \geq |I|$, as we wanted. \qed

2.3. A proof of the main theorem. The proof of Theorem 1 is similar to the proof of Theorem 3.1 in the paper by de Laat, Oliveira, and Vallentin [23]. We first prove the theorem for functions of bounded support and then extend it to $L^1$ functions.

Let $f: M(n) \to \mathbb{R}$ be a function of bounded support satisfying conditions (i)–(iii) in Theorem 1. Given a lattice $L \subseteq \mathbb{R}^n$ whose fundamental cell is big enough so that there is a nonempty periodic packing with periodicity lattice $L$, we use $f$ to define a kernel $K_L: (M(n)/L) \times (M(n)/L) \to \mathbb{R}$ satisfying conditions (i)–(iii) of Theorem 2 for the graph $G_L$, defined in the previous section.

In fact, we let

$$K_L((x,A),(y,B)) = \sum_{v \in L} f((y-v,B)^{-1}(x,A))$$

$$= \sum_{v \in L} f(B^{-1}(x-y+v),B^{-1}A)$$

for every $(x,A),(y,B) \in M(n)/L$.
Since \( f \) has bounded support and \( x, y \in \mathbb{R}^n/L \), the sum above is actually a finite sum. This shows not only that \( K_L \) is well-defined, but also that it is continuous.

We claim that \( K_L \) has the following properties:

K1. it is a positive kernel;
K2. the constant 1 function is an eigenfunction of \( K_L \), with eigenvalue \( \lambda \);
K3. \( K_L((x, A), (y, B)) \leq 0 \) if \((x, A) \neq (y, B)\) are nonadjacent in \( G_L \);
K4. \( f(0, I) \geq K_L((x, A), (x, A)) \) for all \((x, A) \in M(n)/L \).

Once we have established these properties, it becomes clear that the kernel

\[
\tilde{K}_L = \frac{\text{vol}(\mathbb{R}^n/L)}{\lambda} K_L
\]

satisfies conditions (i)–(iii) of Theorem 2 for the graph \( G_L \). In particular, the fact that \( \tilde{K}_L - J \) is positive follows directly from K1 and K2 above, because the constant 1 function is an eigenfunction of both \( \tilde{K}_L \) and \( J \) with associated eigenvalue \( \text{vol}(\mathbb{R}^n/L) \) in both cases.

But then from K4 we may take \( B = f(0, I) \text{vol}(\mathbb{R}^n/L)/\lambda \) in Theorem 2 and obtain the bound

\[
\alpha(G_L) \leq f(0, I) \frac{\text{vol}(\mathbb{R}^n/L)}{\lambda}.
\]

So the maximum density of any periodic packing with periodicity lattice \( L \) is bounded from above by (cf. equation [1])

\[
\frac{\alpha(G_L)}{\text{vol}(\mathbb{R}^n/L)} \text{vol} \mathcal{K} \leq \frac{f(0, I)}{\lambda} \text{vol} \mathcal{K},
\]

and since \( L \) is an arbitrary lattice, we would have a proof of Theorem 1.

So we set out to prove K1–K4. Property K1 is implied by the fact that \( f \) is of positive type. In fact, since \( f(x, A) = \overline{f((x, A)^{-1})} \), kernel \( K_L \) is Hermitian by construction. Now take a function \( \rho \in L^2(M(n)/L) \). We also view \( \rho \) as the periodic function \( \rho: M(n) \to \mathbb{C} \) such that \( \rho(x + v, A) = \rho(x, A) \) for all \( v \in L \). For \( T > 0 \), write \( M_T(n) = [-T, T]^n \times \text{SO}(n) \). Then

\[
\lim_{T \to \infty} \frac{\text{vol}(\mathbb{R}^n/L)}{\text{vol}[-T, T]^n} \int_{M(n)} \int_{M(n)} K_L((x, A), (y, B)) \rho(x, A) \overline{\rho(y, B)} \, d(y, B) \, d(x, A).
\]
Above, from the second to the third line we exchange the sum with the innermost integral and use the fact that, if \( h: \mathbb{R}^n \to \mathbb{C} \) is an integrable function, then
\[
\sum_{v \in L} \int_{\mathbb{R}^n/L} h(x+v) \, dx = \int_{\mathbb{R}^n} h(x) \, dx.
\]

To go from the third to the fourth line we notice that the function \( (x,A) \mapsto \int_{\mathbb{M}(n)} f((y,B)^{-1}(x,A)) \rho(y,B) \, d(y,B) \) is periodic with respect to the lattice \( L \). From the fourth to the fifth line we use the fact that \( f \) is of bounded support. Finally, from the fifth to the sixth line we apply directly the definition of a function of positive type.

To see \( K_2 \), we use (3) and notice that for a fixed \( (x,A) \in \mathbb{M}(n)/L \) we have
\[
\int_{\mathbb{M}(n)/L} K_L((x,A), (y,B)) \, d(y,B) = \int_{\mathbb{M}(n)/L} \sum_{v \in L} f((y-v,B)^{-1}(x,A)) \, d(y,B)
\]
\[
= \int_{\mathbb{M}(n)} f((y,B)^{-1}(x,A)) \, d(y,B)
\]
\[
= \lambda.
\]

To prove \( K_3 \), recall that \( (x,A), (y,B) \in \mathbb{M}(n)/L \) are nonadjacent if for all \( v \in L \) we have \( K^o \cap (B^{-1}(x-x+y) + B^{-1}AK^o) = \emptyset \). But then, since \( f \) satisfies (ii) in the statement of Theorem 1, every summand in (2) will be nonpositive, implying \( K_3 \).

Property \( K_4 \) may be similarly proven. In fact, since from start we assumed \( L \) has a large enough fundamental cell, for \( v \in L \) with \( v \neq 0 \) we have \( K^o \cap (A^{-1}v+K^o) = \emptyset \). But then in expression (2) for \( K_L((x,A), (x,A)) \), all summands but the one for \( v = 0 \) will be nonpositive, and the summand for \( v = 0 \) is exactly \( f(0,I) \), proving \( K_4 \).

So we have \( K_1-K_4 \), and Theorem 1 follows for functions \( f \) of bounded support. To prove the theorem for a given \( L^1 \) function, we approximate it by functions of bounded support as follows.

Let \( f \in L^1(\mathbb{M}(n)) \) be a real-valued function satisfying conditions (i)–(iii) in Theorem 1. For \( T > 0 \), consider the function \( g_T: \mathbb{M}(n) \to \mathbb{R} \) given by
\[
g_T(x,A) = \frac{\text{vol}(B(0,T) \cap B(x,T))}{\text{vol } B(0,T)} f(x,A),
\]
where \( B(x,T) \) is the ball of radius \( T \) centered at \( x \).

Clearly, \( g_T \) is continuous and has bounded support. We claim that it is also a function of positive type.

