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REMARKS ON SPHERE PACKINGS, CLUSTERS AND HALES FERGUSON THEOREM

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1. Introduction

In a short note to one of his friends in 1610 about the structure and the shape of snowflakes crystals (see the remarkable articles of Hales [H] and Oesterlé [O] for historical details), *Strena seu de nive sexangula*, Johannes Kepler claims the following result known as Kepler's conjecture, which is considered today as Hales Ferguson's theorem, since 1998.

THEOREM 1.1 (Hales - Ferguson). — *No packing of identical spheres in three dimensions has density greater than the face-centred cubic packing, namely* $\frac{\pi}{\sqrt{18}} = 0.74048\ldots$.

The Kepler conjecture was an old unsolved problem in discrete geometry.

The face-centred cubic packing is known as the canonballs packing or the pyramid stacking of oranges and is the densest lattice packing of spheres, of density $\pi/\sqrt{18}$. The fundamental question asked by the conjecture was to understand how the density could or not exceed the so-called Kepler bound $\pi/\sqrt{18}$ in the case of aperiodic packings of spheres with respect to lattice sphere packings of $\mathbb{R}^n$. Hales, in a multistep programm abundantly described on the web [H3] [H4], whose one step was Ferguson's thesis [F], announced the proof of the conjecture in 1998 after more than seven years of investigations. In the meantime an incomplete proof by Hsiang [Hs] was published in 1993 and was a source of controversy [H2] [O].

The seminar given by the author was intended to sketch the main ingredients of the proof of Hales as presented in [H].

In this present short note, we will just recall a few questions which seem important about densities of aperiodic and lattice sphere packings in $\mathbb{R}^n$. Comparison will be made with the ingredients developed by Rogers, Hales, Ferguson, Hsiang and others.

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The general context in which we will proceed is that of the set of uniformly discrete sets, suitably topologized, leaving aside spaces of lattices. We will recall the Minkowski-Hermite approach for lattice sphere packings (in section 4) which is generalized by the theory of systoles [B] and generalized systoles [A]. The integer n will be assumed to be greater than 2 in the sequel.

2. Uniformly discrete sets, Delone sets and densities

First, in order to make more accurate the statements and fix the notations, we will recall some definitions about densities and systems of spheres of $\mathbb{R}^n$, $n \geqslant 1$.

Let $t > 0$ be a real number. By definition, we will say that a discrete set Λ of $\mathbb{R}^n$ is an uniformly discrete set of constant $t > 0$ if $\|x - y\| \geqslant t$ as soon as $x \neq y$ with $x,y \in \Lambda$. Examples of uniformly discrete sets of constant t are the empty set $\varnothing$, point sets reduced to one point $\{x\}$, with $x \in \mathbb{R}^n$; let us cite also any $\mathbb{Z}$-module $\mathbb{Z}^k, 1 \leqslant k \leqslant n$, built on the canonical basis of $\mathbb{R}^n$, in particular $\mathbb{Z}^n$, as uniformly discrete set of constant 1. We will say that a discrete point set of $\mathbb{R}^n$ is a uniformly discrete set if there exists $t > 0$ such that it is a uniformly discrete set of constant t. By definition a finite uniformly discrete set of $\mathbb{R}^n$ will be called a cluster.

Take $r > 0$ and assume $\mathscr{A} := (a_i)_{i \in I}$ is a finite or infinite discrete collection of points of $\mathbb{R}^n$ which is a uniformly discrete set of $\mathbb{R}^n$ of constant $2r$. The set $\mathscr{A}$ may be empty. Denote by $B = B(0,r)$ the n-dimensional closed ball of $\mathbb{R}^n$ of volume $v_n(r) = \pi^{n/2} r^n / \Gamma(\frac{n+2}{2})$, centred at the origin and of radius r. By definition, a system of (identical) spheres over $\mathscr{A}$ of radius r is a packing of translates of B where the translation vectors belong to $\mathscr{A}$. We will denote it by

$$\mathscr{B}(\mathscr{A}) := \{a_i + B \mid i \in I\}$$

We will speak of a system of spheres of radius r without mentioning the dependency to $\mathscr{A}$ and will mention it when necessary in the sequel. Two different balls (so-called *spheres* in literature by tradition) in the packing $\mathscr{B}(\mathscr{A})$ may have at most one point in common on the boundary or are of empty intersection.

