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Perfect, strongly eutactic lattices are periodic extreme

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Abstract

We introduce a parameter space for periodic point sets, given as unions of m translates of point lattices. In it we investigate the behavior of the sphere packing density function and derive sufficient conditions for local optimality. Using these criteria we prove that perfect, strongly eutactic lattices cannot be locally improved to yield a periodic sphere packing with greater density. This applies in particular to the densest known lattice sphere packings in dimension $d \leqslant 8$ and $d = 24$.

MSC: 52C17; 11H55

Keywords: Sphere packing; Root lattice; Leech lattice; Periodic point set; Voronoi characterization; Perfect lattice; Strongly eutactic; Spherical design

1. Introduction

The classical and widely studied *sphere packing problem* asks for a non-overlapping arrangement of equally sized spheres in a Euclidean space, such that the fraction of space covered by spheres is maximized. The problem arose from the arithmetical study of positive definite quadratic forms. By the works Thue [29] and Hales [17] the optimal arrangements of spheres are known in dimension 2 and 3. We refer to [15,10,21,27] for details and further reading.

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Table 1
Point sets defining best known sphere packings up to dimension 24.

d	point set	$\delta/\operatorname{vol} B^d$	author(s)
2	A_2	0.2886...	Lagrange, 1773 [19]
3	$\mathsf{A}_3 = \mathsf{D}_3, *$	0.1767...	Gauß, 1840 [13]
4	D_4	0.125	Korkine & Zolotareff, 1877 [18]
5	$\mathsf{D}_5, *$	0.0883...	Korkine & Zolotareff, 1877 [18]
6	$\mathsf{E}_6, *$	0.0721...	Blichfeldt, 1935 [4]
7	$\mathsf{E}_7, *$	0.0625	Blichfeldt, 1935 [4]
8	E_8	0.0625	Blichfeldt, 1935 [4]
9	$\Lambda_9, *$	0.0441...	
10	P_{10c}	0.0390...	Leech & Sloane, 1970 [20]
11	P_{11a}	0.0351...	Leech & Sloane, 1970 [20]
12	K_{12}	0.0370...	
13	P_{13a}	0.0351...	Leech & Sloane, 1970 [20]
14	$\Lambda_{14}, *$	0.0360...	
15	$\Lambda_{15}, *$	0.0441...	
16	$\Lambda_{16}, *$	0.0625	
17	$\Lambda_{17}, *$	0.0625	
18	V_{18}	0.0750...	Bierbrauer & Edel, 1998 [3]
19	$\Lambda_{19}, *$	0.0883...	
20	V_{20}	0.1315...	Vardy, 1995 [30]
21	$\Lambda_{21}, *$	0.1767...	
22	V_{22}	0.3325...	Conway & Sloane, 1996 [9]
23	Λ_{23}	0.5	
24	Λ_{24}	1	Cohn & Kumar, 2004 [7]

In dimensions $d \leqslant 8$ and $d = 24$ the corresponding authors solved the lattice sphere packing problem. The other mentioned authors found the listed, densest known periodic sphere packings. The asterisk $*$ indicates that an equally dense, periodic non-lattice sphere packing is known.

For reasons related to the historical roots of the sphere packing problem, special attention has been on (*point*) *lattices* as the discrete set of sphere centers. In dimension 2 the *hexagonal lattice* and in dimension 3 the *face-centered-cubic lattice* yield optimal sphere packings. For the restriction of the sphere packing problem to lattices, the optimal configurations are known up to dimension 8 and in dimension 24 (see Table 1). Here, solutions are given by fascinating objects, the so-called *root lattices* and the *Leech lattice*. We refer to [10,21,36] for further information on these exceptional objects.

A major *open problem* in the theory of sphere packing is to find a dimension in which there is a non-lattice packing that is denser than any lattice packing. In dimension 10 there exists a non-lattice sphere packing, that is conjectured to have a higher density than any lattice sphere packing (see [20]). As shown in Table 1, below dimension 24 similar sphere packings have been found in dimensions 11, 13, 18, 20 and 22. All of them are *periodic*, that is, a finite union of translates of a lattice sphere packing. By a well-known conjecture, attributed by Gruber [16] to Zassenhaus, optimal sphere packing density can always be attained by periodic sphere packings. It is known that their density comes arbitrarily close to the optimal value (see for example [6, Appendix A]).

A natural idea to obtain a better non-lattice sphere packing, is to "locally modify" one of the optimal known lattice sphere packings in dimensions $d = 4, \ldots, 8$. In this paper we show that such modifications are not possible within the set of all periodic sphere packings (see Corollary 11). We more generally show in Theorem 10 that such modifications are not possible for *perfect, strongly eutactic lattices*.

One may wonder why the restriction to periodic structures is necessary. One could also consider more general discrete sets. However, within the set of all discrete sets, we are not aware of any notion of a "local modification" that on the one hand could potentially lead to an improved sphere packing density, but on the other hand would allow us to generalize the result of this paper. For instance, a natural approach to define the ϵ-neighborhood of a discrete set is as the collection of sets that can be obtained by changing the position of elements by at most an ϵ distance. However, such a local modification would not even change the sphere packing density. It is equal to a constant multiple of the average number of points per unit volume, which could not be changed in such an ϵ-neighborhood. In contrast to that, the local changes of periodic sets considered in this paper allow arbitrarily large displacements of points, if they are far enough from the origin.

The paper is organized as follows. In Section 2 we recall some necessary background on lattices and positive definite quadratic forms. In Section 3 we introduce the so-called Ryshkov polyhedron, and based on it we give a geometrical interpretation of Voronoi's characterization of locally optimal lattice sphere packings. This viewpoint allows a natural generalization to study local optimal periodic sphere packings. For their study we introduce a parameter space in Section 4. We give characterizations of local optimal periodic sphere packings with up to m lattices translates in Section 5. Based on these general characterizations we obtain one of the main results of this paper in Section 6: We show that perfect, strongly eutactic lattices cannot locally be modified to yield a better periodic sphere packing – they are *periodic extreme* (see Definition 8).

2. Background on lattices and quadratic forms

Lattices and periodic sets. A (full rank) *lattice* L in $\mathbb{R}^d$ is a discrete subgroup $L = \mathbb{Z}\boldsymbol{a}_1 + \cdots + \mathbb{Z}\boldsymbol{a}_d$ generated by d linear independent (column) vectors $\boldsymbol{a}_i \in \mathbb{R}^d$. We say that these vectors form a *basis* of L and associate it with the matrix $A = (\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d) \in \mathsf{GL}_d(\mathbb{R})$. We write $L = A\mathbb{Z}^d$. It is well known that L is generated in this way precisely by the matrices AU with $U \in \mathsf{GL}_d(\mathbb{Z})$. We refer to [15] for details and more background on lattices. Given a lattice L and *translational vectors* $\boldsymbol{t}_i$, for say $i = 1, \ldots, m$, the discrete set

$$\Lambda = \bigcup_{i=1}^{m} (\boldsymbol{t}_i + L) \tag{1}$$

is called a *periodic* (*point*) *set*.

The *sphere packing radius* $\lambda(\Lambda)$ of a discrete set Λ (not necessarily periodic) in the Euclidean space $\mathbb{R}^d$ (with norm $\|\cdot\|$) is defined as the infimum of half the distances between distinct points:

$$\lambda(\Lambda) = \frac{1}{2} \inf_{\boldsymbol{x}, \boldsymbol{y} \in \Lambda, \boldsymbol{x} \neq \boldsymbol{y}} \|\boldsymbol{x} - \boldsymbol{y}\|.$$

The sphere packing radius is the largest possible radius λ such that solid spheres of radius λ and with centers in Λ do not overlap. Denoting the solid unit sphere by B^d, the *sphere packing* defined by Λ is the union of non-overlapping spheres

$$\bigcup_{\boldsymbol{x} \in \Lambda} \big(\boldsymbol{x} + \lambda(\Lambda) B^d\big).$$

Its *density* $\delta(\Lambda)$ is, loosely speaking, defined as the fraction of space covered by spheres. We can make this definition more precise by considering a cube $C = \{x \in \mathbb{R}^d\colon |x_i| \leqslant 1/2\}$ and setting

$$\delta(\Lambda) = \lambda(\Lambda)^d \operatorname{vol} B^d \cdot \liminf_{\lambda\to\infty} \frac{\operatorname{card}(\Lambda \cap \lambda C)}{\operatorname{vol} \lambda C}.$$

If the limit inferior above is a true limit, the cube in the definition can be replaced by any other compact set C that is the closure of its interior, without the value of δ changing. We say that a corresponding set Λ is *uniformly dense* in that case. It can be shown that the supremum of $\delta(\Lambda)$ over all discrete sets is attained by a uniformly dense set Λ. We refer to [14] and [6, Appendix A] for further reading.