To see this, we will use a characterization of continuous functions of positive type analogous to the characterization of continuous positive kernels given in 2.2, namely: A continuous function \( f \in L^\infty(\mathbb{M}(n)) \) is of positive type if and only if the matrix
\[
(f((x_j, A_j)^{-1}(x_i, A_i)))_{i,j=1}^m
\]
is positive semidefinite for any \( m \) and any elements \( (x_1, A_1), \ldots, (x_m, A_m) \in \mathbb{M}(n) \) (cf. Folland [17], Proposition 3.35).
Let \((x_1, A_1), \ldots, (x_m, A_m) \in M(n)\) be any given elements. Let \(\chi_i : \mathbb{R}^n \to \{0, 1\}\) be the characteristic function of \(B(x_i, T)\) and denote by \(\langle f, g \rangle\) the standard inner product between functions \(f, g \in L^2(\mathbb{R}^n)\). Then
\[
gr_T((x_j, A_j)^{-1}(x_i, A_i)) = \frac{\operatorname{vol}(B(0, T) \cap B(A_j^{-1}(x_i - x_j), T))}{\operatorname{vol} B(0, T)} f((x_j, A_j)^{-1}(x_i, A_i)) \]
\[
= \frac{\operatorname{vol}(B(x_i, T) \cap B(x_j, T))}{\operatorname{vol} B(0, T)} f((x_j, A_j)^{-1}(x_i, A_i)) \]
\[
= \frac{\langle \chi_i, \chi_j \rangle}{\operatorname{vol} B(0, T)} f((x_j, A_j)^{-1}(x_i, A_i)).
\]

This shows that the matrix
\[
(\langle g_T((x_j, A_j)^{-1}(x_i, A_i)) \rangle_{i,j=1}^m)
\]
is the Hadamard (entrywise) product of the matrices
\[
(f((x_j, A_j)^{-1}(x_i, A_i)))_{i,j=1}^m
\]
and
\[
\frac{1}{\operatorname{vol} B(0, T)} (\langle \chi_i, \chi_j \rangle)_{i,j=1}^m.
\]
The first matrix above is positive semidefinite since \(f\) is of positive type. The second matrix is positive semidefinite since it is a positive multiple of the Gram matrix of vectors \(\chi_1, \ldots, \chi_m\). So we have that \(\frac{1}{\lambda_T}\) is positive semidefinite, and thus \(g_T\) is of positive type.

By construction, whenever \(f(x, A) \leq 0\), also \(g_T(x, A) \leq 0\). So \(g_T\) is a continuous function of bounded support satisfying conditions (i) and (ii) from the statement of Theorem 1. This implies immediately that
\[
\frac{g_T(0, I)}{\lambda_T} \operatorname{vol} \mathcal{K} = \frac{f(0, I)}{\lambda_T} \operatorname{vol} \mathcal{K}
\]
is an upper bound for the density of any packing of congruent copies of \(\mathcal{K}\), where
\[
\lambda_T = \int_{M(n)} g_T(x, A) \ d(x, A).
\]
To finish, notice that \(g_T\) converges pointwise to \(f\) as \(T \to \infty\). Moreover, for all \(T\) we have \(|g_T(x, A)| \leq |f(x, A)|\). So it follows from Lebesgue’s dominated convergence theorem that \(\lambda_T \to \lambda\) as \(T \to \infty\). This together with \(\frac{1}{\lambda_T}\) finishes the proof of Theorem 1

2.4. Using the symmetry of the body. Let \(\mathcal{K} \subseteq \mathbb{R}^n\) be a convex body. Its symmetry group is the subgroup of SO\((n)\) defined as
\[
S(\mathcal{K}) = \{ A \in \text{SO}(n) : A \mathcal{K} = \mathcal{K}\}.
\]
The action by conjugation of an element \(B \in \text{SO}(n)\) on a function \(f \in L^1(M(n))\) is given by
\[
(B \cdot f)(x, A) = f((0, B)^{-1}(x, A)(0, B)).
\]
Suppose now \(G\) is a compact subgroup of \(S(\mathcal{K})\). Then in Theorem 1 we may restrict ourselves to \(G\)-invariant functions \(f \in L^1(M(n))\) without affecting the bound obtained. Here we say that \(f\) is \(G\)-invariant if \(B \cdot f = f\) for all \(B \in G\).

This restriction to \(G\)-invariant functions may make it easier to apply Theorem 1. This is actually the case for our application to pentagon packings, as we will see in 5.
Computing upper bounds for the packing density of congruent copies of a convex body

To see that the restriction to \(G\)-invariant functions does not affect the bound that can be obtained from Theorem 1, notice that, if \(f \in L^1(M(n))\) is a bounded continuous function satisfying conditions (i)–(iii) of Theorem 1, then also \(B \cdot f\), for \(B \in G\), satisfies these conditions.

In fact, to show that \(B \cdot f\) is of positive type, let \((x_1, A_1), \ldots, (x_m, A_m) \in M(n)\). Then
\[
((B \cdot f)((x_j, A_j)^{-1}(x_i, A_i)))_{i,j=1}^m = (f(((0, B)^{-1}(x_j, A_j)^{-1}(x_i, A_i)(0, B))))_{i,j=1}^m
\]
and since \(f\) is of positive type, \(B \cdot f\) is also of positive type (cf. the alternative characterization of continuous functions of positive type in the previous section).

To see that \(B \cdot f\) satisfies condition (ii) of Theorem 1, notice that, since \(B^{-1}K = K\), we have \(K^o \cap (x + AK^o) = \emptyset\) if and only if \(K^o \cap (B^{-1}x + B^{-1}ABK^o) = \emptyset\).

Finally, we have
\[
\int_{M(n)} (B \cdot f)(x, A) d(x, A) = \int_{M(n)} f(x, A) d(x, A),
\]
and so we see that \(B \cdot f\) satisfies the conditions of Theorem 1 and provides the same bound as \(f\).

Now, since \(G\) is compact, it admits a Haar measure \(\mu\) which we normalize so that \(\mu(G) = 1\). Then it is immediate that the function \(\overline{f} \in L^1(M(n))\) such that
\[
\overline{f}(x, A) = \int_G (B \cdot f)(x, A) d\mu(B)
\]
satisfies (i)–(iii) of Theorem 1 and provides the same bound as \(f\). Moreover, \(\overline{f}\) is \(G\)-invariant. So it follows that a restriction to \(G\)-invariant functions does not affect the bound of Theorem 1.

By exploiting the symmetry of the body \(K\), we may also weaken condition (ii) of Theorem 1, obtaining the following version of it:

**Theorem 3.** Let \(K \subseteq \mathbb{R}^n\) be a convex body, \(G\) be a subgroup of \(S(K)\), and \(T\) be a set of representatives of the left cosets of \(G\) in \(SO(n)\).

Let \(f \in L^1(M(n))\) be a bounded real-valued function such that:

(i) \(f\) is continuous and of positive type;
(ii) \(f(x, A) \leq 0\) for all \(x \in \mathbb{R}^n\) and \(A \in T^{-1}T\) such that \(K^o \cap (x + AK^o) = \emptyset\);
(iii) \(\lambda = \int_{M(n)} f(x, A) d(x, A) > 0\).

Then the density of any packing of congruent copies of \(K\) is at most
\[
\frac{f(0, I)}{\lambda} \cdot \text{vol } K,
\]
where \(\text{vol } K\) is the volume of \(K\).

**Proof.** For a lattice \(L \subseteq \mathbb{R}^n\) with large enough fundamental cell, we define kernel \(K_L : (M(n)/L) \times (M(n)/L) \to \mathbb{R}\) as in (2). Following the proof of Theorem 1, we know that \(K_L\) satisfies properties K1, K2, and K4. Because of condition (ii) above, kernel \(K_L\) also satisfies a weaker version of K3, namely we have \(K_L((x, A), (y, B)) \leq 0\) for all \(x, y \in \mathbb{R}^n\) and \(A, B \in T\) such that \((x, A)\) and \((y, B)\) are distinct, nonadjacent vertices of \(G_L\). This can be seen from (2), because since \(A, B \in T\), and therefore \(B^{-1}A \in T^{-1}T\), every summand in (2) is nonpositive.
Since \( K_L \) does not necessarily satisfy condition (ii) of Theorem 2, we may not directly apply this theorem to bound \( \alpha(G_L) \), but we may still use \( K_L \) to find such a bound, by repeating the proof of Theorem 2.

