On Packing Spheres into Containers

About Kepler's Finite Sphere Packing Problem

Achill Schürmann

Received: June 3, 2005
Revised: July 21 2006

Communicated by Günter Ziegler

Abstract. In an Euclidean d-space, the container problem asks to pack n equally sized spheres into a minimal dilate of a fixed container. If the container is a smooth convex body and $d \geq 2$ we show that solutions to the container problem can not have a "simple structure" for large n. By this we in particular find that there exist arbitrary small $r > 0$, such that packings in a smooth, 3-dimensional convex body, with a maximum number of spheres of radius r, are necessarily not hexagonal close packings. This contradicts Kepler's famous statement that the cubic or hexagonal close packing "will be the tightest possible, so that in no other arrangement more spheres could be packed into the same container".

2000 Mathematics Subject Classification: 52C17; 01A45, 05B40
Keywords and Phrases: sphere packing, Kepler, container problem

1 Introduction

How many equally sized spheres can be packed into a given container? In 1611, Kepler discussed this question in his booklet [Kep11] and came to the following conclusion:

> "Coaptatio fiet arctissima, ut nullo praeterea ordine plures globuli in idem vas compingi queant."

> "The (cubic or hexagonal close) packing will be the tightest possible, so that in no other arrangement more spheres could be packed into the same container."

In this note we want to show that Kepler's assertion is false for many containers (see Section 5, Corollary 2). Even more general we show, roughly speaking, that the set of solutions to the finite container problem (see below) in an Euclidean space of dimension $d \geq 2$ has no "simple structure" (see Definition 1).
To make this precise, we consider the Euclidean d-space $\mathbb{R}^d$ endowed with inner product $\langle \cdot, \cdot \rangle$ and norm $|\cdot|$. Let $B^d = \{\boldsymbol{x} \in \mathbb{R}^d : |\boldsymbol{x}| \leq 1\}$ denote the (solid) unit sphere and $S^{d-1} = \{\boldsymbol{x} \in \mathbb{R}^d : |\boldsymbol{x}| = 1\}$ its boundary. Then a discrete set $X \subset \mathbb{R}^d$ is a *packing set* and defines a *sphere packing* $X + \frac{1}{2}B^d = \{\boldsymbol{x} + \frac{1}{2}\boldsymbol{y} : \boldsymbol{x} \in X, \boldsymbol{y} \in B^d\}$, if distinct elements $\boldsymbol{x}$ and $\boldsymbol{x}'$ of X have distance $|\boldsymbol{x} - \boldsymbol{x}'| \geq 1$. The sphere packing is called *finite* if X is of finite cardinality $|X|$. Here we consider finite sphere packings contained in a convex body (*container*) C, that is, a compact, convex subset of $\mathbb{R}^d$ with nonempty interior. The *finite container problem* may be stated as follows.

PROBLEM. *Given $d \geq 2$, $n \in \mathbb{N}$ and a convex body $C \subset \mathbb{R}^d$, determine*

$$\lambda(C, n) = \min\{\lambda > 0 : \lambda C \supset X + \tfrac{1}{2}B^d \text{ a packing, } X \subset \mathbb{R}^d \text{ with } |X| = n\}$$

and packing sets X attaining the minimum.

Many specific instances of this container problem have been considered (see for example [Bez87], [BW04], [Fod99], [Mel97], [NÖ97],[Spe04], [SMC+06]). Independent of the particular choice of the container C, solutions tend to densest infinite packing arrangements for growing n (see Section 5, cf. [CS95]). In dimension 2 these packings are known to be arranged hexagonally. Nevertheless, although close, solutions to the container problem are not hexagonally arranged for all sufficiently large n and various convex disks C, as shown by the author in [Sch02], Theorem 9 (cf. [LG97] for corresponding computer experiments). Here we show that a similar phenomenon is true in arbitrary Euclidean spaces of dimension $d \geq 2$.
We restrict ourselves to *smooth convex bodies C* as containers. That is, we assume the *support function* $h_C(\boldsymbol{u}) = \sup\{\langle \boldsymbol{x}, \boldsymbol{u} \rangle : \boldsymbol{x} \in C\}$ of C is differentiable at all $\boldsymbol{u} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$, or equivalently, we require that C has a unique *supporting hyperplane* through each boundary point (see [Sch93], Chapter 1.7).
Our main result shows that families of packing sets with a "simple structure" can not be solutions to the container problem if C is smooth and n sufficiently large. This applies for example to the family of solutions to the *lattice restricted container problem*. In it, we only consider packing sets which are isometric to a subset of some *lattice* (a discrete subgroup of $\mathbb{R}^d$).

THEOREM 1. *Let $d \geq 2$ and $C \subset \mathbb{R}^d$ a smooth convex body. Then there exists an $n_0 \in \mathbb{N}$, depending on C, such that $\lambda(C, n)$ is not attained by any lattice packing set for $n \geq n_0$.*

2 PACKING FAMILIES OF LIMITED COMPLEXITY

The result of Theorem 1 can be extended to a more general class of packing sets.

DEFINITION 1. *A family $\mathcal{F}$ of packing sets in $\mathbb{R}^d$ is of* limited complexity *(an* lc-family*), if* *(i) there exist isometries $\mathcal{I}_X$, for each $X \in \mathcal{F}$, such that*

$$\{\boldsymbol{x}-\boldsymbol{y} : \boldsymbol{x}, \boldsymbol{y} \in \mathcal{I}_X(X) \text{ and } X \in \mathcal{F}\} \tag{1}$$

has only finitely many accumulation points in any bounded region.

(ii) there exists a $\varrho > 0$, such that for all $\boldsymbol{x} \in X$ with $X \in \mathcal{F}$, every affine subspace spanned by some elements of

$$\{\boldsymbol{y} \in X : |\boldsymbol{x}-\boldsymbol{y}| = 1\}$$

either contains $\boldsymbol{x}$ or its distance to $\boldsymbol{x}$ is larger than ϱ.

Condition (i) shows that point configurations within an arbitrarily large radius around a point are (up to isometries of X and up to finitely many exceptions) arbitrarily close to one out of finitely many possibilities. Condition (ii) limits the possibilities for points at minimum distance further. Note that the existence of a $\varrho > 0$ in (ii) follows if (1) in (i) is finite within S^{d-1}.