For general discrete sets, it may be difficult to compute the density, respectively the limit inferior in the definition. For a lattice the limit inferior can simply be replaced by $1/\det L$, where $\det L = |\det A|$ is the *determinant* of the lattice $L = A\mathbb{Z}^d$. Note that the determinant of L is independent of the particular choice of the basis A. For periodic sets Λ as in (1) we get the estimate

$$\delta(\Lambda) \leqslant \frac{m\lambda(\Lambda)^d \operatorname{vol} B^d}{\det L},$$

with equality if and only if the lattice translates $\boldsymbol{t}_i + L$ are pairwise disjoint.

Positive definite quadratic forms. Among similarity classes of lattices, hence in the space $O_d(\mathbb{R})\backslash \mathsf{GL}_d(\mathbb{R})/\mathsf{GL}_d(\mathbb{Z})$, there exist only finitely many local maxima of δ up to scaling. In order to characterize and to work with them, i.e., enumerate them, it is convenient to use the language of real *positive definite quadratic forms* (PQFs for short). These are simply identified with the set $\mathcal{S}^d_{>0}$ of real symmetric, positive definite matrices. Given a matrix $Q \in \mathcal{S}^d_{>0}$, we set $Q[\boldsymbol{x}] = \boldsymbol{x}^t Q \boldsymbol{x}$ for $\boldsymbol{x} \in \mathbb{R}^d$, defining a corresponding PQF. Note that every matrix $Q \in \mathcal{S}^d_{>0}$ can be decomposed into $Q = A^t A$ with $A \in \mathsf{GL}_d(\mathbb{R})$ and therefore $\mathcal{S}^d_{>0}$ can be identified with the space $O_d(\mathbb{R})\backslash \mathsf{GL}_d(\mathbb{R})$ of lattice bases up to orthogonal transformations. Two PQFs (respectively matrices) Q and Q' are called *arithmetically equivalent* (or *integrally equivalent*) if there exists a matrix $U \in \mathsf{GL}_d(\mathbb{Z})$ with $Q' = U^t Q U$. Thus arithmetical equivalence classes of PQFs are in one-to-one correspondence with similarity classes of lattices.

The *arithmetical minimum* $\lambda(Q)$ of a PQF Q is defined by

$$\lambda(Q) = \min_{\boldsymbol{x}\in\mathbb{Z}^d\backslash\{\boldsymbol{0}\}} Q[\boldsymbol{x}].$$

If $L = A\mathbb{Z}^d$ with $A \in \mathsf{GL}_d(\mathbb{R})$ satisfying $Q = A^t A$ is a corresponding lattice, there is an immediate relation to the packing radius of L: We have $\lambda(Q) = (2\lambda(L))^2$ and therefore

$$\delta(L) = \mathcal{H}(Q)^{d/2} \frac{\operatorname{vol} B^d}{2^d},$$

where

$$\mathcal{H}(Q) = \frac{\lambda(Q)}{(\det Q)^{1/d}}$$

is the so-called *Hermite invariant* of Q. Note that $\mathcal{H}(\cdot)$ is invariant with respect to scaling. A classical problem in the arithmetic theory of quadratic forms is the determination of the *Hermite constant*

$$\mathcal{H}_d = \sup_{Q \in \mathcal{S}^d_{>0}} \mathcal{H}(Q).$$

By the relation described above, it corresponds to determining the supremum of possible lattice sphere packing densities. Local maxima of the Hermite invariant on $\mathcal{S}^d_{>0}$ and corresponding lattices are called *extreme*.

3. Voronoi's characterization of extreme forms

The Ryshkov polyhedron. Since the Hermite invariant is invariant with respect to scaling, a natural approach to maximizing it is to consider all forms with a fixed arithmetical minimum, say 1, and minimize the determinant among them. We may even relax the condition on the arithmetical minimum and only require that it is at least 1. In other words, we have

$$\mathcal{H}_d = 1/\inf_{\mathcal{R}}(\det Q)^{1/d},$$

where

$$\mathcal{R} = \{Q \in \mathcal{S}^d_{>0}\colon \lambda(Q) \geqslant 1\}. \tag{2}$$

We refer to $\mathcal{R}$ as *Ryshkov polyhedron*, as it was Ryshkov [26] who noticed that this view on Hermite's constant allows a simplified description of Voronoi's theory, to be sketched below.

We denote by $\mathcal{S}^d$ the space of real symmetric matrices, respectively of real quadratic forms in d variables. It is a Euclidean vector space of dimension $\binom{d+1}{2}$ with the usual inner product defined by

$$\langle Q, Q'\rangle = \sum_{i,j=1}^{d} q_{ij}q'_{ij} = \operatorname{trace}(Q \cdot Q').$$

Because of the fundamental identity

$$Q[\boldsymbol{x}] = \langle Q, \boldsymbol{x}\boldsymbol{x}^t\rangle,$$

quadratic forms $Q \in \mathcal{S}^d$ attaining a fixed value on a given $\boldsymbol{x} \in \mathbb{R}^d \setminus \{\boldsymbol{0}\}$ lie all in a *hyperplane* (*affine subspace of co-dimension* 1). Thus Ryshkov polyhedra $\mathcal{R}$ are intersections of infinitely many *halfspaces*:

$$\mathcal{R} = \{Q \in \mathcal{S}^d_{>0}\colon \langle Q, \boldsymbol{x}\boldsymbol{x}^t\rangle \geqslant 1 \text{ for all } \boldsymbol{x} \in \mathbb{Z}^d \setminus \{\boldsymbol{0}\}\}. \tag{3}$$

It can be shown that $\mathcal{R}$ is "locally like a polyhedron", meaning that any intersection with a *polytope* (convex hull of finitely many vertices) is itself a polytope. For a proof we refer to

[27, Theorem 3.1]. As a consequence $\mathcal{R}$ has *vertices*, *edges*, *facets* and in general *k-dimensional faces* (*k-faces*). For details on terminology and basic properties of polytopes we refer to [33].

Perfect forms. The vertices Q of the Ryshkov polyhedron are called *perfect forms*. Such forms are characterized by the fact that they are determined uniquely by their arithmetical minimum (here 1) and its representatives

$$\operatorname{Min} Q = \{\boldsymbol{x} \in \mathbb{Z}^d \colon Q[\boldsymbol{x}] = \lambda(Q)\}.$$

A corresponding lattice is called perfect too. The following proposition due to Minkowski implies that the Hermite constant can only be attained among perfect forms, i.e., the maximal lattice sphere packing density can only be attained by perfect lattices.

Proposition 1. *(See Minkowski [22].)* $(\det Q)^{1/d}$ *is a strictly concave function on* $\mathcal{S}^d_{>0}$.

For a proof see for example [15, § 39.2]. Note, that in contrast to $(\det Q)^{1/d}$, the function $\det Q$ is not a concave function on $\mathcal{S}^d_{>0}$ (see [24]). However Minkowski's theorem implies that the set

$$\{Q \in \mathcal{S}^d_{>0} \colon \det Q \geqslant D\} \tag{4}$$

is strictly convex for $D > 0$.

Another property of perfect forms which we use later is the following.

Proposition 2. *If* $Q \in \mathcal{S}^d$ *is perfect, then* $\operatorname{Min} Q$ *spans* $\mathbb{R}^d$.

The existence of d linear independent vectors in $\operatorname{Min} Q$ for a perfect form Q follows from the observation that the rank-1 forms $\boldsymbol{x}\boldsymbol{x}^t$ with $\boldsymbol{x} \in \operatorname{Min} Q$ have to span $\mathcal{S}^d$, since they uniquely determine Q through the linear equations $\langle Q, \boldsymbol{x}\boldsymbol{x}^t\rangle = \lambda(Q)$. If however $\operatorname{Min} Q$ does not span $\mathbb{R}^d$ then these rank-1 forms can maximally span a $\binom{d}{2}$-dimensional subspace of $\mathcal{S}^d$.