Let \( (x_1, A_1), \ldots, (x_m, A_m) \) be an independent set of \( G_L \). For each \( A_i \), let \( \overline{A}_i \in T \) belong to the same coset of \( A_i \). Then \( \overline{A}_i K = A_i \mathcal{K} \), so that \( (x_1, \overline{A}_1), \ldots, (x_m, \overline{A}_m) \) is also an independent set of \( G_L \). Now we have,

\[
mf(0,I) \frac{\text{vol}(\mathbb{R}^n/L)}{\lambda} \geq \sum_{i,j=1}^{m} \frac{\text{vol}(\mathbb{R}^n/L)}{\lambda} K_L((x_i,\overline{A}_i),(x_j,\overline{A}_j)) \geq m^2,
\]

and hence we obtain the bound

\[
\alpha(G_L) \leq f(0,I) \frac{\text{vol}(\mathbb{R}^n/L)}{\lambda}
\]

and the theorem follows. \( \square \)

3. Semidefinite Programming and Sums of Squares

We collect here the basic facts we need from semidefinite programming. For further background we refer to the book by Ben-Tal and Nemirovski [5].

A linear programming problem amounts to maximizing a linear function over a polyhedron, which is the intersection of the nonnegative orthant \( \mathbb{R}^n_0 \) with an affine subspace. A semidefinite programming problem — a rich generalization of linear programming — amounts to maximizing a linear function over a spectrahedron, the intersection of the cone of positive semidefinite matrices \( S^n_0 \) with an affine subspace. A semidefinite programming problem in primal standard form is

\[
\sup \left\{ \langle C, X \rangle : X \in S^n_0, \langle A_j, X \rangle = b_j, j = 1, \ldots, m \right\},
\]

where \( C, A_1, \ldots, A_m \) are given \( n \times n \) matrices and where \( b_1, \ldots, b_m \in \mathbb{C} \). Here \( \langle A, B \rangle = \text{tr}(B^*A) \) denotes the trace inner product between matrices. Matrices \( C \) and \( A_i \) are usually required to be symmetric (or Hermitian). The seemingly more general setting used here can be easily reduced to this restricted version though.

Semidefinite programming problems are conic optimization problems. Sometimes it is convenient to assume that the variable matrix \( X \) has block-diagonal structure, which amounts to changing the cone \( S^n_0 \) to the direct product \( S^n_{0_1} \times \cdots \times S^n_{0_k} \). For solving semidefinite programming problems two types of algorithms are available: the ellipsoid method and interior point methods. The ellipsoid method focuses on the existence of polynomial-time algorithms but no practical implementation is available. In contrast to this there are many very good implementations of interior point methods.

Semidefinite programming is specially useful for certifying the nonnegativity of polynomials or of trigonometric polynomials via sums of squares. We quickly discuss the univariate case — the multivariate case is a simple extension.

A univariate polynomial \( p \in \mathbb{R}[x] \) of degree \( 2d \) is a sum of squares, i.e., it can be written as

\[
p = h_1^2 + \cdots + h_r^2 \quad \text{for some } r \in \mathbb{N} \text{ and } h_1, \ldots, h_r \in \mathbb{R}[x] \text{ of degree at most } d
\]

if and only if there is a positive semidefinite matrix \( Q \) with

\[
p = \langle V, Q \rangle,
\]

where \( V \) is a matrix of polynomials such that \( V_{kl} = P_k(x)P_l(x) \) for some basis \( P_k \) of the space of polynomials of degree at most \( d \).
Note $p = \langle V, Q \rangle$ is an identity between polynomials. One can check it by linear equalities — equating the coefficients — once one writes both sides in terms of some basis.

If a polynomial can be written as a sum of squares, then it is clearly nonnegative. For univariate polynomials, the converse is also true. This is not the case in general, however; Laurent [25] presents a survey.

A similar approach can be applied to trigonometric polynomials. Such is an expression of the sort
\[ p(\theta) = \sum_{k=-n}^{n} c_k e^{ik\theta}, \]
where $c_k = \overline{c_{-k}}$. One way to certify that this trigonometric polynomial is nonnegative for all $\theta$ is to write it as a sum of squares, that is, to write it as
\[ p(\theta) = |h_1(e^{i\theta})|^2 + \cdots + |h_r(e^{i\theta})|^2 \]
for some number $r$ and some univariate polynomials $h_1, \ldots, h_r$. Now, being a sum of squares is equivalent to the existence of an $(n+1) \times (n+1)$ positive semidefinite matrix $Q$ such that
\[ p(\theta) = \langle V(e^{i\theta}), Q \rangle, \]
where $V$ is the matrix with $V_{kl}(z) = z^k - l$.

4. Harmonic analysis on $M(2)$

Our approach to apply Theorem 1 in order to obtain upper bounds for the maximum density of pentagon packings is to specify the function $f$ via its Fourier transform. So here we quickly present the facts from the theory of harmonic analysis on $M(2)$ that we will use. We follow Sugiura [31] closely, though we deviate at some points, mainly concerning choices of normalization, as we will see.

For $x, y \in \mathbb{R}^2$, denote by $x \cdot y = x_1y_1 + x_2y_2$ the Euclidean inner product. Let $S^1$ be the unit circle and for $\varphi, \psi \in L^2(S^1)$ denote by $\langle \varphi, \psi \rangle$ the standard inner product between $\varphi$ and $\psi$, i.e.,
\[ \langle \varphi, \psi \rangle = \frac{1}{\omega(S^1)} \int_{S^1} \varphi(\xi)\overline{\psi(\xi)} d\omega(\xi), \]
where $\omega$ is the Lebesgue measure on the unit circle.

For $a \geq 0$ and $(x, A) \in M(2)$, consider the operator $U^a_{(x, A)}: L^2(S^1) \rightarrow L^2(S^1)$ defined as follows: For $\varphi \in L^2(S^1)$ we have
\[ [U^a_{(x, A)}\varphi](\xi) = e^{2\pi i ax \cdot \xi} \varphi(A^{-1}\xi) \]
for all $\xi \in S^1$. (In the definition of $U^a_{(x, A)}$ we differ from Sugiura [31], who omits the factor $2\pi$, which we include to obtain better formulas — from a computational point of view — later on. Besides changing some normalization parameters, this does not affect the theory as presented by Sugiura.)

Operator $U^a_{(x, A)}$ is a bounded and unitary operator. Moreover, one can easily check that
\[ U^a_{(x, A)(y, B)} = U^a_{(x, A)} U^a_{(y, B)} \]
for all $(x, A), (y, B) \in M(2)$. So the strongly continuous map $\rho_a(x, A) = U^a_{(x, A)}$ provides a representation of $M(2)$ for every $a \geq 0$. Representations $\rho_a$, for $a > 0$, are all irreducible and pairwise nonequivalent.
Given a function \( f \in L^1(M(2)) \), its Fourier transform at \( a \geq 0 \) is the bounded operator \( \hat{f}(a) : L^2(S^1) \to L^2(S^1) \) defined as

\[
\hat{f}(a) = \int_{M(2)} f(x, A) U_{(x, A)}^a \, d(x, A).
\]

Having defined the Fourier transform of \( f \), we would like to have an inversion formula, that is, a way to compute \( f \) back from its Fourier transform. In our case the inversion formula takes the following shape:

\[
f(x, A) = 2\pi \int_0^\infty \text{tr}(U_{(x, A)}^a \hat{f}(a)) \, da,
\]

where \( \text{tr} F \) is the trace of a trace-class operator \( F \) (see, e.g., Conway [14]). Here we again deviate slightly from the exposition of Sugiura. The extra factor of \( 2\pi \) in the above formula as compared to Theorem 3.1 in his book [31] follows from the different normalization he uses for the measure of \( M(2) \).

Of course, it is not always the case that the inversion formula holds or converges everywhere. In the book by Sugiura it is shown that the inversion formula holds for rapidly decreasing functions (see Definition 3 in Chapter IV, §3 in Sugiura [31]).

We will provide explicit formulas for the Fourier transform and hence obtain explicit formulas for \( f \). In this way it will be clear in our application that \( f \) is continuous and \( L^1 \). To ensure that \( f \) is of positive type, the following lemma will be useful.

**Lemma 3.1.** Suppose that for each \( a \geq 0 \) we have that \( \hat{f}(a) \) is a Hilbert-Schmidt, positive, trace-class operator. Then, if the function \( f \) defined in (6) is bounded and continuous, it is of positive type.