There is an obvious one-to-one correspondence between system of spheres of radius r and uniformly discrete sets of constant $2r$ of $\mathbb{R}^n$. Indeed, to obtain a packing of spheres from any arbitrary uniformly discrete set $\mathscr{A}$ of constant r, we chose the real number $t > 0$ as large as possible such that the balls $\{a_i + B(0,t) \mid i \in I\}$ have pairwise disjoint interiors, that is for $t = r$. Conversely, any system of spheres clearly defines a uniformly discrete set which is constituted by the collection of the centres of spheres and its constant is twice the common radius of the spheres.

In chapter 1 of Rogers [R], it is shown that a density can be attributed to the system of spheres $\mathscr{B}(\mathscr{A})$. Let x_0 be an arbitrary element of $\mathbb{R}^n$. Let us call $\delta(\mathscr{B}(\mathscr{A})) \in [0,1]$ its density, computed at x_0, defined by

$$\delta(\mathscr{B}(\mathscr{A})) = \limsup_{R \to +\infty} \left[\mathrm{vol}\left(\left(\bigcup_{i \in I} (a_i + B) \right) \bigcap B(x_0,R) \right) / \mathrm{vol}\,(B(x_0,R)) \right] \in [0,1] \quad (1)$$

The theorem 1.7 in Rogers [R] proves that this value is independent of the point x_0. Therefore we will speak of the density of the sphere packing $\mathscr{B}(\mathscr{A})$ without mentioning x_0 and will take, as it is usual, $x_0 = 0$ for simplicity's sake. It is clear that if $\mathscr{A}$ is the empty set then $\delta(\mathscr{B}(\varnothing)) = 0$; similarly, if $\mathscr{A}$ is a finite uniformly discrete set of arbitrary strictly positive constant, we have $\delta(\mathscr{B}(\mathscr{A})) = 0$. Even though $\mathscr{A}$ is an infinite uniformly discrete set of arbitrary strictly positive constant, the notion of density becomes interesting, i.e. non zero, when $\mathscr{A}$ has *enough* points say at infinity in a sense we will precise below. It is the case of lattices which were extensively studied (Conway and Sloane [CS], Martinet [M]) and remains a wonderful subject.

By the theorem 1.7 in Rogers [R], we know that any non-singular affine transformation of $\mathbb{R}^n$ leaves invariant the density of a sphere packing of $\mathbb{R}^n$. Therefore, we will restrict ourselves in the following to the study of densest systems of spheres of $\mathbb{R}^n$ which arise from uniformly discrete sets of $\mathbb{R}^n$ of constant 1 (say 1 for simplicity's sake). It amounts to make a dilation of $\mathbb{R}^n$ to have $r = 1/2$. We will denote by $\mathscr{UD}$ the set of uniformly discrete sets of constant 1 and by $\mathscr{UD}$-sets its elements. Take $R > 0$ a real number. We will denote by X_R the subset of $\mathscr{UD}$ constituted by the discrete sets Λ of $\mathbb{R}^n$ such that

$$\Lambda \text{ is a } \mathscr{UD}\text{-set}$$

and obeys the following condition of relative denseness:

$$\forall z \in \mathbb{R}^n \quad \exists \lambda \in \Lambda \text{ such that } \lambda \in B(z,R).$$

The elements of X_R are said to be Delone sets of constants $(1,R)$. In general, if a discrete set Λ belongs to $\mathscr{UD}$ and is such that there exists a real number $R > 0$ such that $\Lambda \in X_R$, then we will say that Λ is a Delone set (*ensemble de Delaunay* in french), without mentioning necessarily the constants $(1,R)$.