Finiteness up to equivalence. The arithmetical equivalence operation $Q \mapsto U^t QU$ of $\mathsf{GL}_d(\mathbb{Z})$ on $\mathcal{S}^d_{>0}$ leaves $\lambda(Q)$, $\operatorname{Min} Q$ and also $\mathcal{R}$ invariant. In fact, $\mathsf{GL}_d(\mathbb{Z})$ acts on the sets of faces of a given dimension, thus in particular on the sets of vertices, edges and facets of $\mathcal{R}$. The following theorem shows that the Ryshkov polyhedron $\mathcal{R}$ contains only finitely many arithmetically inequivalent vertices. By Proposition 1 this implies in particular that $\mathcal{H}_d$ is actually attained, namely by some perfect forms. For a proof we refer to [27, Theorem 3.4].

Theorem 3 *(Voronoi [32]). Up to arithmetical equivalence and scaling there exist only finitely many perfect forms in a given dimension* $d \geqslant 1$.

Thus the classification of perfect forms in a given dimension, respectively the enumeration of vertices of the Ryshkov polyhedron up to arithmetical equivalence, yields the Hermite constant. Perfect forms have been classified up to dimension 8 (see [11]).

Characterization of extreme forms. From dimension 6 onwards not every perfect form is extreme (see [21]). In order to characterize extreme forms within the set of perfect forms the notion of *eutaxy* is used: A PQF Q is called *eutactic* if its inverse Q^{-1} is contained in the (relative) interior relint $\mathcal{V}(Q)$ of its *Voronoi domain*

$$\mathcal{V}(Q) = \operatorname{cone}\{\boldsymbol{x}\boldsymbol{x}^t\colon \boldsymbol{x} \in \operatorname{Min} Q\}.$$

Here cone M denotes the *conic hull*

$$\left\{\sum_{i=1}^{n} \alpha_i \boldsymbol{x}_i\colon n \in \mathbb{N} \text{ and } \boldsymbol{x}_i \in M, \alpha_i \geqslant 0 \text{ for } i = 1, \dots, n\right\}$$

of a set M. Note that the Voronoi domain is full-dimensional (of dimension $\binom{d+1}{2}$) if and only if Q is perfect. Note also that the rank-1 forms $\boldsymbol{x}\boldsymbol{x}^t$ give inequalities $\langle Q, \boldsymbol{x}\boldsymbol{x}^t\rangle \geqslant 1$ defining the Ryshkov polyhedron and by this the Voronoi domain of Q is equal to the *normal cone*

$$\{N \in \mathcal{S}^d\colon \langle N, Q/\lambda(Q)\rangle \leqslant \langle N, Q'\rangle \text{ for all } Q' \in \mathcal{R}\} \tag{5}$$

of $\mathcal{R}$ at its boundary point $Q/\lambda(Q)$.

Algebraically the eutaxy condition $Q^{-1} \in \operatorname{relint} \mathcal{V}(Q)$ is equivalent to the existence of positive $\alpha_{\boldsymbol{x}}$ with

$$Q^{-1} = \sum_{\boldsymbol{x} \in \operatorname{Min} Q} \alpha_{\boldsymbol{x}} \boldsymbol{x}\boldsymbol{x}^t. \tag{6}$$

Thus computationally eutaxy of Q can be tested by solving the *linear program*

$$\max \alpha_{\min} \quad \text{such that } \alpha_{\boldsymbol{x}} \geqslant \alpha_{\min} \text{ and (6) holds.} \tag{7}$$

The form Q is eutactic if and only if the maximum is greater 0.

Voronoi [32] showed that perfection together with eutaxy implies extremality and vice versa:

Theorem 4 *(Voronoi [32]). A PQF $Q \in \mathcal{S}^d_{>0}$ is extreme if and only if Q is perfect and eutactic.*

We here give a proof providing a geometrical viewpoint that turns out to be quite useful for the intended generalization discussed in the following sections.

Proof. The function $\det Q$ is a positive real valued polynomial on $\mathcal{S}^d$, depending on the $\binom{d+1}{2}$ different coefficients q_{ij} of Q. Using the expansion theorem we obtain

$$\det Q = \sum_{i=1}^{d} q^{\#}_{ji} q_{ij}$$

for any fixed column index $j \in \{1, \dots, d\}$. Here, $q^{\#}_{ij} = (-1)^{i+j} \det Q_{ij}$ (with Q_{ij} the minor matrix of Q, obtained by removing row i and column j) denote the coefficients of the *adjoint form* $Q^{\#} = (\det Q) Q^{-1} \in \mathcal{S}^d_{>0}$ of Q. Thus

$$\operatorname{grad} \det Q = (\det Q) Q^{-1} \tag{8}$$

and the tangent hyperplane T in Q of the smooth *determinant*-det Q-*surface*

$$S = \{Q' \in \mathcal{S}^d_{>0}\colon \det Q' = \det Q\}$$

is given by

$$T = \{Q' \in \mathcal{S}^d\colon \langle Q^{-1}, Q' \rangle = \langle Q^{-1}, Q \rangle\}.$$

Or in other words, Q^{-1} is a normal vector of the tangent plane T of S at Q. By Proposition 1 and the observation that (4) is convex, we know that S is contained in the halfspace

$$\{Q' \in \mathcal{S}^d\colon \langle Q^{-1}, Q' - Q \rangle \geqslant 0\}, \tag{9}$$

with Q being the unique intersection point of S and T.

As a consequence, a perfect form Q attains a local minimum of $\det Q$ (hence is extreme) if and only if the halfspace (9) contains the Ryshkov polyhedron $\mathcal{R}$, and its boundary meets $\mathcal{R}$ only in Q. This is easily seen to be equivalent to the condition that the normal cone (Voronoi domain) $\mathcal{V}(Q)$ of $\mathcal{R}$ at Q contains Q^{-1} in its interior. $\square$

Note that eutaxy alone does not suffice for extremality. However, there exist only finitely many eutactic forms in every dimension and they can (in principle) be enumerated too (see [21, Section 9.5]). Nevertheless, this seems computationally more difficult than the enumeration of perfect forms (see [28,5,1,12]). By the geometry of S and T a eutactic form attains always a unique minimum of δ (maximum of det) on its face of the Ryshkov polyhedron. However, not all faces of the Ryshkov polyhedron contain a eutactic form.

4. Parameter spaces for periodic sets

We want to study the more general situation of periodic sphere packings. Recall from (1) that a periodic set with m lattice translates (an *m-periodic set*) in $\mathbb{R}^d$ is of the form

$$\Lambda' = \bigcup_{i=1}^{m} (\boldsymbol{t}'_i + L), \tag{10}$$

with a lattice $L \subset \mathbb{R}^d$ and translation vectors $\boldsymbol{t}'_i \in \mathbb{R}^d$, $i = 1, \ldots, m$.

We want to work with a parameter space for m-periodic sets similar to $\mathcal{S}^d_{>0}$ for lattices. For this, we consider Λ' as a linear image $\Lambda' = A\Lambda_{\boldsymbol{t}}$ of a *standard periodic set*

$$\Lambda_{\boldsymbol{t}} = \bigcup_{i=1}^{m} (\boldsymbol{t}_i + \mathbb{Z}^d). \tag{11}$$

Here, $A \in \mathsf{GL}_d(\mathbb{R})$ satisfies in particular $L = A\mathbb{Z}^d$. Since we are only interested in properties of periodic sets up to isometries, we encode Λ' by $Q = A^t A \in \mathcal{S}^d_{>0}$, together with the m translation vectors $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$. Since every property of periodic sets we deal with here is invariant up to translations, we may assume without loss of generality that $\boldsymbol{t}_m = \boldsymbol{0}$. Thus we consider the parameter space

$$\mathcal{S}^{d,m}_{>0} = \mathcal{S}^d_{>0} \times \mathbb{R}^{d\times(m-1)} \tag{12}$$

for m-periodic sets (up to isometries). We hereby in particular generalize the space $\mathcal{S}^{d,1}_{>0} = \mathcal{S}^d_{>0}$ in a natural way. We call the elements of $\mathcal{S}^{d,m}_{>0}$ *periodic forms* and denote them usually by $X = (Q, \boldsymbol{t})$, where $Q \in \mathcal{S}^d_{>0}$ and

$$\boldsymbol{t} = (\boldsymbol{t}_1, \dots, \boldsymbol{t}_{m-1}) \in \mathbb{R}^{d\times(m-1)}$$

is a real valued matrix containing $m-1$ columns with vectors $\boldsymbol{t}_i \in \mathbb{R}^d$. One should keep in mind: although we omit $\boldsymbol{t}_m = \boldsymbol{0}$, we implicitly keep it as a translation vector. Note that a periodic set Λ' as in (10) has many *representations* by periodic forms. In particular, m may vary and we have different choices for A. A similar approach for periodic sets in dimension 3 has been considered in [25].