**Proof.** Take \((x_1, A_1), \ldots, (x_m, A_m) \in M(2)\). Recalling the alternative characterization of continuous functions of positive type given in [2,3] we show that the matrix

\[
(f((x_j, A_j)^{-1}(x_i, A_i)))_{i,j=1}^m
\]

is positive semidefinite.

By construction, this is a Hermitian matrix. From (6), to prove it is positive semidefinite it suffices to show that for all \( a \geq 0 \) the matrix

\[
(\text{tr}(U_{(x, A)}^a \hat{f}(a)))_{i,j=1}^m
\]

is positive semidefinite.

Notice that since each \( \hat{f}(a) \) is trace-class, and since \( U_{(x, A)}^a \) is a bounded operator, then \( U_{(x, A)}^a \hat{f}(a) \) is trace-class for all \( (x, A) \in M(2) \), and so each entry of (7) is well-defined.
To compute this, we express
\[ A \]
and we see \( A \) as
\[ \chi \]
for \( \phi \).

We define the
\[ \hat{A} \]
self-adjoint operator such that \( \hat{A} \) is a trace-class, positive, Hilbert-Schmidt operator, it has a square-root system of \( L^2 \) form. We identify both \( \text{SO}(2) \) and \( m \) being the Gram matrix of a unitary operator, \( U \).

Here, we go from the second to the third line by noticing that, since \( U_{(x,A)}^{-1} \) is a unitary operator, \( U_{(x,A)}^{-1} \) is also a complete orthonormal system of \( L^2(\mathbb{S}^1) \). Finally, from the fifth to the sixth line, we observe that since \( \hat{f}(a) \) is a trace-class, positive, Hilbert-Schmidt operator, it has a square-root \( \hat{f}^{1/2}(a) \), a self-adjoint operator such that \( \hat{f}(a) = \hat{f}^{1/2}(a) \hat{f}^{1/2}(a) \).

So we see that (7) is a sum of positive semidefinite matrices, the \( k \)th summand being the Gram matrix of \( m \) vectors, and we are done. \( \square \)

We finish this section by computing a more explicit formula for the inverse transform. We identify both \( \text{SO}(2) \) and \( \mathbb{S}^1 \) with the torus \( \mathbb{R}/(2\pi \mathbb{Z}) \), and by an abuse of language with the interval \([0, 2\pi]\). We equip \( L^2([0, 2\pi]) \) with the inner product
\[
\langle \varphi, \psi \rangle = \frac{1}{2\pi} \int_0^{2\pi} \varphi(\xi)\overline{\psi(\xi)} \, d\xi
\]
for \( \varphi, \psi \in L^2([0, 2\pi]) \). Then the functions \( \chi_r \in L^2([0, 2\pi]) \), for \( r \in \mathbb{Z} \), defined as \( \chi_r(\xi) = e^{ir\xi} \) provide a complete orthonormal system of \( L^2([0, 2\pi]) \).

We define the matrix coefficients of the operator \( U_{(x,A)}^a \) on the basis \( \chi_r \) as
\[
u_{r,s}(x,A) = \langle U_{(x,A)}^a \chi_s, \chi_r \rangle \] with \( r, s \in \mathbb{Z} \).

To compute this, we express \( x \) in polar coordinates as
\[
x = \rho(\cos \theta, \sin \theta)
\]
and we see \( A \) as the rotation matrix
\[
A = A(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix},
\]
which rotates vectors counter-clockwise by an angle of $\alpha$. Then

$$u^a_{r,s}(\rho, \theta, \alpha) = \langle U^a_{(x,A)} \chi_s, \chi_r \rangle$$

$$= \frac{1}{2\pi} \int_{0}^{2\pi} [U^a_{(x,A)} \chi_s](\xi) \chi_r(\xi) d\xi$$

$$= \frac{1}{2\pi} \int_{0}^{2\pi} e^{2\pi i a \rho (\cos \theta, \sin \theta) \cdot (\cos \xi, \sin \xi)} e^{ia(s-\alpha)} e^{-ir \xi} d\xi$$

(9)

$$= \frac{1}{2\pi} e^{-isa} \int_{0}^{2\pi} e^{2\pi i a \rho \cos(\xi-\theta)} e^{i(s-r)\xi} d\xi$$

$$= \frac{1}{2\pi} e^{-isa} \int_{0}^{2\pi} e^{2\pi a \rho \cos \xi} e^{i(s-r)(\xi+\theta)} d\xi$$

$$= \frac{1}{2\pi} e^{-isa} \int_{0}^{2\pi} e^{i(s-r)\xi} e^{2\pi i a \rho \cos \xi} d\xi$$

$$= e^{-isa} J_{s-r}(2\pi a \rho).$$

Here, $J_n(z)$ is the Bessel function of parameter $n$. To obtain the last line, we apply Bessel’s integral (cf. Watson [32], (1) in Chapter II, §2.2).

We may then rewrite (6) by expressing the operators $\hat{f}(a)$ on the basis $\chi_r$, for $r \in \mathbb{Z}$. This gives us

$$f(\rho, \theta, \alpha) = \int_{0}^{\infty} \sum_{r,s \in \mathbb{Z}} \hat{f}(a)_{r,s} u^a_{r,s}(\rho, \theta, \alpha) a \, da$$

(10)

$$= \int_{0}^{\infty} \sum_{r,s \in \mathbb{Z}} \hat{f}(a)_{r,s} e^{-isa} e^{-i(sa+(r-s)\theta)} J_{s-r}(2\pi a \rho) a \, da.$$

5. Computations for pentagon packings

In this section we present a semidefinite programming problem and show how from its solution a function $f$ can be derived that satisfies conditions (i)–(iii) of Theorem 1 when $K$ is a regular pentagon. We describe the semidefinite programming problem in detail, and then discuss how it can be solved with the computer and how a function $f$ can be obtained from its solution that provides the bound of 0.98103 for the maximum density of packings of regular pentagons in $\mathbb{R}^2$.

Throughout this section, $K$ will denote the regular pentagon on $\mathbb{R}^2$ whose vertices are the points

$$\frac{1}{2}(\cos(k2\pi/5), \sin(k2\pi/5)) \quad \text{for } k = 0, \ldots, 4.$$

Note the circumscribed circle of $K$ has radius $1/2$.

The symmetry group of $K$ is isomorphic to $C_5$, the cyclic group of order 5. It consists of the rotation matrices $A(k2\pi/5)$, for $k = 0, \ldots, 4$, where $A(\alpha)$ is given in [8].

5.1. Specifying the function. Our approach is to specify the function $f$ required by Theorem 1 via its Fourier transform. In this section we discuss our choice for the Fourier transform of $f$, give explicit formulas for $f$ in terms of its transform, and show which constraints must be imposed on the transform so that $f$ is a real-valued, $L^1$ and continuous function of positive type which is $S(K)$-invariant.
Let \( N > 0 \) be an integer and \( d \geq 1 \) be an odd integer. Consider the matrix-valued function \( \varphi \) given by

\[
\varphi(a) = \left( \varphi_{r,s}(a) \right)_{r,s=-N}^{N} = \left( \sum_{k=0}^{d} f_{r,s,k} a^{2k} \right)_{r,s=-N}^{N}.
\]

Notice that each \( \varphi(a) \) is a \((2N + 1) \times (2N + 1)\) matrix whose entries are even univariate polynomials in the variable \( a \).

We define \( f \) as the function whose Fourier transform is

\[
\hat{f}(a) = \varphi(a) e^{-\pi a^2}.
\]

Note that we express the operator \( \hat{f}(a) \) in the basis \( \chi_r \) for \( r \in \mathbb{Z} \), as discussed in [1]. Clearly, each \( \hat{f}(a) \) is a trace-class, Hilbert-Schmidt operator. In fact, each \( \hat{f}(a) \) has finite rank.