An example of an lc-family in which isometries can be chosen so that (1) is finite in any bounded region, is the family of *hexagonal packing sets*. These are isometric copies of subsets of a *hexagonal lattice*, in which every point in the plane is at minimum distance 1 to six others. For the hexagonal packing sets, condition (ii) is satisfied for all $\varrho < \frac{1}{2}$. More general, isometric copies of subsets of a fixed lattice give finite sets (1) in any bounded region and satisfy (ii) for suitable small $\varrho > 0$. Similar is true for more general families of packing sets, as for example for the *hexagonal close configurations* in dimension 3 (see Section 5).

An example of an lc-family, in which the sets (1) are not necessarily finite in any bounded region, are the solutions to the lattice restricted container problem. As shown at the end of Section 3, condition (ii) in Definition 1 is nevertheless satisfied. Thus we are able to derive Theorem 1 from the following, more general result.

Theorem 2. *Let $d \geq 2$, $C \subset \mathbb{R}^d$ a smooth convex body and $\mathcal{F}$ an lc-family of packing sets in $\mathbb{R}^d$. Then there exists an $n_0 \in \mathbb{N}$, depending on $\mathcal{F}$ and C, such that $\lambda(C, n)$ is not attained by any packing set in $\mathcal{F}$ for $n \geq n_0$.*

Proofs are given in the next section. In Section 4 we briefly mention some possible extensions of Theorem 2. In Section 5 we discuss consequences for the quoted assertion of Kepler, if interpreted as a container problem (see Corollary 2).

3 Proofs

Idea. The proof of Theorem 2 is subdivided into four preparatory steps and corresponding propositions. These technical ingredients are brought together at the end of this section. Given an lc-family $\mathcal{F}$ of packing sets, the idea is the following: We show that packing sets $X \in \mathcal{F}$, with $|X|$ sufficiently large, allow the construction of packing sets X' with $|X'| = |X|$ and with $X' + \frac{1}{2}B^d$ fitting into a smaller dilate of C. Roughly speaking, this is accomplished in two steps. First we show that "rearrangements" of spheres near the boundary of C are possible for sufficiently large n. This allows us to obtain arbitrarily large regions in which spheres have no contact, respectively in which points of X' have distance greater than 1 to all other points (Proposition 2, depending on property (i) of Definition 1). Such an initial modification then allows rearrangements of all spheres (Proposition 3 and 4, depending on property (ii) of Definition 1), so that the resulting packing fits into a smaller dilate of C. For example, consider a hexagonal packing in the plane: It is sufficient to initially rearrange (or remove) two disks in order to subsequently rearrange all other disks, so that no disk is in contact with others afterwards (see Figure 1, cf. [Sch02]).

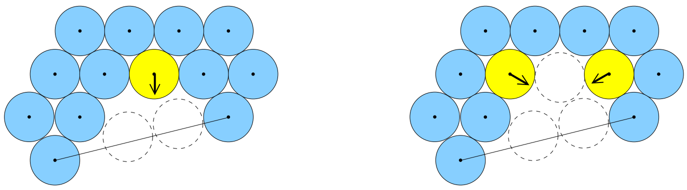


Figure 1: Local rearrangements in a hexagonal circle packing.

How do we know that the new sphere packings $X' + \frac{1}{2}B^d$ fit into a smaller dilate of C? Consider

$$\lambda(C, X) = \min\{\lambda > 0 : \lambda C \supset \boldsymbol{t} + X + \tfrac{1}{2}B^d \text{ for some } \boldsymbol{t} \in \mathbb{R}^d\}$$

for a fixed finite packing set X. Here and in the sequel we use $\boldsymbol{t} + X$ to abbreviate $\{\boldsymbol{t}\} + X$. Clearly

$$\lambda(C, n) = \min\{\lambda(C, X) : \ X \text{ is a packing set with } |X| = n\ \},$$

and $\lambda(C, X') < \lambda(C, X)$ whenever the *convex hull* $\operatorname{conv} X'$ of X' (and hence X' itself) is contained in the interior $\operatorname{int}\operatorname{conv} X$ of the convex hull of X. Thus in order to prove that X does not attain $\lambda(C, |X|)$ for any convex container C, it is sufficient to describe a way of attaining a packing set X' with $|X'| = |X|$ and

$$X' \subset \operatorname{int}\operatorname{conv} X. \tag{2}$$

I. Let us first consider the "shapes" of packing sets X_n attaining $\lambda(C, n)$. Here and in what follows, X_n denotes a packing set with $|X_n| = n$.
In order to define the "shape", let

$$R(M) = \min\{R \geq 0 : M \subset \boldsymbol{t} + RB^d \text{ for some } \boldsymbol{t} \in \mathbb{R}^d\}$$

denote the circumradius of a compact set $M \subset \mathbb{R}^d$ and let $\boldsymbol{c}(M)$ denote the center of its circumsphere. Hence $M \subseteq \boldsymbol{c}(M) + R(M)B^d$. Then the *shape* of M is defined by

$$\mathcal{S}(M) = (\operatorname{conv}(M) - \boldsymbol{c}(M))\,/R(M) \subset B^d.$$

The family of nonempty compact subsets in $\mathbb{R}^d$ can be turned into a metric space, for example with the *Hausdorff metric* (cf. [Sch93]). Shapes of packing sets X_n attaining $\lambda(C,n)$ converge to the shape of C, that is,

$$\lim_{n\to\infty} \mathcal{S}\left(X_n\right) = \mathcal{S}(C). \tag{3}$$

This is seen by "reorganizing elements" in a hypothetical convergent subsequence of $\{X_n\}_{n\in\mathbb{N}}$ not satisfying (3).
The convergence of shapes leads for growing n to shrinking sets of *outer (unit) normals*

$$\{\boldsymbol{v} \in S^{d-1} : \langle \boldsymbol{v}, \boldsymbol{x}\rangle \geq \langle \boldsymbol{v}, \boldsymbol{y}\rangle \text{ for all } \boldsymbol{y} \in \operatorname{conv} X_n\} \tag{4}$$

at boundary points $\boldsymbol{x}$ of the *center polytope* $\operatorname{conv} X_n$. For general terminology and results on convex polytopes used here and in the sequel we refer to [Zie97].
Since C is smooth, the sets of outer normals (4) at boundary points of $\operatorname{conv} X_n$ become uniformly small for large n. Also, within a fixed radius around a boundary point, the boundary of $\operatorname{conv} X_n$ becomes "nearly flat" for growing n.