The parameter space $\mathcal{S}^{d,m}_{>0}$ is contained in the space

$$\mathcal{S}^{d,m} = \mathcal{S}^d \times \mathbb{R}^{d\times(m-1)}. \tag{13}$$

It can be turned into a Euclidean space with inner product $\langle\cdot,\cdot\rangle$, defined for $X = (Q, \boldsymbol{t})$ and $X' = (Q', \boldsymbol{t}')$ by

$$\langle X, X'\rangle = \langle Q, Q'\rangle + \sum_{i=1}^{m-1} \boldsymbol{t}_i^t \boldsymbol{t}_i'.$$

Note, for the sake of simplicity we use the same symbol for the inner products on all spaces $\mathcal{S}^{d,m}$.

We extend the definition of the arithmetical minimum λ, by defining the *generalized arithmetical minimum*

$$\lambda(X) = \min\bigl\{Q[\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v}]\colon\ 1 \leqslant i, j \leqslant m \text{ and } \boldsymbol{v} \in \mathbb{Z}^d,\ \text{with } \boldsymbol{v} \neq \boldsymbol{0} \text{ if } i = j\bigr\}$$

for the periodic form $X = (Q, \boldsymbol{t}) \in \mathcal{S}^{d,m}_{>0}$. Note that we have $\lambda(X) = 0$ in the case of intersecting lattice translates $(\boldsymbol{t}_i + \mathbb{Z}^d) \cap (\boldsymbol{t}_j + \mathbb{Z}^d) \neq \emptyset$ with $i \neq j$. The set of *representations of the generalized arithmetical minimum* $\operatorname{Min} X$ is the set of all $\boldsymbol{w} = \boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v}$ attaining $\lambda(X)$. Computationally, $\operatorname{Min} X$ and $\lambda(X)$ can be obtained by solving a sequence of *closest vector problems* (CVPs), one for each pair i, j with $i \neq j$. In addition one shortest vector problem (SVP) has to be solved, taking care of the cases where $i = j$. Implementations of algorithms solving CVPs and SVPs are provided for example in MAGMA [35] or GAP [34].

In order to define the sphere packing density function $\delta : \mathcal{S}^{d,m}_{>0} \to \mathbb{R}$ we set $\det X = \det Q$ for periodic forms $X = (Q, \boldsymbol{t})$. Then

$$\delta(X) = \left(\frac{\lambda(X)}{(\det X)^{1/d}}\right)^{\frac{d}{2}} m \operatorname{vol} B^d / 2^d. \tag{14}$$

In analogy to the lattice case, we call a periodic form $X \in \mathcal{S}^{d,m}_{>0}$ *m-extreme* if it attains a local maximum of δ within $\mathcal{S}^{d,m}_{>0}$.

The relation (14) shows that the supremum of δ among m-periodic sphere packings is up to some power and a constant factor equal to the "Hermite like constant"

$$\sup_{X \in \mathcal{S}^{d,m}_{>0}} \lambda(X)/(\det X)^{1/d} = 1/\inf_{X \in \mathcal{R}_m} (\det X)^{1/d},$$

where the set $\mathcal{R}_m$ on the right side is the (*generalized*) *Ryshkov set*

$$\mathcal{R}_m = \{X \in \mathcal{S}^{d,m}_{>0}\colon \lambda(X) \geqslant 1\}. \tag{15}$$

The condition $\lambda(X) \geqslant 1$ gives infinitely many linear inequalities

$$p_{\boldsymbol{v}}(X) = Q[\boldsymbol{v}] = \langle X, (\boldsymbol{v}\boldsymbol{v}^t, 0)\rangle \geqslant 1$$

for $\boldsymbol{v} \in \mathbb{Z}^d \setminus \{\mathbf{0}\}$, as in the case $m = 1$. For $m > 1$ we additionally have the infinitely many polynomial inequalities

$$p_{i,j,\boldsymbol{v}}(X) = Q[\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v}] \geqslant 1, \tag{16}$$

where $i, j \in \{1, \dots, m\}$ with $i \neq j$ and $\boldsymbol{v} \in \mathbb{Z}^d$. These polynomials are of degree 3 in the parameters q_{kl}, t_{kl} of X. Note that they are linear for a fixed $\boldsymbol{t}$. Observe also that $p_{i,m,\boldsymbol{v}}$ and $p_{m,j,\boldsymbol{v}}$ are special due to our assumption $\boldsymbol{t}_m = \mathbf{0}$ and that there is a symmetry $p_{i,j,\boldsymbol{v}} = p_{j,i,-\boldsymbol{v}}$ by which we may restrict our attention to polynomials with $i \leqslant j$. For $i = j$ we have the linear function $p_{i,j,\boldsymbol{v}} = p_{\boldsymbol{v}}$.

5. Local analysis of periodic sphere packings

Characterizing local optima. Before we generalize perfection and eutaxy to a notion of *m-perfection* and *m-eutaxy* (in order to obtain a sufficient condition for a periodic form to be m-extreme from it) we discuss a rather general setting: Assume we want to minimize a smooth function on a *basic closed semialgebraic set*, that is, on a region which is described by finitely many (non-strict) polynomial inequalities. Let E denote a Euclidean space with inner product $\langle\cdot,\cdot\rangle$. Further, let $f : E \to \mathbb{R}$ be *smooth* (infinitely differentiable) and $g_1, \dots, g_k$ be (real valued) polynomials on E. Assume we want to determine whether or not we have a local minimum of f at X_0 on the boundary of

$$G = \{X \in E\colon g_i(X) \geqslant 0 \text{ for } i = 1, \dots, k\}. \tag{17}$$

For simplicity, we further assume $(\operatorname{grad} f)(X_0) \neq 0$ and $g_i(X_0) = 0$, as well as $(\operatorname{grad} g_i)(X_0) \neq 0$, for $i = 1, \dots, k$. Then, in a sufficiently small neighborhood of X_0, the function f as well as the polynomials g_i can be approximated arbitrarily close by corresponding affine functions. For example, f is approximated by the *beginning of its Taylor series*

$$f(X_0) + \langle (\operatorname{grad} f)(X_0), X - X_0\rangle.$$

From this one easily derives the following well-known criterion (see for example [2, Theorem 4.2.2]) for an isolated local minimum of f at X_0, depending on the normal cone

$$\mathcal{V}(X_0) = \operatorname{cone}\{(\operatorname{grad} g_i)(X_0)\colon\ i = 1, \ldots, k\}.$$

The function f attains an isolated local minimum on G if

$$(\operatorname{grad} f)(X_0) \in \operatorname{int} \mathcal{V}(X_0), \tag{18}$$

and f does not attain a local minimum if

$$(\operatorname{grad} f)(X_0) \notin \mathcal{V}(X_0). \tag{19}$$

The behavior in the case $(\operatorname{grad} f)(X_0) \in \operatorname{bd} \operatorname{cone} \mathcal{V}(X_0)$ depends on the involved functions f and g_i and has to be treated depending on the specific problem.