The reason for our choice for the Fourier transform is that it makes it easy to compute the function \( f \). Let

\[
C_{r,s,k}(\rho) = \frac{\Gamma(k + 1 + |r - s|/2)(\rho \sqrt{\pi})^{|r-s|}}{2\pi^{k+1} \Gamma(|r-s| + 1)}.
\]

Then using (4.11.24) in Andrews, Askey, and Roy [1], since \( J_n(z) = (-1)^n J_{-n}(z) \), we have

\[
\int_{0}^{\infty} a^{2k+1} e^{-\pi a^2} J_{s-r}(2\pi \rho a) da = (-1)^{s-r} \int_{0}^{\infty} a^{2k+1} e^{-\pi a^2} J_{|r-s|}(2\pi \rho a) da
\]

\[
= (-1)^{s-r} C_{r,s,k}(\rho) \; _1F_1 \left( \frac{|r-s|/2 + k}{|r-s| + 1}; \pi \rho^2 \right) e^{-\pi \rho^2},
\]

where \( _1F_1 \) is the hypergeometric series. Together with (10) and (11), this implies for \( f \) the formula

\[
f(\rho, \theta, \alpha) = \sum_{r,s=-N}^{N} \sum_{k=0}^{d} (-1)^{s-r} t^{r-s} e^{-i(s \alpha + (r-s) \theta)} f_{r,s,k} C_{r,s,k}(\rho)
\]

\[
\cdot _1F_1 \left( \frac{|r-s|/2 + k}{|r-s| + 1}; \pi \rho^2 \right) e^{-\pi \rho^2},
\]

where \( (\rho, \theta, \alpha) \) parametrizes an element of \( M(2) \) as in [1].

It is immediately clear that, thanks to our choice of Fourier transform, \( f \) is an \( L^1 \) and continuous function; actually, it is rapidly decreasing. So, by using Lemma 3.1 we see that if \( \hat{f}(a) \) is a positive kernel for each \( a \geq 0 \), then \( f \) is a function of positive type. From the definition of \( \hat{f}(a) \), we see that \( \hat{f}(a) \) is positive for every \( a \geq 0 \) if and only if the matrices \( \varphi(a) \) are positive semidefinite for every \( a \). Notice that requiring \( \varphi(a) \) to be positive semidefinite includes requiring \( \varphi(a) \) to be Hermitian. This on its turn we achieve by imposing the constraint

\[
f_{r,s,k} = f_{s,r,k} \text{ for all } r, s, \text{ and } k.
\]

We may further simplify (13) by imposing two extra conditions on the coefficients \( f_{r,s,k} \). Namely, when \( r - s \) is even and \( |r-s|/2 - k \leq 0 \), the hypergeometric
series in \( [13] \) becomes a Laguerre polynomial. Indeed we have (cf. (6.2.2) in Andrews, Askey, and Roy [1])

\[
_{1}F_{1}\left(\left|\frac{r-s}{2}\right|; \pi \rho^{2}\right) = \frac{n!}{(\pi \rho^{2})^{n}} L_{n}^{r-s}(\pi \rho^{2}),
\]

where \( n = k - \frac{|r-s|}{2} \),

\[
(a)_{n} = a(a+1) \cdots (a+n-1)
\]

and \( L_{n}^{\alpha} \) is the Laguerre polynomial of degree \( n \) and parameter \( \alpha \).

So we impose on the coefficients \( f_{r,s;k} \) the constraints

\[
f_{r,s;k} = 0 \quad \text{if } r - s \text{ is odd or } k < \frac{|r-s|}{2}.
\]

Then \( [13] \) becomes

\[
f(\rho, \theta, \alpha) = \sum_{r,s=-N}^{N} \sum_{k=-|r-s|/2}^{d} (-1)^{|r-s|/2} e^{-i(s\alpha+(r-s)\theta)} f_{r,s;k}
\cdot D_{r,s;k}(\rho)L_{n}^{r-s}(\pi \rho^{2})e^{-\pi \rho^{2}},
\]

where \( D_{r,s;k}(\rho) = C_{r,s;k}(\rho) n!/(|r-s|+1)_{n} \).

To ensure that \( f \) is a real-valued function, we observe from \( [9] \) that when \( r - s \) is even, \( u_{r,s}^{\alpha}(\rho, \theta, \alpha) = \overline{u_{r,s}^{\alpha}(\rho, \theta, \alpha)} \). Then from \( [10] \) it is clear that if \( \varphi_{r,s}(a) = \overline{\varphi_{r,s}(a)} \) for all \( a \geq 0 \) and \( r, s \), function \( f \) is real-valued. So to ensure that \( f \) is real-valued it suffices to impose the constraint

\[
f_{r,s;k} = \overline{f_{r,s;k}} \quad \text{for all } r, s, \text{ and } k.
\]

Finally, we would like to impose constraints on the coefficients \( f_{r,s;k} \) so as to make function \( f \) \( S(K) \)-invariant, that is, so as to have

\[
f(\rho, \theta + l2\pi/5, \alpha) = f(\rho, \theta, \alpha) \quad \text{for } l = 0, \ldots, 4.
\]

From \( [15] \), it is easy to see that one way of achieving this is to require that

\[
f_{r,s;k} = 0 \quad \text{whenever } r - s \equiv 0 \pmod{5}.
\]

Since we already set \( f_{r,s;k} = 0 \) when \( r - s \) is odd, we end up with the constraint

\[
f_{r,s;k} = 0 \quad \text{whenever } r - s \equiv 0 \pmod{10}.
\]

To finish, we summarize the constraints imposed on the coefficients \( f_{r,s;k} \):

1. We consider only the pairs \( r, s \) such that \( r - s \equiv 0 \pmod{10} \) and we set \( f_{r,s;k} = 0 \) if \( k < \frac{|r-s|}{2} \). This has a double effect: It simplifies the hypergeometric series into a Laguerre polynomial and makes the function \( S(K) \)-invariant;
2. We set \( f_{r,s;k} = \overline{f_{r,s;k}} \) for all \( r, s, \) and \( k \). This makes the matrices \( \varphi(a) \) Hermitian. We then require these matrices to be positive semidefinite; this ensures that function \( f \) is of positive type;
3. We set \( f_{r,s;k} = \overline{f_{r-s,k}} \) for all \( r, s, \) and \( k \). This ensures that function \( f \) is real-valued.
With these constraints, we obtain the following formula for $f$:

$$f(\rho, \theta, \alpha) = \sum_{r,s=-N}^{N} \sum_{k=-\lfloor r-s/2 \rfloor}^{\lfloor r-s/2 \rfloor} (-1)^{|r-s|/2} e^{-i(s\alpha+(r-s)\theta)} f_{r,s,k}$$

$$\cdot D_{r,s,k}(\rho) L^{|r-s|/2} \pi^2 e^{-\pi \rho^2}.$$

### 5.2. A semidefinite programming formulation: basic setup

Recall our goal is to describe a semidefinite programming problem whose solutions correspond to functions $f \in L^1(M(n))$ satisfying the conditions of Theorem 1. In this section, we take a first step by showing how to formulate the problem of finding a function $f$ like (11) as a semidefinite programming problem.

We start by making an extra assumption, namely that all coefficients $f_{r,s,k}$ are real. This allows us to work exclusively with real matrices, making the semidefinite programming problem we obtain smaller. In principle, however, everything we describe can be extended to the more general setting of complex coefficients. It could be, though we do not know, that such a restriction to real numbers greatly worsens the bound that can be obtained via our approach.