Proposition 1. *Let $d \geq 2$ and $C \subset \mathbb{R}^d$ a smooth convex body. Let $\{X_n\}$ be a sequence of packing sets in $\mathbb{R}^d$ attaining $\lambda(C,n)$. Then*

(i) for $\varepsilon > 0$ there exists an $n_1 \in \mathbb{N}$, depending on C and ε, such that for all $n \geq n_1$, outer normals $\boldsymbol{v}, \boldsymbol{v}' \in S^{d-1}$ of $\operatorname{conv} X_n$ at $\boldsymbol{x} \in X_n$ satisfy

$$|\boldsymbol{v} - \boldsymbol{v}'| < \varepsilon;$$

(ii) for $\varepsilon > 0$ and $r > 0$ there exists an $n_1 \in \mathbb{N}$, depending on C, ε and r, such that for all $n \geq n_1$, and for $\boldsymbol{x}, \boldsymbol{x}' \in \operatorname{bd}\operatorname{conv} X_n$ with $|\boldsymbol{x} - \boldsymbol{x}'| \leq r$, outer normals $\boldsymbol{v} \in S^{d-1}$ of $\operatorname{conv} X_n$ at $\boldsymbol{x}$ satisfy

$$\langle \boldsymbol{v}, \boldsymbol{x} - \boldsymbol{x}'\rangle > -\varepsilon.$$

II. In what follows we use some additional terminology. Given a packing set X, we say $\boldsymbol{x} \in X$ is in a *free position*, if the set

$$\mathcal{N}_X(\boldsymbol{x}) = \{\boldsymbol{y} \in X : |\boldsymbol{x} - \boldsymbol{y}| = 1\}$$

is empty. If some $\boldsymbol{x} \in X$ is not contained in $\operatorname{int}\operatorname{conv} \mathcal{N}_X(\boldsymbol{x})$, then it is possible to obtain a packing set $X' = X \setminus \{\boldsymbol{x}\} \cup \{\boldsymbol{x}'\}$ in which $\boldsymbol{x}'$ is in a free position. We say $\boldsymbol{x}$ is *moved to a free position* in this case (allowing $\boldsymbol{x}' = \boldsymbol{x}$). We say $\boldsymbol{x}$ is *moved into or within a set M* (to a free position), if $\boldsymbol{x}' \in M$. Note, in the resulting packing set X' less elements may have minimum distance 1 to others, and therefore possibly further elements can be moved to free positions.
Assuming $X \in \mathcal{F}$ attains $\lambda(C, |X|)$ with $|X|$ sufficiently large, the following proposition shows that it is possible to move elements of X into free positions within an arbitrarily large region, without changing the center polytope $\operatorname{conv} X$.

PROPOSITION 2. *Let $d \geq 2$ and $R > 0$. Let $C \subset \mathbb{R}^d$ a smooth convex body and $\mathcal{F}$ a family of packing sets in $\mathbb{R}^d$ satisfying (i) of Definition 1. Then there exists an $n_2 \in \mathbb{N}$, depending on R, $\mathcal{F}$ and C, such that for all $X \in \mathcal{F}$ attaining $\lambda(C, |X|)$ with $|X| \geq n_2$, there exists a $\boldsymbol{t}_X \in \mathbb{R}^d$ with*

(i) $(\boldsymbol{t}_X + RB^d) \subset \operatorname{conv} X$*, and*

(ii) all elements of $X \cap \operatorname{int}(\boldsymbol{t}_X + RB^d)$ can be moved to free positions by subsequently moving elements of $X \cap \operatorname{int}\operatorname{conv} X$ to free positions within $\operatorname{int}\operatorname{conv} X$.

Proof. Preparations. By applying suitable isometries to the packing sets in $\mathcal{F}$ we may assume that

$$\{\boldsymbol{y} :\ \boldsymbol{y} \in X - \boldsymbol{x} \text{ with } |\boldsymbol{y}| < r \text{ for } \boldsymbol{x} \in X \text{ and } X \in \mathcal{F}\} \tag{5}$$

has only finitely many accumulation points for every $r > 1$. For each X, the container C is transformed to possibly different isometric copies. This is not a problem though, since the container is not used aside of Proposition 1, which is independent of the chosen isometries. Note that the smoothness of C is implicitly used here.

We say $\boldsymbol{x} \in X$ is *moved in direction* $\boldsymbol{v} \in S^{d-1}$, if it is replaced by an $\boldsymbol{x}'$ on the ray $\{\boldsymbol{x} + \lambda \boldsymbol{v} : \lambda \in \mathbb{R}_{>0}\}$. Note that it is possible to move $\boldsymbol{x}$ in direction $\boldsymbol{v} \in S^{d-1}$ to a free position, if

$$\mathcal{N}_X(\boldsymbol{x}, \boldsymbol{v}) = \{\boldsymbol{w} \in \mathcal{N}_X(\boldsymbol{x}) - \boldsymbol{x} : \langle \boldsymbol{v}, \boldsymbol{w} \rangle > 0\} \tag{6}$$

is empty. If we want a fixed $\boldsymbol{x} \in X$ to be moved to a free position, in direction $\boldsymbol{v} \in S^{d-1}$ say, we have to move the elements $\boldsymbol{y} \in \boldsymbol{x} + \mathcal{N}_X(\boldsymbol{x}, \boldsymbol{v})$ first. In order to do so, we move the elements of $\boldsymbol{y} + \mathcal{N}_X(\boldsymbol{y}, \boldsymbol{v})$ to free positions, and so on. By this we are lead to the definition of the *access cone*

$$\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v}) = \operatorname{pos}\{\mathcal{N}_X(\boldsymbol{x}, \boldsymbol{v}) : \boldsymbol{x} \in X \text{ for } X \in \mathcal{F} \text{ with } |X| \geq n\} \tag{7}$$

of $\mathcal{F}$ and n in direction $\boldsymbol{v} \in S^{d-1}$. Here,

$$\operatorname{pos}(M) = \{\sum_{i=1}^{m} \lambda_i \boldsymbol{x}_i : m \in \mathbb{N}, \lambda_i \geq 0 \text{ and } \boldsymbol{x}_i \in M \text{ for } i = 1, \ldots, m\ \}$$

denotes the *positive hull* of a set $M \subset \mathbb{R}^d$, which is by definition a convex cone. Note that $\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v})$ is contained in the halfspace $\{\boldsymbol{x} \in \mathbb{R}^d : \langle \boldsymbol{v}, \boldsymbol{x} \rangle \geq 0\}$ and that $\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v}) \subseteq \operatorname{acc}_{\mathcal{F},n'}(\boldsymbol{v})$ whenever $n \geq n'$.