For the lattice sphere packing problem we have $E = \mathcal{S}^d$ and $f = \det^{1/d}$. For $Q_0 \in \mathcal{S}^d_{>0}$ we set $g_i(Q) = Q[\boldsymbol{v}_i] - \lambda(Q_0)$ with $(\operatorname{grad} g_i)(Q) = \boldsymbol{v}_i \boldsymbol{v}_i^t$ for each pair $\pm\boldsymbol{v}_i$ in $\operatorname{Min} Q_0$. By Theorem 4 we have a local minimum of $f(Q) = (\det Q)^{1/d}$ at Q_0 on G (as in (17)) if and only if Q_0 is perfect and eutactic, respectively if $\mathcal{V}(Q_0)$ is full-dimensional and $(\operatorname{grad} f)(Q_0) \in \operatorname{int} \mathcal{V}(Q_0)$. Here, $(\operatorname{grad} f)(Q_0)$ is a positive multiple of Q_0^{-1}. Thus in this special case (due to Proposition 1) we do not have a local minimum of f where $(\operatorname{grad} f)(Q_0) \in \operatorname{bd} \operatorname{cone} \mathcal{V}(Q_0)$.

Let us consider the case of m-periodic sets, hence of $E = \mathcal{S}^{d,m}$ with $m > 1$. We want to know if a periodic form $X_0 \in \mathcal{S}^{d,m}_{>0}$ attains a local minimum of $f = \det^{1/d}$. We may assume $\lambda(X_0) > 0$. The set $\operatorname{Min} X_0$ is finite and moreover, for $X = (Q, \boldsymbol{t})$ in a small neighborhood of $X_0 = (Q_0, \boldsymbol{t}^0)$, every $\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v} \in \operatorname{Min} X$ corresponds to a $\boldsymbol{t}_i^0 - \boldsymbol{t}_j^0 - \boldsymbol{v} \in \operatorname{Min} X_0$. Thus locally at X_0, the generalized Ryshkov set $\mathcal{R}_m$ is given by the basic closed semialgebraic set G defined by the inequalities $p_{i,j,\boldsymbol{v}}(X) - \lambda(X_0) \geqslant 0$, one for each pair $\pm(\boldsymbol{t}_i^0 - \boldsymbol{t}_j^0 - \boldsymbol{v})$ in $\operatorname{Min} X_0$. As explained in Section 4, we may assume $1 \leqslant i \leqslant j \leqslant m$ and $\boldsymbol{t}_j^0 = \boldsymbol{0}$ if $j = m$. An elementary calculation yields

$$(\operatorname{grad} p_{i,j,\boldsymbol{v}})(X) = \big(\boldsymbol{w}\boldsymbol{w}^t, \boldsymbol{0}, \ldots, \boldsymbol{0}, 2Q\boldsymbol{w}, \boldsymbol{0}, \ldots, \boldsymbol{0}, -2Q\boldsymbol{w}, \boldsymbol{0}, \ldots, \boldsymbol{0}\big), \tag{20}$$

where we set $X = (Q, \boldsymbol{t})$ and use $\boldsymbol{w}$ to abbreviate $\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v}$. This is to be understood as a vector in $\mathcal{S}^{d,m} = \mathcal{S}^d \times \mathbb{R}^{d\times(m-1)}$, with its "$\mathcal{S}^d$-component" being the rank-1 form $\boldsymbol{w}\boldsymbol{w}^t$ and its "translational-component" containing the zero-vector $\boldsymbol{0}$ in all but the ith and jth column. If $j = m$, the jth column is omitted and if $i = j$ the corresponding column is $\boldsymbol{0}$. For $(\operatorname{grad} f)(X)$ we obtain a positive multiple of $(Q^{-1}, \boldsymbol{0})$.

A sufficient condition for local m-periodic sphere packing optima. Generalizing the notion of perfection, we say a periodic form $X = (Q, \boldsymbol{t}) \in \mathcal{S}^{d,m}_{>0}$ (and a corresponding periodic set represented by X) is *m-perfect* if the *generalized Voronoi domain*

$$\mathcal{V}(X) = \operatorname{cone}\{(\operatorname{grad} p_{i,j,\boldsymbol{v}})(X)\colon\ \boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v} \in \operatorname{Min} X \text{ for some } \boldsymbol{v} \in \mathbb{Z}^d\} \tag{21}$$

is full-dimensional, that is, if $\dim \mathcal{V}(X) = \dim \mathcal{S}^{d,m} = \binom{d+1}{2} + (m-1)d$. Generalizing the notion of eutaxy, we say that X (and a corresponding periodic set) is *m-eutactic* if

$$\left(Q^{-1}, \mathbf{0}\right) \in \operatorname{relint} \mathcal{V}(X).$$

So the general discussion at the beginning of this section yields the following sufficient condition for a periodic form X to be *isolated m-extreme*, that is, for X having the property that any sufficiently small change which preserves $\lambda(X)$, necessarily lowers $\delta(X)$.

Theorem 5. *If a periodic form $X \in \mathcal{S}^{d,m}_{>0}$ is m-perfect and m-eutactic, then X is isolated m-extreme.*

Note that the theorem gives a computational tool to certify isolated m-extremeness of a given periodic form $X = (Q, \boldsymbol{t}) \in \mathcal{S}^{d,m}_{>0}$: First, we compute $\operatorname{Min} X$ and use Eq. (20) to obtain generators of the generalized Voronoi domain $\mathcal{V}(X)$. From the generators it can be easily checked if the domain is full-dimensional, hence if X is m-perfect. Next, we can computationally test whether $(Q^{-1}, \mathbf{0})$ is in $\mathcal{V}(X)$ or not; for example by solving a linear program similar to (7).

If we find $(Q^{-1}, \mathbf{0}) \in \operatorname{relint} \mathcal{V}(X)$ (or equivalently in $\operatorname{int} \mathcal{V}(X)$ as $\mathcal{V}(X)$ is assumed to be full-dimensional), the periodic form X represents an isolated m-extreme periodic set. If $(Q^{-1}, \mathbf{0}) \notin \mathcal{V}(X)$, the periodic form X does not represent an m-extreme periodic set. In this situation, we can even find a "direction" $N \in \mathcal{S}^{d,m}$, for which we can improve the sphere packing density of the periodic form X, that is, such that $\delta(X + \epsilon N) > \delta(X)$ for all sufficiently small $\epsilon > 0$.

Remark 6. Let $X \in \mathcal{S}^{d,m}_{>0}$ with $(Q^{-1}, \mathbf{0}) \notin \mathcal{V}(X)$. Then we can improve the sphere packing density of X in direction N given by the nearest point to $-(Q^{-1}, \mathbf{0})$ in the polyhedral cone

$$\mathcal{P}(X) = \left\{N \in \mathcal{S}^{d,m} \colon \langle V, N \rangle \geqslant 0 \text{ for all } V \in \mathcal{V}(X)\right\}. \tag{22}$$

Note that the cone $\mathcal{P}(X)$ is dual to the generalized Voronoi domain $\mathcal{V}(X)$ and (added to X) gives locally a linear approximation of the generalized Ryshkov set $\mathcal{R}_m$.

Fluid diamond packings. For general m we are confronted with a difficulty which does not show up in the lattice case $m = 1$: There may be non-isolated m-extreme sets, which are not m-perfect. The *fluid diamond packings* in dimension 9, described by Conway and Sloane in [8], give such an example.

Example. The *root lattice* D_d can be defined by

$$\mathsf{D}_d = \left\{\boldsymbol{x} \in \mathbb{Z}^d \colon \sum_{i=1}^{d} x_i \equiv 0 \bmod 2\right\}.$$

The *fluid diamond packings* are 2-periodic sets

$$\mathsf{D}_9\langle \boldsymbol{t}\rangle = \mathsf{D}_9 \cup (\mathsf{D}_9 + \boldsymbol{t})$$

with $\boldsymbol{t} \in \mathbb{R}^9$ such that the minimal distance among elements is equal to the minimum distance $\sqrt{2}$ of D_9 itself. We may choose for example $\boldsymbol{t} = \boldsymbol{t}_\alpha = (\frac{1}{2}, \ldots, \frac{1}{2}, \alpha)^t$ with any $\alpha \in \mathbb{R}$. For integers α we obtain the densest known packing lattice $\Lambda_9 = \mathsf{D}_9\langle \boldsymbol{t}_\alpha \rangle$ in dimension 9, showing that it is part of a family of uncountably many equally dense 2-periodic sets.