A Delone set of constants $(1,R)$ does not contain say any *deep hole* of diameter greater than $2R$ by definition. A feature common to all Delone sets of $\mathbb{R}^n$ is that the $\mathbb{R}$-span of an arbitrary Delone set is always $\mathbb{R}^n$ itself. Lattices which are uniformly discrete sets of $\mathbb{R}^n$ of constant 1 are Delone sets, for instance $\mathbb{Z}^n$. The empty set is not a Delone set. For all $R' \geqslant R > 0$, then $X_R \subset X_{R'}$. For all Delone set Λ of $\mathbb{R}^n$, let us denote by

$$R(\Lambda) := \inf\{R \mid \Lambda \in X_R\}$$

the *covering radius* of Λ, namely the smallest real number R such that $\Lambda \in X_R$; obviously $R(\Lambda) > 0$. We have

$$\Lambda \in X_{R(\Lambda)} \text{ with } \Lambda \notin X_{R'}$$

for all $R' > 0$ strictly less than $R(\Lambda)$. Let $R_{\min} := \inf_{\Lambda \text{ Delone}} R(\Lambda)$ the minimal covering radius over all Delone sets of $\mathbb{R}^n$. If R' is such that $0 < R' < R_{\min}$ then obviously $X_{R'} = \varnothing$.

The terminology about uniformly discrete sets and Delone sets did not appear in Rogers [R] but this author has studied sphere packings over Delone sets (see Chapter 7

in [R]) in the scope of defining nonzero local densities and bounded Voronoi polyhedra. This concept of Delone set of $\mathbb{R}^n$ was also implicitely used by Hales since one of his first operation on a given sphere packing, in the search for densest sphere packings, is *saturation* [H3]. Saturation means that each time a sphere packing has a sufficiently large hole, a sphere may be put inside; and so on, up till it becomes impossible to do it. Let us precise this notion.

PROPOSITION 2.1. — *Packings of identical spheres of maximal density in* $\mathbb{R}^n$ *arise from Delone sets of constants* $(2t,2t)$ *where* $t > 0$ *is the common radius of the spheres. In other terms*

$$\sup_{\mathscr{A}\in X_1} \delta(\mathscr{B}(\mathscr{A})) = \sup_{\mathscr{A}\in \mathscr{UD}} \delta(\mathscr{B}(\mathscr{A}))$$

Proof. — Assume $t = 1/2$ for simplicity's sake and that $\mathscr{A} \in \mathscr{UD}$ is an arbitrary $\mathscr{UD}$-set in $\mathbb{R}^n$. If there exists $z \in \mathbb{R}^n$ such that $\|z - \lambda\| \geqslant 1$ for all $\lambda \in \mathscr{A}$, then we put a ball B of radius $1/2$ at z. We repeat this adding process indefinitely up till there is no more points of $\mathbb{R}^n$ which satisfy this property. This adding process of balls creates a sequence of uniformly discrete sets from which we extract a subsequence which is converging in the d-topology (see theorem 2.2 below) and for which the limit is a Delone set. This adding process of balls favours an increase of the density of $\mathscr{A}$ along this subsequence to give rise to a Delone set of constant $(1,1)$ of higher density (not necessarily strictly) made of the whole collection of old and new sphere centres. This adding process does not necessarily stop after a finite number of steps. If a $\mathscr{UD}$-set cannot be added a ball by this adding process, then it is already necessarily a Delone set of constants $(1,1)$. Note that this adding process can eventually be used for some Delone sets $\mathscr{A}$ of constants $(1,1)$ to densify them: if there is a point $z \in \mathbb{R}^n$ such that the closest $\lambda \in \mathscr{A}$ is at distance 1 from z, we put a ball B at z. Therefore sphere packings of maximal density arise from Delone sets of constants $(1,1)$. Conversely, it is not known whether an arbitrary Delone set of constants $(1,1)$ gives rise to a sphere packing of density equal to

$$\sup_{\mathscr{A}\in X_1} \delta(\mathscr{B}(\mathscr{A}))$$

Possibly not since presumably the density function is not constant on X_1. □

Let us remark that if we remove a finite number of points from a $\mathscr{UD}$-set, its density will not change. The previous proposition means that all the information about densest sphere packings is contained in X_1.