By the assumption that (5) has only finitely many accumulation points for $r > 1$, there exist only finitely many limits $\lim_{n\to\infty}\left(\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v}) \cap B^d\right)$. Here, limits are defined using the Hausdorff metric on the set of nonempty compact subsets of $\mathbb{R}^d$ again.

Strategy. We choose a $\boldsymbol{v} \in S^{d-1}$ such that there exists an $\varepsilon > 0$ with

$$\lim_{n\to\infty}\left(\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v}) \cap B^d\right) = \lim_{n\to\infty}\left(\operatorname{acc}_{\mathcal{F},n}(\boldsymbol{v}') \cap B^d\right),$$

for all $\boldsymbol{v}'$ in the ε*-neighborhood* $S_\varepsilon(\boldsymbol{v}) = S^{d-1} \cap (\boldsymbol{v} + \varepsilon B^d)$ of $\boldsymbol{v} \in S^{d-1}$.

In order to prove the proposition, we show the following for every $X \in \mathcal{F}$, attaining $\lambda(C, |X|)$ with $|X|$ sufficiently large: There exists a $\boldsymbol{t}_X \in \mathbb{R}^d$ such that (i') $(\boldsymbol{t}_X + RB^d) + \mathrm{acc}_{\mathcal{F},n}(\boldsymbol{v})$ does not intersect $X \cap \mathrm{bd}\,\mathrm{conv}\,X$, while

(ii') $(\boldsymbol{t}_X + RB^d) \subset \mathrm{conv}\,X$.

It follows that $\mathrm{bd}\,\mathrm{conv}\,X$ has to intersect the unbounded set

$$(\boldsymbol{t}_X + RB^d) + \mathrm{acc}_{\mathcal{F},n}(\boldsymbol{v}) \tag{8}$$

and by the definition of the access cone it is possible to move the elements in $X \cap \mathrm{int}(\boldsymbol{t}_X + RB^d)$ to free positions as asserted. For example, after choosing a direction $\boldsymbol{v}' \in S_\varepsilon(\boldsymbol{v})$, we may subsequently pick non-free elements $\boldsymbol{x}$ in (8) with maximal $\langle \boldsymbol{x}, \boldsymbol{v}' \rangle$. These elements can be moved to a free position within $\mathrm{int}\,\mathrm{conv}\,X$, since $\mathcal{N}_X(\boldsymbol{x}, \boldsymbol{v}')$ is empty by the definition of the access cone.

Bounding the boundary intersection. We first estimate the size of the intersection of (8) with $\mathrm{bd}\,\mathrm{conv}\,X$. For $\boldsymbol{v}' \in S_\varepsilon(\boldsymbol{v})$ and $n \in \mathbb{N}$, we consider the sets

$$M(\boldsymbol{v}', n) = \{\boldsymbol{x} \in RB^d + \mathrm{acc}_{\mathcal{F},n}(\boldsymbol{v}) : \langle \boldsymbol{x}, \boldsymbol{v}' \rangle = R\}.$$

By the definition of the access cones (7), $M(\boldsymbol{v}', n) \subseteq M(\boldsymbol{v}', n')$ for $n \geq n'$. We choose

$$r > \sup\{|\boldsymbol{x} - \boldsymbol{y}| : \boldsymbol{x}, \boldsymbol{y} \in M(\boldsymbol{v}', n) \text{ with } \boldsymbol{v}' \in S_\varepsilon(\boldsymbol{v})\},$$

as a common upper bound on the diameter of the sets $M(\boldsymbol{v}', n)$ with n sufficiently large, say $n \geq n'$. Note that R as well as $\mathcal{F}$, $\boldsymbol{v}$ and ε have an influence on the size of r and n'.

By Proposition 1 (ii) we can choose n' possibly larger to ensure the following for all $X \in \mathcal{F}$ attaining $\lambda(C, |X|)$ with $|X| \geq n'$: *The intersection of* (8) *with* $\mathrm{bd}\,\mathrm{conv}\,X$ *has a diameter less than r, no matter which* $\boldsymbol{t}_X \in \mathrm{conv}\,X$ *at distance* R *to* $\mathrm{bd}\,\mathrm{conv}\,X$ *we choose. Moreover,* $(\boldsymbol{t}_X + RB^d) \subset \mathrm{conv}\,X$.

Ensuring an empty intersection. It remains to show that for $X \in \mathcal{F}$, attaining $\lambda(C, |X|)$ with $|X|$ sufficiently large, $\boldsymbol{t}_X$ can be chosen such that (8) does not intersect $X \cap \mathrm{bd}\,\mathrm{conv}\,X$. For this we prove the following claim: *There exists an n'', depending on r, $\boldsymbol{v}$ and ε, such that for all $X \in \mathcal{F}$ with $|X| \geq n''$, there exists a vertex $\boldsymbol{x}$ of* $\mathrm{conv}\,X$ *with outer normal $\boldsymbol{v}' \in S_\varepsilon(\boldsymbol{v})$ and*

$$\{\boldsymbol{x}\} = X \cap (\mathrm{bd}\,\mathrm{conv}\,X) \cap (\boldsymbol{x} + rB^d). \tag{9}$$

Thus these vertices $\boldsymbol{x}$ have a distance larger than r to any other element of $X \cap \mathrm{bd}\,\mathrm{conv}\,X$. Therefore, by choosing $n_2 \geq \max\{n', n''\}$, we can ensure that there exists a $\boldsymbol{t}_X \in \mathbb{R}^d$ at distance R to $\mathrm{bd}\,\mathrm{conv}\,X$ such that (i') and (ii') are satisfied for all $X \in \mathcal{F}$ attaining $\lambda(C, |X|)$ with $|X| \geq n_2$. Note that n', n'', and hence n_2, depend on the choice of $\boldsymbol{v}$ and ε. But we may choose $\boldsymbol{v}$ and ε, depending on $\mathcal{F}$, so that n_2 can be chosen as small as possible. In this way we get an n_2 which solely depends on R, $\mathcal{F}$ and C.