The sets $\mathsf{D}_9\langle \boldsymbol{t}_\alpha \rangle$ give examples of non-isolated 2-extreme sets, which are 2-eutactic, but not 2-perfect. In order to see this, let us consider a representation $X_\alpha \in \mathcal{S}^{9,2}_{>0}$ for $\mathsf{D}_9\langle \boldsymbol{t}_\alpha \rangle$. We choose a basis A of D_9. Then $X_\alpha = (Q, A^{-1}\boldsymbol{t}_\alpha)$, with $Q = A^t A$, is a representation of $\mathsf{D}_9\langle \boldsymbol{t}_\alpha \rangle$.

For non-integral α we find $\operatorname{Min} X_\alpha = \operatorname{Min} Q$ (using MAGMA for example). It follows (for example by Lemma 9 below) that X_α is 2-eutactic, but not 2-perfect. For integral α we find

$$\operatorname{Min} X_\alpha = \operatorname{Min} Q \cup \left\{ (x_1, \ldots, x_8, 0)^t \in \{0,1\}^9 \colon \sum_{i=1}^{8} x_i \equiv 0 \bmod 2 \right\}.$$

Thus the vectors in $\operatorname{Min} X_\alpha \setminus \operatorname{Min} Q$ span only an 8-dimensional space. Therefore X_α is not 2-perfect. Nevertheless, a corresponding calculation shows that X_α is 2-eutactic, as in the case of non-integral α.

In order to see that X_α is non-isolated 2-extreme, we can apply Proposition 7 below. One easily checks that for integral α (hence for the lattice Λ_9) we have only one degree of freedom for a local change of $\boldsymbol{t}_\alpha$ giving an equally dense sphere packing. For non-integral α we have nine degrees of freedom for such a modification.

Non-isolated m-extreme sets as in this example can occur for periodic forms $X \in \mathcal{S}^{d,m}_{>0}$, only if $(Q^{-1}, \mathbf{0}) \in \operatorname{bd} \mathcal{V}(X)$ (which is for example always the case if X is m-eutactic, but not m-perfect). In this case it is in general not clear what an infinitesimal change of X in a direction $N \in \mathcal{S}^{d,m}$ leads to (already assuming it is orthogonal to $(Q^{-1}, \mathbf{0})$ as well as in the boundary of the set $\mathcal{P}(X)$ in (22)). If $\mathcal{F}(X)$ denotes the unique face of $\mathcal{V}(X)$ containing $(Q^{-1}, \mathbf{0})$ in its relative interior, then this "set of uncertainty" is equal to the face of $\mathcal{P}(X)$ dual to $\mathcal{F}(X)$, that is, equal to

$$\mathcal{U}(X) = \bigl\{ N \in \mathcal{P}(X) \colon \langle V, N \rangle = 0 \text{ for all } V \in \mathcal{F}(X) \bigr\}. \tag{23}$$

Or in other words, the set $\mathcal{U}(X)$ is the intersection of $\mathcal{P}(X)$ with the hyperplane orthogonal to $(Q^{-1}, \mathbf{0})$. Note that it is possible to determine $\mathcal{F}(X)$ (and hence a description of $\mathcal{U}(X)$ by linear inequalities) computationally, using linear programming techniques.

Purely translational changes. Below we give an additional sufficient condition for m-extremeness. For this we consider the case when all directions in $\mathcal{U}(X)$ are "*purely translational changes*" $N = (0, \boldsymbol{t}^N) \in \mathcal{S}^{d,m}$. A vivid interpretation of a purely translational change can be given by thinking of the corresponding modification of a periodic sphere packing. The spheres of each lattice translate are jointly moved. If in such a local change all contacts among spheres are lost, we can increase their radius and obtain a new sphere packing with larger density. If some contacts among spheres are preserved however, the sphere packing density remains the same. The latter case is captured in the following proposition, which gives an easily testable criterion for m-extremeness. We apply this proposition in Section 6, where we consider potential local improvements of best known packing lattices to periodic non-lattice sets.

Proposition 7. *For a periodic form $X = (Q, \boldsymbol{t}) \in \mathcal{S}^{d,m}_{>0}$ with $(Q^{-1}, \boldsymbol{0}) \in \operatorname{bd} \mathcal{V}(X)$, let $\mathcal{U}(X)$ be contained in*

$$\left\{(\boldsymbol{0}, \boldsymbol{t}^N) \in \mathcal{S}^{d,m}\colon\ \boldsymbol{t}_i^N = \boldsymbol{t}_j^N \text{ for at least one } \boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v} \in \operatorname{Min} X \text{ with } \boldsymbol{v} \in \mathbb{Z}^d\right\}.$$

Then X is (possibly non-isolated) m-extreme.

Note, if X is m-eutactic (possibly not m-perfect), the set $\mathcal{U}(X)$ is the *orthogonal complement* $\mathcal{V}(X)^{\perp}$ of the linear hull of $\mathcal{V}(X)$. Note also that Proposition 7 includes in particular the special case where some $\boldsymbol{v} \in \mathbb{Z}^d$ are in $\operatorname{Min} X$ (and therefore $\boldsymbol{t}_i = \boldsymbol{t}_j = \boldsymbol{0}$ for $i = j = m$). This situation occurs for the 2-periodic, fluid diamond packings in the example above.

From the sphere packing interpretation of the proposition its assertion is clear. Nevertheless, we give a proof below, based on a local analysis in $\mathcal{S}^{d,m}_{>0}$. More than actually needed for the proof, we analyze how δ changes locally at a periodic form $X \in \mathcal{S}^{d,m}_{>0}$ in a direction $N \in \mathcal{U}(X)$. As a byproduct, we obtain tools allowing a computational analysis of possible local optimality for a given periodic form (not necessarily covered by the proposition). These can for example be used in a numerical search for good periodic sphere packings.

Proof of Proposition 7. The generalized Voronoi domain $\mathcal{V}(X)$ is spanned by gradients $(\operatorname{grad} p_{i,j,\boldsymbol{v}})(X)$ (as given in (20)), one for each pair of vectors $\pm\boldsymbol{w} \in \operatorname{Min} X$. The assumption that a direction $N = (Q^N, \boldsymbol{t}^N)$ is in $\mathcal{U}(X)$ for a periodic form $X = (Q, \boldsymbol{t})$, implies $\langle Q^{-1}, Q^N\rangle = 0$. Moreover, for the unique maximal face $\mathcal{F}(X)$ of $\mathcal{V}(X)$ with $(Q^{-1}, \boldsymbol{0}) \in \operatorname{relint} \mathcal{F}(X)$, the condition that N is orthogonal to some $(\operatorname{grad} p_{i,j,\boldsymbol{v}})(X)$ in $\mathcal{F}(X)$ translates into

$$\left\langle(\operatorname{grad} p_{i,j,\boldsymbol{v}})(X), N\right\rangle = Q^N[\boldsymbol{w}] + 2\left(\boldsymbol{t}_i^N - \boldsymbol{t}_j^N\right)^t Q\boldsymbol{w} = 0, \tag{24}$$

with $\boldsymbol{w} = (\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v})$. Recall that in the special case $i = j$ (and for $m = 1$ anyway) $p_{i,j,\boldsymbol{v}}$ is linear and (24) reduces to the condition $Q^N[\boldsymbol{w}] = 0$; if then N satisfies this linear condition, $p_{i,j,\boldsymbol{v}}(X + \epsilon N)$ is a constant function in ϵ.

When $p_{i,j,\boldsymbol{v}}(X + \epsilon N)$ is a cubic polynomial in ϵ we need to use higher order information in order to judge its behavior. An elementary calculation yields for the *Hessian*

$$(\operatorname{hess} p_{i,j,\boldsymbol{v}})(X)[N] = 2Q\left[\boldsymbol{t}_i^N - \boldsymbol{t}_j^N\right] + 4\left(\boldsymbol{t}_i^N - \boldsymbol{t}_j^N\right)^t Q^N\boldsymbol{w}. \tag{25}$$

Now how does δ change at X in direction N, assuming it is in the set of uncertainty $\mathcal{U}(X)$? Among the polynomials $p_{i,j,\boldsymbol{v}}$ with N satisfying (24), the fastest decreasing polynomial in direction N determines $\lambda(X + \epsilon N)$ for small enough ϵ. Thus for the local change of δ in direction N, we may restrict our attention to a polynomial $p_{i,j,\boldsymbol{v}}$ with the smallest value (25) of its Hessian.