Muraz and Verger-Gaugry [MVG] have shown that a certain uniform topology can be put on $\mathscr{UD}$. Moreover, they have constructed a distance d on $\mathscr{UD}$ for which $(\mathscr{UD},d)$ is a metric space and proved the following result.

THEOREM 2.2. — *The space* $(\mathscr{UD},d)$ *is a compact metric space. For all* $R \geqslant 1$, *the subset* $X_R \subset \mathscr{UD}$ *of Delone sets of constants* $(1,R)$ *is compact in the* d*-topology.*

Since the proof of the theorem in [MVG] can obviously be extended to any $R \geqslant R_{\min}$, we deduce that X_R is compact for all $R \geqslant R_{\min}$ and that the space $\bigcup_{R>0} X_R$ of all Delone sets of $\mathbb{R}^n$ is locally compact in the d-topology.

We now pull back the d-topology on $\mathcal{UD}$ to the set of systems of spheres of radius 1/2, denoted by SS, without mentioning 'n' the dimension of the ambiant space $\mathbb{R}^n$. We define, keeping the same notation 'd' for the distance,

$$d(\mathcal{B}(\mathcal{A}),\mathcal{B}(\mathcal{A}')) := d(\mathcal{A},\mathcal{A}') \quad \text{for all } \mathcal{A},\mathcal{A}' \in \mathcal{UD}$$

COROLLARY 2.3. — *The set of systems of spheres of radius 1/2 endowed with the d-topology, (SS, d), is a compact space.*

Let us recall the classical definition of the packing constant of $\mathbb{R}^n$:

$$\delta_n^+ := \sup_{\mathcal{A}\in\mathcal{UD}} \delta(\mathcal{B}(\mathcal{A}))$$

Obviously, we have:

$$\delta_n^+ = \sup_{\mathcal{A}\in X_1} \delta(\mathcal{B}(\mathcal{A})) = \sup_{\mathcal{A}\in X_R} \delta(\mathcal{B}(\mathcal{A}))$$

where $R \geqslant 1$ is an arbitrary real number. Let us define in a similar way

$$\delta_n^- := \inf_{\mathcal{A}\in X_1} \delta(\mathcal{B}(\mathcal{A}))$$

(Q0) For all integer $n \geqslant 1$, does there exist systems of spheres $\mathcal{B}$ of $\mathbb{R}^n$ of maximal density, i.e. such that their density reaches the packing constant

$$\delta(\mathcal{B}) = \delta_n^+ \ ?$$

Does there exists a topology on $\mathcal{UD}$ such that δ is continuous?

If the answer is yes, we will say that a system of spheres (or a sphere packing) is *extreme* if it corresponds to a local maximum of the density function δ. Some questions can now be formulated as far as we are concerned with densest sphere packings of $\mathbb{R}^n$.

(Q1) How many extreme systems of spheres does there exist (up to translation, rotation and symmetry) and how can they be characterized?

In particular

(Q2) Which are among them the densest ones, and for which value of δ_n^+?

If δ cannot be made continuous for any non trivial topology on $\mathcal{UD}$, we cannot speak of extreme lattices, but we will only consider those sphere packings of density close to δ_n^+, without knowing whether this value is reached by a system of spheres.

We have only a very partial answer to question (Q0) by the following proposition (2.5).

First, let us mention a useful lemma correlating the proximity of $\mathcal{UD}$-sets in the d-topology and their respective points in $\mathbb{R}^n$.