It remains to prove the claim. Since (5) has only finitely many accumulation points, the set of normals $\boldsymbol{v}' \in S^{d-1}$ with hyperplane $\{\boldsymbol{y} \in \mathbb{R}^d : \langle \boldsymbol{v}', \boldsymbol{y} \rangle = 0\}$ running through

$\mathbf{0}$ and an accumulation point $\boldsymbol{y}$ of (5) all lie in the union $\mathcal{U}_r$ of finitely many linear subspaces of dimension $d-1$. Thus for any $\delta > 0$ the normals of these hyperplanes all lie in $\mathcal{U}_{r,\delta} = \mathcal{U}_r + \delta B^d$ if we choose $|X|$ sufficiently large, depending on δ. By choosing δ small enough, we find a $\boldsymbol{v}' \in S_\varepsilon(\boldsymbol{v})$ with $\boldsymbol{v}' \notin \mathcal{U}_{r,\delta}$. Moreover, there exists an $\varepsilon' > 0$ such that $S_{\varepsilon'}(\boldsymbol{v}') \cap \mathcal{U}_{r,\delta} = \emptyset$. Since every center polytope $\operatorname{conv} X$ has a vertex $\boldsymbol{x}$ with outer normal $\boldsymbol{v}'$, we may choose $|X|$ sufficiently large by Proposition 1 (i) (applied to $2\varepsilon'$), such that $\operatorname{conv} X$ has no outer normal in $\mathcal{U}_{r,\delta}$ at $\boldsymbol{x}$.
Moreover, for sufficiently large $|X|$, faces of $\operatorname{conv} X$ intersecting $\boldsymbol{x} + rB^d$ can not contain any vertex in $X \cap (\boldsymbol{x} + rB^d)$ aside of $\boldsymbol{x}$. Thus by construction, there exists an n'' such that (9) holds for all $X \in \mathcal{F}$ with $|X| \geq n''$. This proves the claim and therefore the proposition. $\square$

Note that the proof offers the possibility to loosen the requirement on $\mathcal{F}$ a bit, for the price of introducing another parameter: For suitable large r, depending on $\mathcal{F}$, the proposition holds, if instead of (i) in Definition 1 we require

(i') there exist isometries $\mathcal{I}_X$ for each $X \in \mathcal{F}$, such that

$$\{\boldsymbol{x} - \boldsymbol{y} : \boldsymbol{x}, \boldsymbol{y} \in \mathcal{I}_X(X) \text{ and } X \in \mathcal{F}\}$$

has only finitely many accumulation points within rB^d.

III. For all $X \in \mathcal{F}$ attaining $\lambda(C, |X|)$, with $|X|$ sufficiently large, we are able to obtain *contact free regions* $(\boldsymbol{t}_X + RB^d) \subset \operatorname{conv} X$, with R as large as we want, by Proposition 2. That is, we can modify these packing sets X by moving elements to free positions within $\operatorname{int}(\boldsymbol{t}_X + RB^d)$. By choosing R large enough, such an initial contact free region allows to move further elements to free positions. The following proposition takes care of interior points.

Proposition 3. *Let $d \geq 2$ and $\mathcal{F}$ a family of packing sets in $\mathbb{R}^d$ satisfying (ii) in Definition 1 with $\varrho > 0$. Let $R \geq \frac{1}{\varrho}$, $X \in \mathcal{F}$ and $\boldsymbol{x} \in X \cap \operatorname{int}\operatorname{conv} X$. Let $\boldsymbol{t} \in \mathbb{R}^d$ with $|\boldsymbol{t} - \boldsymbol{x}| \leq R + \frac{\varrho}{2}$ and with all elements of $X \cap (\boldsymbol{t} + RB^d)$ in a free position. Then $\boldsymbol{x}$ can be moved to a free position within* $\operatorname{int}\operatorname{conv} X$.

Proof. Assume $\boldsymbol{x} \in \operatorname{int}\operatorname{conv} \mathcal{N}_X(\boldsymbol{x})$. By the assumption on $\mathcal{F}$,

$$\boldsymbol{x} + \varrho B^d \subset \operatorname{int}\operatorname{conv} \mathcal{N}_X(\boldsymbol{x}).$$

Thus there exists a $\boldsymbol{y} \in \mathcal{N}_X(\boldsymbol{x})$, such that the orthogonal projection $\boldsymbol{y}'$ of $\boldsymbol{y}$ onto the line through $\boldsymbol{x}$ and $\boldsymbol{t}$ satisfies $|\boldsymbol{y}' - \boldsymbol{x}| \geq \varrho$ and $|\boldsymbol{y}' - \boldsymbol{t}| \leq R - \frac{\varrho}{2}$. Then

$$|\boldsymbol{y} - \boldsymbol{t}|^2 = |\boldsymbol{y}' - \boldsymbol{t}|^2 + |\boldsymbol{y} - \boldsymbol{y}'|^2 \leq \left(R - \tfrac{\varrho}{2}\right)^2 + \left(1 - \varrho^2\right) < R^2.$$

Thus $\boldsymbol{y}$ is in a free position by the assumptions of the proposition, which contradicts $\boldsymbol{y} \in \mathcal{N}_X(\boldsymbol{x})$. $\square$

IV. After Propositions 2 and 3 it remains to take care of points in $X \cap \operatorname{bd}\operatorname{conv} X$, for $X \in \mathcal{F}$ attaining $\lambda(C, |X|)$, and with $|X|$ sufficiently large. It turns out that these points can all be moved to free positions within $\operatorname{int}\operatorname{conv} X$. As a consequence we obtain the following.