By Proposition 1 we know that $\det^{1/d}$ decreases strictly at X in a direction $N \in \mathcal{U}(X)$ if and only if $Q^N \neq 0$.

For a purely translational change with $Q^N = 0$, the function $\det^{1/d}$ remains constant. On the other hand, because of (25) and since Q is positive definite, we have $(\operatorname{hess} p_{i,j,\boldsymbol{v}})(X)[N] \geqslant 0$, with equality if and only if $\boldsymbol{t}_i^N - \boldsymbol{t}_j^N = \boldsymbol{0}$. The latter implies that $p_{i,j,\boldsymbol{v}}(X + \epsilon N)$ is a constant function of ϵ. Thus for purely translational changes $N = (0, \boldsymbol{t}^N) \in \mathcal{U}(X)$, the density function $\delta(X + \epsilon N)$ is constant for small enough $\epsilon \geqslant 0$, if $\boldsymbol{t}_i^N = \boldsymbol{t}_j^N$ for some pair (i, j) with $\boldsymbol{t}_i - \boldsymbol{t}_j - \boldsymbol{v} \in \operatorname{Min} X$ (for a suitable $\boldsymbol{v} \in \mathbb{Z}^d$). This proves the proposition. $\square$

Note that our argumentation in the proof also shows that $\delta(X+\epsilon N)$ increases for small $\epsilon>0$, for a purely translational change $N=(0,\boldsymbol{t}^N)\in\mathcal{U}(X)$ with $\boldsymbol{t}_i^N\neq\boldsymbol{t}_j^N$ for all pairs (i,j) with $\boldsymbol{t}_i-\boldsymbol{t}_j-\boldsymbol{v}\in\operatorname{Min}X$ (for some $\boldsymbol{v}\in\mathbb{Z}^d$). This case corresponds to a modification of a periodic sphere packing in which all contacts among spheres are lost.

6. Periodic extreme sets

A given periodic set has many representations by periodic forms, in spaces $\mathcal{S}^{d,m}_{>0}$ with varying m. For example, by choosing some sublattice of $\mathbb{Z}^d$, we can add additional translational parts.

It could happen that a periodic set Λ with a given representation $X\in\mathcal{S}^{d,m}_{>0}$ is m-extreme, whereas a second representation $X'\in\mathcal{S}^{d,m'}$ is not m'-extreme. We are not aware of an example though. However, in some cases we are certain that the packing density of no representation of Λ can locally be improved.

Definition 8. A periodic set is *periodic extreme* if it is m-extreme for all possible representations $X\in\mathcal{S}^{d,m}_{>0}$.

Theorem 10 below gives a sufficient condition for a lattice to be periodic extreme. For its statement we need the notion of *strong eutaxy* for lattices, respectively PQFs: A form $Q\in\mathcal{S}^d_{>0}$ (and a corresponding lattice) is called *strongly eutactic* if

$$Q^{-1}=\alpha\sum_{\boldsymbol{x}\in\operatorname{Min}Q}\boldsymbol{x}\boldsymbol{x}^t \tag{26}$$

for some $\alpha>0$, i.e., if the coefficients in the eutaxy condition (6) are all equal. It is well known that a PQF Q is strongly eutactic if and only if the vectors in $\operatorname{Min}Q$ form a so-called *spherical 2-design* with respect to Q (see [31], [21, Corollary 16.1.3]).

Lemma 9. *Any representation $X\in\mathcal{S}^{d,m}_{>0}$ of a strongly eutactic lattice (respectively PQF) is m-eutactic.*

Proof. Let $Q\in\mathcal{S}^d_{>0}$ be strongly eutactic, satisfying (26) for some $\alpha>0$. Let $X=(Q^X,\boldsymbol{t}^X)\in\mathcal{S}^{d,m}_{>0}$ be some representation of Q, e.g. with $m>1$. Let the corresponding eutactic lattice be denoted by Λ. Then Q^X is the Gram matrix of a basis $A\in\mathsf{GL}_d(\mathbb{R})$ of a sublattice L of Λ. The columns of $\boldsymbol{t}^X$ are the coordinates of lattice points of Λ relative to A.

For a fixed $\boldsymbol{w}\in\operatorname{Min}X$ we define an abstract graph, whose vertices are the indices in $\{1,\dots,m\}$. Two vertices i and j are connected by an edge whenever there is some $\boldsymbol{v}\in\mathbb{Z}^d$ such that $\boldsymbol{w}=\boldsymbol{t}_i^X-\boldsymbol{t}_j^X-\boldsymbol{v}$. In other words, the graph reflects via an edge (i,j) that spheres of packing radius $\lambda(\Lambda)$ around points of the two sublattice translates $A(\boldsymbol{t}_i^X+Z^d)$ and $A(\boldsymbol{t}_j^X+Z^d)$ touch. For $\boldsymbol{z}\in Z^d$, the sphere with center $A(\boldsymbol{t}_j^X+\boldsymbol{z})$ touches the sphere with center $A(\boldsymbol{t}_j^X+\boldsymbol{z}+\boldsymbol{w})$. Since the periodic form X represents a lattice Λ, we find a chain of touching spheres at centers $A(\boldsymbol{t}_j^X+\boldsymbol{z}+k\boldsymbol{w})$, with $k=0,1,\dots$. Modulo some natural number less or equal to m these centers belong to the same lattice translate of L. As a consequence, we find that the graph defined above is a disjoint union of cycles. So $\boldsymbol{w}$ induces a partition $(I_1,\dots,I_k)$ of $\{1,\dots,m\}$.

Let I be an index set of this partition (containing the indices of a fixed cycle of the defined graph). Summing over all triples $(i, j, \boldsymbol{v})$ with $i, j \in I$ and $\boldsymbol{v} \in \mathbb{Z}^d$ such that $\boldsymbol{w} = \boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{v} \in \operatorname{Min} X$, we find (using (20)):

$$\sum_{\substack{(i,j,\boldsymbol{v}) \in I^2 \times \mathbb{Z}^d \\ \text{with } \boldsymbol{v} = \boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{w}}} (\operatorname{grad} p_{i,j,\boldsymbol{v}})(X) = 2|I| \big(\boldsymbol{w}\boldsymbol{w}^t, \boldsymbol{0}\big).$$

The factor 2 comes from the symmetry $\operatorname{grad} p_{i,j,\boldsymbol{v}} = \operatorname{grad} p_{j,i,-\boldsymbol{v}}$. Summation over all index sets I of the partition yields

$$\sum_{\substack{(i,j,\boldsymbol{v}) \in \{1,\dots,m\}^2 \times \mathbb{Z}^d \\ \text{with } \boldsymbol{v} = \boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{w}}} (\operatorname{grad} p_{i,j,\boldsymbol{v}})(X) = 2m \big(\boldsymbol{w}\boldsymbol{w}^t, \boldsymbol{0}\big). \tag{27}$$

As a consequence we find by the strong eutaxy condition (26) that

$$\big(Q^{-1}, \boldsymbol{0}\big) = (\alpha/2m) \sum_{\substack{\boldsymbol{w} \in \operatorname{Min} X, (i,j,\boldsymbol{v}) \in \{1,\dots,m\}^2 \times \mathbb{Z}^d \\ \text{with } \boldsymbol{v} = \boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{w}}} (\operatorname{grad} p_{i,j,\boldsymbol{v}})(X),$$

with a suitable $\alpha > 0$. Thus X is m-eutactic. $\square$

Not all PQFs (or lattices) which are strongly eutactic have to be perfect. For example the lattices $\mathbb{Z}^n$ for $n \geqslant 2$ are of this kind. But if a strongly eutactic PQF is in addition also perfect, then the following theorem shows that this is sufficient for it to be periodic extreme. Note that this applies in particular to so called *strongly perfect* lattices and PQFs. For these lattices the vectors in $\operatorname{Min} Q$ form a spherical 4-design with respect to Q (see [23] or [21, Chapter 16] for further details).