So let $\varphi$ be given as in (11) with

$$f_{s,r,k} = f_{r,s,k} = f_{-r,-s,k} = f_{-s,-r,k}$$

as we require. Write $y = (y_{-N}, \ldots, y_N)$ and consider the polynomial

$$\sigma(a, y) = \sum_{r,s=-N}^{N} \sum_{k=-\lfloor r-s/2 \rfloor}^{\lfloor r-s/2 \rfloor} f_{r,s,k} a^{2k} y_r y_s.$$

Then $\varphi(a)$ is positive semidefinite for all $a$ if and only if $\sigma$ is a sum of squares (see §3). (Here, it is easy to see that if $\sigma$ is a sum of squares, then $\varphi(a)$ is positive semidefinite for all $a$. The converse is also true; for a proof see Choi, Lam, and Reznick [11]. This fact is related to the Kalman-Yakubovich-Popov lemma in systems and control; see the discussion in Aylward, Itani, and Parrilo [4].)

The constraint that $\sigma$ is a sum of squares can on its turn be formulated in terms of positive semidefinite matrices. Following the recipe given on §3, one would obtain a semidefinite programming formulation in terms of a single variable matrix of large size. In our case, however, since $\sigma$ is an even polynomial in $a$ and since the product $y_r y_s$ only appears when $r-s \equiv 0 \pmod{10}$, we may block-diagonalize the variable matrix, obtaining a formulation in terms of smaller matrices, as we show now.

To this end, let $P_0, P_1, \ldots$ be a sequence of real, even, univariate polynomials such that $P_k$ has degree $2k$. For $j = 0, \ldots, 9$, let

$$I_j = \{ r \in \mathbb{Z} : -N \leq r \leq N \text{ and } r \equiv j \pmod{10} \}.$$

For $i = 0, 1$ and $j = 0, \ldots, 9$, consider the matrix $V^{ij}$ with rows and columns indexed by $\{0, \ldots, [d/2]\} \times I_j$ such that

$$V^{ij}_{(l,r)(l',s)} = a^{2i} P_i(a) P_{l'}(a) y_r y_s$$

for all $l, l' = 0, \ldots, [d/2]$ and $r, s \in I_j$. Notice the entries of $V^{ij}$ are even polynomials in $a$. 
Then \( \sigma \) is a sum of squares if and only if there are real, positive semidefinite matrices \( Q^{ij} \), of appropriate dimensions, such that

\[
\sigma = \sum_{i=0}^{9} \sum_{j=0}^{9} (Q^{ij}, V^{ij}),
\]

where \( (A, B) = \text{tr}(B^*A) \) denotes the trace inner product between matrices \( A \) and \( B \).

Here, it is also important to observe that the symmetry constraints \( f_{r,s:k} = f_{s,r:k} \) are implied by the fact that the matrices \( Q^{ij} \) are symmetric.

So finding real numbers \( f_{r,s:k} \) such that \( f_{r,s:k} = f_{s,r:k} \) and such that \( \varphi(a) \) is positive semidefinite for all \( a \) amounts to finding real positive semidefinite matrices \( Q^{ij} \). Also the other constraints that we imposed on the coefficients \( f_{r,s:k} \) can be represented as linear constraints on the entries of the \( Q^{ij} \) matrices, as we show now.

For \( r, s, k \) with \( r - s \equiv 0 \pmod{10} \), let \( j \in \{0, \ldots, 9\} \) be such that \( r, s \in \mathcal{I}_j \). For \( i = 0, 1 \), consider the matrix \( F^i_{r,s:k} \) with rows and columns indexed by \( \{0, \ldots, [d/2]\} \times \mathcal{I}_j \) such that

\[
(F^i_{r,s:k})(l,r)(l',s) = \text{coeff}(a^{2k}, a^{2i} P_l(a) P_l'(a))
\]

for all \( l, l' = 0, \ldots, [d/2] \), where for a given polynomial \( p \), \( \text{coeff}(a^k, p) \) is the coefficient of monomial \( a^k \) in \( p \). Then we obtain the coefficients \( f_{r,s:k} \) from the matrices \( Q^{ij} \) by the formula

\[
f_{r,s:k} = \sum_{i=0}^{1} (F^i_{r,s:k}, Q^{ij}).
\]

So constraints \( (14) \) and \( (16) \) become

\[
\sum_{i=0}^{1} (F^i_{r,s:k}, Q^{ij}) = 0 \quad \text{if } k < |r - s|/2,
\]

\[
\sum_{i=0}^{1} ((F^i_{r,s:k}, Q^{ij}) - (F^i_{-r,-s:k}, Q^{ij})) = 0 \quad \text{for all } r, s, \text{ and } k,
\]

where \( r, s \equiv j \pmod{10} \) and \( -r, -s \equiv j' \pmod{10} \). Notice that constraint \( (17) \) is already implicit in our formulation, because we enforce by construction that only pairs \( r, s \) with \( r - s \equiv 0 \pmod{10} \) occur.

Also the function \( f \) can be computed from matrices \( Q^{ij} \). To see how, for \( r, s = -N, \ldots, N \) such that \( r - s \equiv 0 \pmod{10} \) and for \( k \geq |r - s|/2 \), set

\[
\tau_{r,s}(a^{2k})(\rho, \theta, \alpha) = (-1)^{|r-s|/2} e^{-i(\alpha + (r-s)\theta)} D_{r,s,k}(\rho) L_n|^{r-s}(|\pi\rho^2|),
\]

where \( n = k - |r - s|/2 \). When \( k < |r - s|/2 \), we set \( \tau_{r,s}(a^{2k}) = 0 \), and then we extend \( \tau_{r,s} \) linearly to all even polynomials in the variable \( a \).

For \( i = 0, 1 \) and \( j = 0, \ldots, 9 \), consider the matrix \( F^{ij} \) with rows and columns indexed by \( \{0, \ldots, [d/2]\} \times \mathcal{I}_j \) such that

\[
[F^{ij}(\rho, \theta, \alpha)](l,r)(l',s) = \tau_{r,s}(a^{2i} P_l(a) P_l'(a))
\]
for all \( l, s, t \in \mathbb{Z} \) and \( r, s \in \mathbb{I} \). Then, in view of (18) and since \( f_{r,s,k} = 0 \) whenever \( k < |r - s|/2 \), we have

\[
\tag{20}
f(\rho, \theta, \alpha) = \sum_{i=0}^{1} \sum_{j=0}^{9} \langle F^{ij}(\rho, \theta, \alpha), Q^{ij} \rangle e^{-\pi \rho^2}.
\]

5.3. **Ensuring nonpositiveness.** How can we ensure that function \( f \), given by (20), satisfies constraint (ii) of Theorem 1? This we do also in terms of semidefinite programming constraints.

First, observe that we require \( f(x, A) \leq 0 \) whenever \( \mathcal{K}^0 \cap (x + \mathcal{A}^0) = \emptyset \). The latter happens if and only if \( x \notin (\mathcal{K} - \mathcal{A})^0 \), where \( \mathcal{K} - \mathcal{A} \) is the Minkowski difference of \( \mathcal{K} \) and \( \mathcal{A} \):

\[
\mathcal{K} - \mathcal{A} = \{ y - z : y \in \mathcal{K}, z \in \mathcal{A} \}.
\]

The Minkowski difference \( \mathcal{K} - \mathcal{A} \) is a polygon for all \( A \in \text{SO}(2) \). Its vertices can be explicitly determined; Figure 1 shows the Minkowski difference when \( A = A(\alpha) \) (as defined in (8)) for \( \alpha \in [-2\pi/10, 2\pi/10] \). By the symmetry of \( \mathcal{K} \), this gives a full characterization of the shape of the Minkowski difference for all \( \alpha \).

Our approach to ensure that \( f \) is nonpositive outside of \((\mathcal{K} - \mathcal{A})^0 \) consists of two steps. First, we observe that all vertices of \( \mathcal{K} - \mathcal{A} \) have norm at most 1. This implies that we must have \( f(x, A) \leq 0 \) whenever \( ||x|| \geq 1 \). This condition on \( f \) can be expressed in terms of sums of squares constraints.