Proposition 4. *Let $d \geq 2$, $C \subset \mathbb{R}^d$ a smooth convex body and $\mathcal{F}$ a family of packing sets in $\mathbb{R}^d$ satisfying (ii) of Definition 1. Then there exists an $n_4 \in \mathbb{N}$, depending on C and $\mathcal{F}$, such that $X \in \mathcal{F}$ with $|X| \geq n_4$ does not attain $\lambda(C, |X|)$, if all elements of $X \cap \operatorname{int}\operatorname{conv} X$ are in a free position.*

Proof. Let $\varrho > 0$ as in (ii) of Definition 1. We choose n_4 by Proposition 1 (ii), applied to $\varepsilon = \varrho$ and $r = 1$. Assume $X \in \mathcal{F}$ with $|X| \geq n_4$ attains $\lambda(C, |X|)$ and all elements of $X \cap \operatorname{int}\operatorname{conv} X$ are in a free position. We show that every element $\boldsymbol{x} \in X \cap \operatorname{bd}\operatorname{conv} X$ can be moved to a free position into $\operatorname{int}\operatorname{conv} X$. This gives the desired contradiction, because after moving (in an arbitrary order) all $X \cap \operatorname{bd}\operatorname{conv} X$ to free positions into $\operatorname{int}\operatorname{conv} X$, we obtain a packing set X' with $|X'| = |X|$ and $X' \subset \operatorname{int}\operatorname{conv} X$.
It is possible to move a given $\boldsymbol{x} \in X \cap \operatorname{bd}\operatorname{conv} X$ to a free position $\boldsymbol{x}' = \boldsymbol{x} + \delta \boldsymbol{v}$ for a (sufficiently small) $\delta > 0$, if $\boldsymbol{v} \in S^{d-1}$ is contained in the non-empty polyhedral cone

$$C_{\boldsymbol{x}} = \left\{ \boldsymbol{v} \in \mathbb{R}^d : \langle \boldsymbol{v}, \boldsymbol{y} - \boldsymbol{x} \rangle \leq 0 \text{ for all } \boldsymbol{y} \in \mathcal{N}_X(\boldsymbol{x}) \right\}.$$

If $\boldsymbol{v} \in C_{\boldsymbol{x}}$ can be chosen, so that $\boldsymbol{x}' \in \operatorname{int}\operatorname{conv} X$, the assertion follows. Otherwise, because $C_{\boldsymbol{x}}$ and $\operatorname{conv} X$ are convex, there exists a hyperplane through $\boldsymbol{x}$, with normal $\boldsymbol{w} \in S^{d-1}$, which separates $\operatorname{conv} X$ and $\boldsymbol{x} + C_{\boldsymbol{x}}$. That is, we may assume that

$$\boldsymbol{w} \in \operatorname{pos}\{\boldsymbol{y} - \boldsymbol{x} : \boldsymbol{y} \in \mathcal{N}_X(\boldsymbol{x})\}$$

and $-\boldsymbol{w}$ is an outer normal of $\operatorname{conv} X$ at $\boldsymbol{x}$.
Then for some $\delta > 0$, there exists a point $\boldsymbol{z} = \boldsymbol{x} + \delta \boldsymbol{w} \in \operatorname{bd}\operatorname{conv} \mathcal{N}_X(\boldsymbol{x})$, which is a convex combination of some $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_k \in \mathcal{N}_X(\boldsymbol{x})$. That is, there exist $\alpha_i \geq 0$ with $\sum_{i=1}^k \alpha_i = 1$ and $\boldsymbol{z} = \sum_{i=1}^k \alpha_i \boldsymbol{y}_i$. Therefore

$$\delta = \langle \boldsymbol{z} - \boldsymbol{x}, \boldsymbol{w} \rangle = \sum_{i=1}^k \alpha_i \langle \boldsymbol{y}_i - \boldsymbol{x}, \boldsymbol{w} \rangle < \varrho,$$

because $\langle \boldsymbol{y}_i - \boldsymbol{x}, \boldsymbol{w} \rangle < \varrho$ due to $|X| \geq n_4$ and $\boldsymbol{y}_i \in \operatorname{bd}\operatorname{conv} X$. This contradicts the assumption on $\mathcal{F}$ with respect to ϱ though. ☐

Finish. The proof of Theorem 2 reduces to the application of Propositions 1, 2, 3 and 4. Let $\mathcal{F}$ be an lc-family of packing sets in $\mathbb{R}^d$, with a $\varrho > 0$ as in (ii) of Definition 1. We choose $R \geq 1/\varrho$ and n_2 and n_4 according to Propositions 2 and 4. By Proposition 1 (ii), we choose n_1 such that packing sets X attaining $\lambda(C, |X|)$ with $|X| \geq n_1$ satisfy the following: For each $\boldsymbol{x} \in X$, there exists a $\boldsymbol{t} \in \mathbb{R}^d$ with $|\boldsymbol{x} - \boldsymbol{t}| = R + \frac{\varrho}{2}$ and $\boldsymbol{t} + RB^d \subset \operatorname{conv} X$.
We choose $n_0 \geq \max\{n_1, n_2, n_4\}$ and assume that $X \in \mathcal{F}$ with $|X| \geq n_0$ attains $\lambda(C, |X|)$. By Proposition 2 we can modify the packing set X to obtain a new packing

set X' with a contact free region $(\boldsymbol{t}_X + RB^d) \subset \operatorname{int}\operatorname{conv} X$, and with the same points $X' \cap \operatorname{bd}\operatorname{conv} X' = X \cap \operatorname{bd}\operatorname{conv} X$ on the boundary of the center polytope $\operatorname{conv} X' = \operatorname{conv} X$.
The following gives a possible order, in which we may subsequently move non-free elements $\boldsymbol{x} \in X \cap \operatorname{int}\operatorname{conv} X$ to free positions: By the choice of n_0 we can guarantee that for each $\boldsymbol{x} \in X \cap \operatorname{int}\operatorname{conv} X$, there exists a $\boldsymbol{t}$ with $|\boldsymbol{x} - \boldsymbol{t}| \leq R + \frac{\varrho}{2}$ and $\boldsymbol{t} + RB^d \subset \operatorname{conv} X$. Let $\boldsymbol{t}_{\boldsymbol{x}}$ be the $\boldsymbol{t}$ at minimal distance to $\boldsymbol{t}_X$. Then among the non-free $\boldsymbol{x} \in \operatorname{int}\operatorname{conv} X$, the one with minimal distance $|\boldsymbol{t}_{\boldsymbol{x}} - \boldsymbol{t}_X|$ satisfies the assumptions of Proposition 3, because a non-free element $\boldsymbol{y} \in X \cap (\boldsymbol{t}_{\boldsymbol{x}} + B^d)$ would satisfy $|\boldsymbol{t}_{\boldsymbol{y}} - \boldsymbol{t}_X| < |\boldsymbol{t}_{\boldsymbol{x}} - \boldsymbol{t}_X|$ due to $\operatorname{conv}\{\boldsymbol{t}_{\boldsymbol{x}}, \boldsymbol{t}_X\} + B^d \subset \operatorname{conv} X$.
Thus by Proposition 3 we can subsequently move the non-free elements within $X \cap \operatorname{int}\operatorname{conv} X$ to free positions. By this we obtain a contradiction to Proposition 4, which proves the theorem.