Theorem 10. *Perfect, strongly eutactic lattices* (*respectively PQFs*) *are periodic extreme.*

Proof. Let $Q \in \mathcal{S}^d_{>0}$ be perfect and strongly eutactic. Hence the vectors in $\operatorname{Min} Q$ span $\mathbb{R}^d$ (by Proposition 2) and satisfy (26) for some $\alpha > 0$. Let $X = (Q^X, \boldsymbol{t}^X) \in \mathcal{S}^{d,m}_{>0}$ be a representation of Q. By Lemma 9, X is m-eutactic. If X is m-perfect as well, we know by Theorem 5 that X is also m-extreme.

So let us assume that X is not m-perfect; hence the generalized Voronoi domain $\mathcal{V}(X)$ is not full-dimensional. We want to apply Proposition 7. For this we choose

$$N = \big(Q^N, \boldsymbol{t}^N\big) \in \mathcal{U}(X) = \mathcal{V}(X)^{\perp} \quad \text{with} \quad N \neq 0.$$

(Recall the definition of $\mathcal{U}(X)$ from (23) and that $\mathcal{U}(X) = \mathcal{V}(X)^{\perp}$ if X is m-eutactic.) By this assumption we have in particular

$$\big\langle N, (\operatorname{grad} p_{i,j,\boldsymbol{v}})(X)\big\rangle = 0$$

for all triples $(i, j, \boldsymbol{v})$ with $\boldsymbol{w} = \boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{v} \in \operatorname{Min} X$. Using Eq. (27), which we obtained in the proof of Lemma 9, we get $\langle N, (\boldsymbol{w}\boldsymbol{w}^t, \boldsymbol{0})\rangle = Q^N[\boldsymbol{w}] = 0$ for every fixed $\boldsymbol{w} \in \operatorname{Min} X$.

By Proposition 2 there exist d linearly independent $\boldsymbol{w}$ in $\operatorname{Min} X$, which implies $Q^N = 0$. Using (24), we obtain

$$0 = \langle N, (\operatorname{grad} p_{i,j,\boldsymbol{v}})(X)\rangle = 2\big(\boldsymbol{t}_i^N - \boldsymbol{t}_j^N\big)^t Q\boldsymbol{w}. \tag{28}$$

If $\boldsymbol{t}_i^N - \boldsymbol{t}_j^N = \boldsymbol{0}$ for some pair (i, j) we can apply Proposition 7. Note that this includes in particular the case $i = j = m$ ($\boldsymbol{t}_i^N = \boldsymbol{t}_j^N = \boldsymbol{0}$) if $\boldsymbol{v} \in \mathbb{Z}^d \cap \operatorname{Min} X$. So we may assume that such $\boldsymbol{v}$ do not exist.

We choose d linearly independent vectors $\boldsymbol{w}_1, \dots, \boldsymbol{w}_d \in \operatorname{Min} X$ (that exist by Proposition 2). By the assumption that non of the $\boldsymbol{w}_i$ is integral and by the assumption that X represents a lattice, each $\boldsymbol{w}_i$ connects the origin $\boldsymbol{t}_m^X = \boldsymbol{0}$ to another translation vector $\boldsymbol{t}_j^X$ (with $j \neq m$) via $\boldsymbol{w}_i = \boldsymbol{t}_j^X - \boldsymbol{v}$ for some $\boldsymbol{v} \in \mathbb{Z}^d$. In the same way each of the chosen minimal vectors connects the translation vector with index i to other translation vectors. We denote by I the subset of $\{1, \dots, m\}$ that is connected to the index m (respectively to the origin $\boldsymbol{0}$) via a sequence of such links through the chosen d minimal vectors. For each index $i \in I$ we get from the minimal vectors d independent linear conditions (28) for the differences $\boldsymbol{t}_i^N - \boldsymbol{t}_j^N$, with suitable $j \in I \setminus \{i\}$. Overall we obtain $d|I|$ independent equations for $d|I|$ differences. We deduce that all of them vanish. Moreover, as $\boldsymbol{t}_m^N = \boldsymbol{0}$ we even find $\boldsymbol{t}_i^N = \boldsymbol{0}$ for all indices $i \in I$. $\square$

The root lattices A_d, D_d and E_d, as well as the Leech lattice are known to be perfect and strongly eutactic (cf. [21]). These lattices are known to solve the lattice sphere packing problem in dimensions $d \leqslant 8$ and $d = 24$ (see Table 1). As an immediate consequence of Theorem 10, we find that they cannot locally be improved to a periodic non-lattice set with greater sphere packing density.

Corollary 11. *The lattices A_d, for $d \geqslant 2$, D_d, for $d \geqslant 3$, and E_d, for $d = 6, 7, 8$, as well as the Leech lattice are periodic extreme.*

We also checked whether or not Theorem 10 can be applied to other dimensions $d \leqslant 24$. For these dimensions the so-called *laminated lattices* Λ_d and *sections K_d of the Leech lattice* give the densest known lattice sphere packings. The lattices K_d are different from Λ_d (and at the same time give the densest known lattice sphere packings) only in dimensions $d = 11, 12, 13$. For these d, the lattice K_d is strongly eutactic only for $d = 12$, when K_d is also known as *Coxeter–Todd lattice*. The laminated lattices Λ_d give the densest known packing lattices in dimensions $d = 9, 10$ and $d = 14, \dots, 24$ (for $d = 18, \dots, 24$ they coincide with K_d). Among those values for d, the laminated lattices Λ_d are strongly eutactic if and only if $d = 15, 16$ or $d \geqslant 20$. Concluding, we cannot exclude that densest known lattice sphere packings in dimensions $d \in \{9, 10, 11, 13, 14, 17, 18, 19\}$ can locally be improved to better periodic sphere packings. Further analysis is required here.

7. Floating and strict periodic extreme lattices

The last step of the proof of Theorem 10 has a vivid interpretation if we think of a sphere packing described by the given lattice. Let $X = (Q^X, \boldsymbol{t}^X)$ be one of its representations and let A

denote a sublattice basis with Gram matrix Q^X. Then the sublattice translates $A(\boldsymbol{t}_i^X + Z^d)$ with $i \in I$ form a "rigid component" of the sphere packing. If we do not want to decrease the sphere packing density in a local deformation we have to move all of its translates simultaneously. This rigid component may actually be larger than the one used in the proof of Theorem 10. It may even consist of the whole packing. A maximal rigid component of translates can be described via an abstract graph with vertices in $\{1, \ldots, m\}$: (i, j) is an edge whenever there is some $\boldsymbol{v} \in \mathbb{Z}^d$ such that $\boldsymbol{t}_i^X - \boldsymbol{t}_j^X - \boldsymbol{v} \in \operatorname{Min} X$. Let I be the set of indices i (vertices of the graph) connected by a path with m. If $|I| = m$ the whole packing forms one rigid component. If I is a strict subset of $\{1, \ldots, m\}$ we say a corresponding packing or lattice is *floating*.

In a floating packing each connected component of the graph above corresponds to a union of translates which can jointly locally be moved without changing $\lambda(X)$ and $\delta(X)$ respectively. Examples are the fluid diamond packings described in the example of Section 5. The same applies to their higher-dimensional generalizations $\mathsf{D}_d^+ = \mathsf{D}_d \cup (\mathsf{D}_d + (\frac{1}{2}, \ldots, \frac{1}{2}))$ for $d \geqslant 10$ (see [10, Section 4.7.3]). For even d these 2-periodic sets are actually lattices (hence 1-periodic). In fact $\mathsf{E}_8 = D_8^+$.

We note that Theorem 10 and Corollary 11 give statements about local optimality of lattices, but not about strict local optimality. With the assumptions of Theorem 10 alone strict local optimality cannot be ensured, as shown by floating lattices like D_d^+ for even $d \geqslant 10$. These lattices have the same minimal vectors as the corresponding root lattice D_d and therefore they give a series of perfect and strongly eutactic lattices that are periodic extreme by Theorem 10. However, they can locally be modified to other 2-periodic sets of the same density.

We think that a strengthening of Corollary 11 is possible for certain lattices that are non-floating, perfect and strongly eutactic. These include in particular the E_8 root lattice and the Leech lattice. We think it is possible to show that these lattices are *strict periodic extreme*, meaning they are isolated m-extreme for all possible representations $X \in \mathcal{S}_{>0}^{d,m}$. By Lemma 9 and Theorem 5 one has to show that a given non-floating, perfect and strongly eutactic lattice is m-perfect for every m. Here some further work is required. . . .

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