Indeed, by writing \( z_1 = e^{i\theta} \) and \( z_2 = e^{i(\alpha - \theta)} \), we may rewrite (19) as

\[
[\tau_{r,s}(a^{2k})](\rho, z_1, z_2) = (-1)^{|r-s|/2} z_1^{-r} z_2^{-s} D_{r,s,k}(\rho) L_n^{r-s}(\pi \rho^2).
\]

In view of (20), if we then have

\[
\sum_{i=0}^{1} \sum_{j=0}^{9} \langle F^{ij}(\rho, z_1, z_2), Q^{ij} \rangle \leq 0 \quad \text{for all } \rho \geq 1,
\]

we have \( f(\rho, \theta, \alpha) \leq 0 \) whenever \( \rho \geq 1 \), as we want.

For \( j = 0, \ldots, 9 \), consider the set

\[
\mathcal{P}_j = \{ (r, s) : 0 \leq r, s \leq N \quad \text{and} \quad r - s \equiv j \pmod{10} \}.
\]

For \( i = 0, 1, j = 0, \ldots, 9 \), consider the matrix \( W^{ij} \) with rows and columns indexed by \( \{0, \ldots, \lfloor d/2 \rfloor \} \times \mathcal{P}_j \) such that

\[
W^{ij}_{(l,p)(l',p')}(\rho, z_1, z_2) = (\rho^l P_l(\rho) z_1^{-u} z_2^{-v})(\rho^{l'} P_{l'}(\rho) z_1^{u'} z_2^{v'}),
\]

where \( p = (u, v) \) and \( p' = (u', v') \) with \( p, p' \in \mathcal{P}_j \), and \( l, l' = 0, \ldots, \lfloor d/2 \rfloor \).

If there are real positive semidefinite matrices \( R^{ij} \) for \( i = 0, 1 \) and \( j = 0, \ldots, 9 \), and \( S^j \) for \( j = 0, \ldots, 9 \), such that

\[
\tag{21}
\sum_{i=0}^{1} \sum_{j=0}^{9} \langle (F^{ij}(\rho, z_1, z_2), Q^{ij}) + (W^{ij}(\rho, z_1, z_2), R^{ij}) \rangle
\]

and

\[
\sum_{j=0}^{9} \langle (\rho^2 - 1)W^{0j}(\rho, z_1, z_2), S^j \rangle = 0,
\]

then \( f(\rho, \theta, \alpha) \leq 0 \) for all \( \rho \geq 1 \). Notice (21) is a polynomial identity on variables \( \rho, z_1, z_1^{-1}, z_2, \) and \( z_2^{-1} \). In other words, the left-hand side defines a polynomial and the identity above states that this polynomial must be identically zero. To see
Figure 1. From left to right, top to bottom. In the first three pictures, we see the Minkowski difference $K - A(\alpha)K$ (the outer shape) for $\alpha = -2\pi/10, 0, \pi/10$. The dashed pentagon in the center corresponds to $A(\alpha)K$. The vertices of the pentagons are numbered from 0 to 4. The vertices of the Minkowski difference are numbered $ij$, meaning that they correspond to $x - y$, where $x$ is the $i$th vertex of $K$ and $y$ is the $j$th vertex of $A(\alpha)K$. In the last picture we show the three-dimensional set $\{(x, \alpha) : x \in K - A(\alpha)K\}$. Here, $\alpha$ is on the vertical axis; every section perpendicular to the vertical axis corresponds to a Minkowski difference $K - A(\alpha)K$. 
that (21) implies that \( f(\rho, \theta, \alpha) \leq 0 \) whenever \( \rho \geq 1 \), one only has to notice that, for \( \rho \geq 1 \) and \( \theta, \alpha \in [0, 2\pi] \), the Hermitian matrices
\[
W^{ij}(\rho, e^{i\theta}, e^{i(\alpha - \theta)}) \quad \text{and} \quad (\rho^2 - 1)W^{0j}(\rho, e^{i\theta}, e^{i(\alpha - \theta)})
\]
are positive semidefinite, and then all inner products in (21) become nonnegative.

Constraint (21) is not enough to ensure, however, that \( f \) is nonpositive outside of the Minkowski difference. To ensure nonpositiveness in the remaining region, we use a discretization heuristic: We pick a sample of triples \((\rho, \theta, \alpha)\) with \( \rho \leq 1 \) for which we have to ensure that \( f(\rho, \theta, \alpha) \leq 0 \) and we do so explicitly for every point of the sample using (20). Afterwards, we have to analyze the solution obtained in order to check that it indeed satisfies condition (ii) of Theorem 1. We will give details on this approach in the next section.

One may model the constraint that \( f \) is nonpositive outside the Minkowski difference using only sums of squares, without using the discretization approach. The sizes of the matrices get very large, however, making this approach computationally infeasible.

5.4. The semidefinite programming problem and how to solve it. We now describe the semidefinite programming problem we solve to obtain upper bounds for the pentagon packing density.

Let \( N > 0 \) be an integer and \( d \geq 1 \) be an odd integer. Let \( S \) be a finite set of triples \((\rho, \theta, \alpha)\) with \( \rho \leq 1 \) corresponding to elements \((x, A) \in \text{M}(2)\) such that \( K^o \cap (x + AK^o) = \emptyset \). We consider the following semidefinite programming problem:

**Problem A.** Find real, positive semidefinite matrices \( Q^{ij}, R^{ij} \) for \( i = 0, 1 \) and \( j = 0, \ldots, 9 \), and \( S^j \) for \( j = 0, \ldots, 9 \), that minimize
\[
\frac{1}{9} \sum_{i=0}^{9} \sum_{j=0}^{9} \langle F^{ij}(0, 0, 0), Q^{ij} \rangle
\]
subject to the constraints

(22) \[ \sum_{i=0}^{1} \langle F^{i}_{r,s,k}, Q^{ij} \rangle = 0 \quad \text{if} \quad k < |r - s|/2, \quad \text{where} \quad r, s \equiv j \pmod{10}, \]

(23) \[ \sum_{i=0}^{1} (\langle F_{r,s,k}^{i}, Q^{ij} \rangle - \langle F_{-r,-s,k}^{i}, Q^{ij} \rangle) = 0 \quad \text{where} \quad r, s \equiv j \pmod{10} \quad \text{and} \quad -r, -s \equiv j' \pmod{10}, \]

(24) \[ \sum_{i=0}^{1} \sum_{j=0}^{9} \left( \langle F^{ij}(\rho, z_1, z_2), Q^{ij} \rangle + \langle W^{ij}(\rho, z_1, z_2), R^{ij} \rangle \right) \]
\[ \quad + \sum_{j=0}^{9} \langle (\rho^2 - 1)W^{0j}(\rho, z_1, z_2), S^j \rangle = 0, \]

(25) \[ \sum_{i=0}^{1} \sum_{j=0}^{9} \langle F^{ij}(\rho, \theta, \alpha), Q^{ij} \rangle \leq 0 \quad \text{for all} \quad (\rho, \theta, \alpha) \in S, \]

(26) \[ \sum_{i=0}^{1} \langle F^{i}_{0,0,0}, Q^{ij} \rangle = 1. \]
Conditions (22)–(25) were already discussed in the previous sections. Notice this is indeed a semidefinite programming problem. In fact, the objective function and all constraints but (24) are clearly linear. As for the polynomial identity (24), one only has to observe that it can be turned into linear constraints by using the fact that a polynomial is identically zero if and only if each monomial has a zero coefficient (cf. §3).