THE LATTICE PACKING CASE. We end this section with the proof of Theorem 1. We may apply Theorem 2 after showing that the family of solutions to the lattice restricted container problem is of limited complexity. The space of lattices can be turned into a topological space (see [GL87]). The convergence of a sequence $\{\Lambda_n\}$ of lattices to a lattice Λ in particular involves that sets of lattice points within radius r around a lattice point tend to translates of $\Lambda \cap rB^d$ for growing n. As a consequence, a convergent sequence of packing lattices, as well as subsets of them, form an lc-family. Solutions to the lattice restricted container problem tend for growing n towards subsets of translates of *densest packing lattices* (see [Zon99]). These lattices are the solutions of the *lattice (sphere) packing problem.* Up to isometries, there exist only finitely many of these lattices in each dimension (see [Zon99]). Thus the assertion follows, since a finite union of lc-families is an lc-family.

4 EXTENSIONS

Let us briefly mention some possible extensions of Theorem 2. These have been treated in [Sch02] for the 2-dimensional case and could be directions for further research.

Packings of other convex bodies. Instead of sphere packings, we may consider packings $X + K$ for other convex bodies K. If the *difference body* $DK = K - K$ is strictly convex, then the proofs can be applied after some modifications: Instead of measuring distances with the norm $|\cdot|$ given by B^d, we use the norm $|\boldsymbol{x}|_{DK} = \min\{\lambda > 0 : \lambda\boldsymbol{x} \in DK\}$ given by DK. The strict convexity of DK is then used for the key fact, that elements $\boldsymbol{x}$ of a packing set X can be moved to a free position, whenever they are not contained in $\operatorname{int}\operatorname{conv}\mathcal{N}_X(\boldsymbol{x})$ (see II in Section 3). Note though that the sets in (6) and depending definitions have to be adapted for general convex bodies.

Packings in other containers. The restriction to smooth convex containers simplifies the proof, but we strongly believe that Theorem 2 is valid for other containers as well, e.g. certain polytopes. On the other hand there might exist containers for which

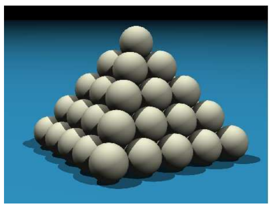
Theorem 2 is not true. In particular in dimension 3 it seems very likely that Theorem 2 is not true for polytopal containers C with all their facets lying in planes containing hexagonal sublattices of the *fcc lattice* (see Section 5). That is, for these polytopal containers C we conjecture the existence of infinitely many n, for which subsets of the *fcc lattice* attain $\lambda(C, n)$. An example for at least "local optimality" of sphere packings (with respect to differential perturbations) in suitable sized, but arbitrarily large tetrahedra was given by Dauenhauer and Zassenhaus [DZ87]. A proof of "global optimality" seems extremely difficult though, as it would provide a new proof of the sphere packing problem ("Kepler conjecture", see Section 5).

Other finite packing problems. Similar "phenomena" occur for other packing problems. For example, if we consider finite packing sets X with minimum diameter or surface area of $\operatorname{conv} X$, or maximum parametric density with large parameter (cf. [FCG91], [BHW94], [Bör04], [BP05]). This is due to the fact that the shapes of solutions tend to certain convex bodies, e.g. a sphere.

5 Kepler's assertion

Kepler's statement, quoted in the introduction, was later referred to as the origin of the famous sphere packing problem known as the *Kepler conjecture* (cf. e.g. [Hal02] p.5, [Hsi01] p.4). In contrast to the original statement, this problem asks for the maximum sphere packing density (see (10) below) of an infinite arrangement of spheres, where the "container" is the whole Euclidean space. As a part of Hilbert's famous problems [Hil01], it attracted many researchers in the past. Its proof by Hales with contributions of Ferguson (see [Hal02], [Hal05], [Hal06]), although widely accepted, had been a matter of discussion (cf. [Lag02], [Szp03], [FL06]).

Following Kepler [Kep11], the *cubic or hexagonal close packings* in $\mathbb{R}^3$ can be described via two dimensional layers of spheres, in which every sphere center belongs to a planar square grid, say with minimum distance 1. These layers are stacked (in a unique way) such that each sphere in a layer touches exactly four spheres of the layer above and four of the layer below.



The packing attained in this way is the well known *face centered cubic (fcc) lattice packing*. We can build up the fcc lattice by planar hexagonal layers as well, but then there are two choices for each new layer to be placed, and only one of them yields an fcc lattice packing. All of them, including the uncountably many non-lattice packings, are referred to as *hexagonal close packings (hc-packings)*. Note that the family of hc-packings is of limited complexity, because up to isometries they can be built from a fixed hexagonal layer.
Let

$$n(C) = \max\{|X| : C \supset X + \tfrac{1}{2}B^d \text{ is a packing }\}.$$

Then in our terminology Kepler asserts that, in $\mathbb{R}^3$, $n(C)$ is attained by hc-packings. His assertion, if true, would imply an "answer" to the sphere packing problem (Kepler conjecture), namely that the density of the densest infinite sphere packing

$$\delta_d = \limsup_{\lambda\to\infty} \frac{n(\lambda C)\cdot \mathrm{vol}(\frac{1}{2}B^d)}{\mathrm{vol}(\lambda C)} \tag{10}$$

is attained by hc-packings for $d = 3$; hence $\delta_3 = \pi/\sqrt{18}$. Note that this definition of density is independent of the chosen convex container C (see [Hla49] or [GL87]). As a consequence of Theorem 2, Kepler's assertion turns out to be false though, even if we think of arbitrarily large containers. Consider for example the containers $\lambda(C, n)C$ for $n \geq n_0$.