Of Problem A we have to explain our choice of objective function and also the meaning of constraint (26). To obtain the best possible bound from Theorem 1, we wish to minimize \( \lambda = \int_{M(2)} f(x, A) d(x, A) \), where

\[
\int_{M(2)} f(x, A) d(x, A) = \lambda \langle 1, 1 \rangle
\]

Constraint (26) is a normalization constraint, setting \( \lambda = 1 \). Indeed, one has \( \lambda = f_{0,0,0} \), since from the definition of \( \hat{f} \) and the inversion formula (cf. §4) we have

\[
\langle \hat{f}\rangle_{0,0} = \langle \int_{M(2)} f(x, A) U^0_{(x,A) - 1} d(x, A), 1 \rangle
\]

\[
= \lambda \langle 1, 1 \rangle
\]

where \( 1 \in L^2(S^1) \) is the constant one function, so that \( U^0_{(x,A) - 1} = 1 \). Now, the objective function evaluates \( f(0, I)/\lambda \), that we wish to minimize.

To be able to solve Problem A on the computer, the choice of the sequence \( P_0, P_1, \ldots \) of polynomials which we use to define our matrices is essential. A bad choice here can lead to numerical instability that might prevent us from solving the problem.

In particular, we have observed that the monomial basis performs specially badly. A much better choice are normalized Laguerre polynomials, as had been observed in a similar setting by de Laat, Oliveira, and Vallentin [23]. Namely, we set

\[
P_k(x) = \mu_k^{-1} L_k^0(2\pi x^2),
\]

where \( \mu_k \) is the absolute value of the coefficient of \( L_k^0(2\pi x^2) \) with largest absolute value.

Also essential to the stability of Problem A is the choice of the basis used to express polynomial identity (24). Again, the monomial basis is a poor choice. Instead we use the basis

\[
P_k(\rho^2 z_1^{-r} z_2^{-s})
\]

for \( k = 0, \ldots, d \) and \( -N \leq r, s \leq N \) such that \( r - s \equiv 0 \pmod{10} \).

This means that in order to express constraint (24), we expand the corresponding polynomial in the above basis, and then require each coefficient of the expansion to be zero.

In preliminary tests with reasonably dense samples for constraint (25), we observed that most variables in Problem A did not seem to play a role, at least for the values of \( d \) and \( N \) that we considered. So we decided to discard all variable matrices except for \( Q^{00}, Q^{05}, Q^{10}, Q^{15}, R^{00}, R^{05}, S^0, \) and \( S^5 \).
Figure 2. The points in gray are an example of a sample used in Problem A; here we show the points in the sample for $\alpha = \pi/10$. Each facet $F$ of the Minkowski difference defines a line $l_F$, its supporting hyperplane, and for the sample we would then pick all points in the grid that are inside the circle of radius 1 and that lie, for some facet $F$ of the Minkowski difference, on the side of $l_F$ that does not contain the origin. Since we work with $S(K)$-invariant functions, however, we need not choose all these points: It suffices to consider only two adjacent facets of the Minkowski difference, instead of all the facets.

and we observed that this did not have much effect on the optimal value of the problem, while providing for simpler and more stable problems. From now on, when we refer to Problem A it should be understood that we only use the variables listed above.

We now have a complete description of the semidefinite programming problem to be solved, let us sketch how we obtained the bound of 0.98103 for the pentagon packing density.

We first solve Problem A (with less variables, as explained above) for $d = 11$ and $N = 5$, using a sample with 537 points. This sample we pick as follows. We first pick 5 uniformly spaced values for $\alpha$ in $[-2\pi/10, 0]$, starting with $-2\pi/10$ and ending with 0. For each such value of $\alpha$, we pick in the square $[-1, 1]^2$ a uniformly spaced grid of $50 \times 50$ points, and add to the sample all triples $(\rho, \theta, \alpha)$, where $(\rho, \theta)$ corresponds to a grid point outside of the Minkowski difference ($K - A(\alpha)K$) and such that $\rho \leq 1$. Moreover, the symmetry of $K$ allows us to restrict our sample considerably — Figure 2 has an example.

We observed, by evaluating the function $f$ obtained via this approach, that this small sample is already enough to enforce condition (ii) of Theorem 1 on most of the required domain. To really obtain a function $f$ satisfying the conditions of Theorem 1, however, we have to work a bit more.
Since we use a numerical solver for semidefinite programming, the solutions we obtain for Problem A are not really feasible, but almost feasible. So we cannot be a priori certain that the bound given by Problem A is really an upper bound.

To deal with this issue, we use the same approach outlined by de Laat, Oliveira, and Vallentin [23], which we briefly explain here. First, we solve Problem A in order to get an estimate of its optimal value; say \( z^* \) is the numerical optimal value obtained. Then, we solve a version of Problem A in which the objective function is removed but a constraint

\[
\sum_{i=0}^{1} \sum_{j=0}^{9} \langle F^{ij}(0,0,0), Q^{ij} \rangle \leq z^* + 10^{-5}
\]

is added.

This problem is a feasibility problem, and for this reason the solver will return a solution that is strictly feasible, i.e., a solution in which the solution matrices are positive definite, if one can be found.

In this way, we manage to obtain a solution of Problem A having objective value close to what the optimal value is supposed to be, in which each matrix has a minimum eigenvalue around \( 10^{-6} \), whereas the constraints are satisfied up to an absolute error of \( 10^{-9} \). By projecting the solution obtained onto the affine subspace generated by constraints (22), (23), (24), and (26), using double-precision floating-point arithmetic, we manage to drop the absolute error to \( 10^{-22} \), while not changing much the minimum eigenvalues of the solution matrices.

So the approach detailed by de Laat, Oliveira, and Vallentin [23] applies. Namely, since the minimum eigenvalues of the solution matrices are big compared to the absolute errors, we may be sure that by changing the solution matrices slightly, we may ensure that the constraints are satisfied, thus obtaining a truly feasible solution, without significantly changing the objective value. Notice that we do not need to carry out this change in practice, it suffices to know that it can be done.

Finally, we still have to show that the function \( f \) thus obtained satisfies condition (ii) of Theorem 1. We have said that \( f \) satisfies condition (ii) for most of the points on the required domain. For instance, since we have constraint (24), we know that \( f(\rho, \theta, \alpha) \leq 0 \) for all \( \rho \geq 1 \). There are, however, points \( (\rho, \theta, \alpha) \) with \( \rho \leq 1 \) for which we have \( f(\rho, \theta, \alpha) \) positive, while (ii) would require this value to be nonpositive.

Though \( f \) does not satisfy condition (ii) of Theorem 1 for the pentagon \( K \), it satisfies this condition once we enlarge \( K \) slightly. Indeed, \( f \) satisfies condition (ii) for the pentagon \( 1.02K \). This we may verify by picking a fine enough sample of points \( (\rho, \theta, \alpha) \) with \( \rho \leq 1 \) for which \( f \) has to be nonpositive, and computing the minimum value of \( f \) on this sample using 256-bit-precision floating-point. By computing the derivatives of \( f \), we may estimate how fine the sample has to be and how large the absolute value of the minimum of \( f \) on the sample has to be, in order for us to be sure that \( f \) is nonpositive in the whole required region.

A side effect of our restriction of the variables is that the function \( f \) we obtain is by construction such that

\[
f(\rho, \theta, \alpha + l2\pi/5) = f(\rho, \theta, \alpha)
\]

for all integer \( l \) (cf. (18)). This and the symmetry of \( K \) helps us restrict the sample to points \( (\rho, \theta, \alpha) \) with \( \alpha \in [-2\pi/10, 2\pi/10] \). To obtain our bound, we had to
use a sample of about 6.5 million points to check that $f$ satisfies condition (ii) of Theorem 1.

Enlarging the body $\mathcal{K}$ worsens the bound given by Theorem 1 but since we consider a small enlargement of $\mathcal{K}$, we still manage to obtain the bound of 0.98103.

Finally, we mention some of the computational tools used to generate the semidefinite programming problem and solve it. To generate the problem, we use a C++ program with a custom-made C++ library for generating semidefinite programming problems, in particular dealing with sums of squares constraints. As a solver we used CSDP [8], and to analyze the resulting solution and check that it is feasible we used a mix of SAGE [30] and C++.

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