Corollary 1. *Let $d \geq 2$, $C \subset \mathbb{R}^d$ a smooth convex body and $\mathcal{F}$ an lc-family of packing sets in $\mathbb{R}^d$. Then there exist arbitrarily large λ such that $n(\lambda C)$ is not attained by packing sets in $\mathcal{F}$.*

We may as well think of arbitrarily small spheres packed into a fixed container C. For $r > 0$, we call $X + rB^d$ a sphere packing if distinct elements $\boldsymbol{x}$ and $\boldsymbol{x}'$ of X have distance $|\boldsymbol{x} - \boldsymbol{x}'| \geq 2r$. Specializing to $\mathbb{R}^3$, the following corollary of Theorem 2 refers directly to Kepler's assertion.

Corollary 2. *Let $C \subset \mathbb{R}^3$ a smooth convex body. Then there exist arbitrarily small $r > 0$, such that*

$$\max\{|X| : C \supset X + rB^d \text{ is a packing }\}$$

is not attained by fcc or hexagonal close packing sets.

Acknowledgments

I like to thank Thomas C. Hales, Tyrrell B. McAllister, Frank Vallentin, Jörg M. Wills, Günter M. Ziegler and the two anonymous referees for many helpful suggestions.

References

[BHW94] U. Betke, M. Henk and J.M. Wills, *Finite and infinite packings*, J. Reine Angew. Math. 453 (1994), 165–191.

[Bez87] K. Bezdek, *Densest packing of small number of congruent spheres in polyhedra*, Ann. Univ. Sci. Budapest Eötvös Sect. Math., 30 (1987), 177–194.

[Bör04] K. Böröczky Jr., *Finite packing and covering*, Cambridge university press, Cambridge, 2004.

[BW04] K. Böröczky Jr., G. Wintsche, *Sphere packings in the regular crosspolytope*, Ann. Univ. Sci. Budapest Eötvös Sect. Math., 43 (2000), 151–157.

[BP05] P. Brass and J. Pach, *Problems in discrete geometry*, Springer, New York, 2005.

[CS95] J.H. Conway and N.J.A. Sloane, *What are all the best sphere packings in low dimensions?*, Discrete Comput. Geom., 13 (1995), 282–403.

[DZ87] M.H. Dauenhauer and H.J. Zassenhaus, *Local optimality of the critical lattice sphere-packing of regular tetrahedra*, Discrete Math. 64 (1987), 129–146.

[FCG91] K.J. Falconer H.T. Croft and R.K. Guy, *Unsolved problems in geometry*, Springer, New York, 1991.

[FL06] G. Fejes Tóth and J.C. Lagarias, *Guest Editors Foreword*, Discrete Comput. Geom., 36 (2006), 1–3.

[Fod99] F. Fodor, *The densest packing of 19 congruent circles in a circle*, Geom. Dedicata, 74 (1999), 139–145.

[GL87] P.M. Gruber and C.G. Lekkerkerker, *Geometry of numbers*, North-Holland, Amsterdam, 1987.

[Hal02] T.C. Hales, *An overview of the Kepler conjecture*, 16 pages, first in a series, arXiv:math.MG/9811071 (v2).

[Hal05] T.C. Hales, *A proof of the Kepler conjecture*, Ann. of Math (2), 162 (2005), 1065–1185.

[Hal06] T.C. Hales, *A proof of the Kepler conjecture (unabridged version)*, Discrete Comput. Geom., 36 (2006), 1–265.

[Hil01] D. Hilbert, *Mathematische Probleme*, Archiv Math. Physik 1 (1901), 44–63.

[Hla49] E. Hlawka, *Ausfüllung und Überdeckung konvexer Körper durch konvexe Körper.*, Monatsh. Math. 53 (1949), 81–131.

[Hsi01] W.Y. Hsiang, *Least action principle of crystal formation of dense packing type and Kepler's conjecture.*, World Scientific, Singapore, 2001.

[Kep11] J. Kepler, *Strena seu de nive sexangula*, Godefridum Tampach, Francofvrti Ad Moenum (Frankfurt), 1611, English translation: Hardy, *The six-cornered snowflake*, Clarendon Pr., Oxford, 1966.

[Lag02] J.C. Lagarias, *Bounds for local density of sphere packings and the Kepler conjecture.*, Discrete Comput. Geom. 27 (2002), 165–193.

[LG97] B.D. Lubachevsky and R.L. Graham, *Curved hexagonal packings of equal disks in a circle*, Discrete Comput. Geom. 18 (1997), 179–194.

[Mel97] J.B.M. Melissen, *Packing and covering with circles*, PhD thesis, University of Utrecht, 1997.

[NÖ97] K.J. Nurmela and P.R.J. Östergard, *More Optimal Packings of Equal Circles in a Square*, Discrete Comput. Geom. 22 (1999), 439–457.

[Sch93] R. Schneider, *Convex bodies: the Brunn-Minkowski theory.*, Cambridge University Press, Cambridge, 1993.

[Sch02] A. Schürmann, *On extremal finite packings*, Discrete Comput. Geom. 28 (2002), 389–403.

[Spe04] E. Specht, *Packomania*, `http://www.packomania.com/`.

[SMC+06] P.G. Szabó, M.Cs. Markót, T. Csendes, E. Specht, L.G. Casado, I. García, *New Approaches to Circle Packing in a Square*, Springer-Verlag, Berlin, to appear.

[Szp03] G. Szpiro, *Does the proof stack up?*, Nature 424 (2003), 12–13.

[Zie97] G.M. Ziegler, *Lectures on polytopes*, Springer-Verlag, New York, 1997.

[Zon99] C. Zong, *Sphere packings*, Springer-Verlag, New York, 1999.

Achill Schürmann
Mathematics Department
University of Magdeburg
39106 Magdeburg
Germany
achill@math.uni-magdeburg.de