LEMMA 2.4. — *Let Λ,Λ' be two non-empty $\mathcal{UD}$-sets. Let $l = dist(0,\Lambda) < +\infty$ denote the distance from the origin to Λ in the Euclidean norm. Let ϵ be an arbitrary real number in the interval $]0,\frac{1}{1+2l}[$ and assume that*

$$d(\Lambda,\Lambda') < \epsilon$$

Then for all $\lambda \in \Lambda$ such that

$$\|\lambda\| < \frac{1-\epsilon}{2\epsilon}$$

(i) there exists an unique $\lambda' \in \Lambda'$ such that $\|\lambda - \lambda'\| < 1/2$, (ii) this pairing (λ,λ') satisfies the inequality:

$$\|\lambda - \lambda'\| \leqslant (1/2 + \|\lambda\|)\epsilon$$

Proof. — See section 2 in [MVG]. □

Let us define the class

$$\mathcal{C} = \left\{ \mathcal{B}(\Lambda) \mid n\Lambda \in \mathcal{UD}, \right.$$
$$\left. \liminf_{R\to+\infty} \frac{\text{vol}\,((\bigcup_{i\in I}(a_i + B)) \cap B(0,R))}{\text{vol}\,(B(0,R))} = \limsup_{R\to+\infty} \frac{\text{vol}\,((\bigcup_{i\in I}(a_i + B)) \cap B(0,R))}{\text{vol}\,(B(0,R))} \right\}$$

The following proposition is a very partial counterpart of the Minkowski-Hermite approach for lattices (recalled in section 4) and shows the usefulness of the d-topology to study aperiodic systems of spheres of $\mathbb{R}^n$ as far as the class $\mathcal{C}$ is known.

PROPOSITION 2.5. — *The restriction of the density map δ to the class $\mathcal{C}$ is continuous in the d-topology.*

Proof. — Let $\epsilon > 0$. Assume that $\mathcal{A} = (a_i)_{i\in\mathbb{Z}}$ and $\mathcal{A}' = (a'_i)_{i\in\mathbb{Z}}$ are two elements of $\mathcal{C}$ such that

$$|\delta(\mathcal{B}(\mathcal{A})) - \delta(\mathcal{B}(\mathcal{A}'))| \leqslant \epsilon \qquad (2)$$

We are looking for $\eta > 0$ such that $d(\mathcal{A},\mathcal{A}') < \eta$ implies the inequality (2). Take $R > 1$ a real number (we will chose it in a suitable way below). Let us denote by

$$\delta_R(\mathcal{B}(\mathcal{A})) = \frac{1}{\text{vol}\,(B(0,R))}\text{vol}\left(\left(\bigcup_{i\in I}(a_i + B)\right) \bigcap B(0,R)\right)$$

By the fact that the density function is a true limit on the class $\mathcal{C}$, there exists R_0 such that $R \geqslant R_0$ implies

$$|\delta(\mathcal{B}(\mathcal{A})) - \delta_R(\mathcal{B}(\mathcal{A}))| \leqslant \epsilon/3 \quad \text{and} \quad |\delta(\mathcal{B}(\mathcal{A}')) - \delta_R(\mathcal{B}(\mathcal{A}'))| \leqslant \epsilon/3 \qquad (3)$$

We will show that

$$|\delta_R(\mathscr{B}(\mathscr{A})) - \delta_R(\mathscr{B}(\mathscr{A}'))| \leqslant \epsilon/3$$

as soon as $d(\mathscr{A},\mathscr{A}') < \eta$ with $\eta > 0$ small enough. Indeed, by lemma 2.4 we know that if $\eta > 0$ is small enough, then the inequality $d(\mathscr{A},\mathscr{A}') < \eta$ implies that all the points of $\mathscr{A}$ are uniquely paired to points of $\mathscr{A}'$ within a big ball, say $B(0,T)$ with $T = \frac{1-\eta}{2\eta}$. Let us take η such that

$$0 < \eta < \frac{1}{2R_0 + 3}$$

Then $T > R_0 + 1$. The number of points a_i of $\mathscr{A} \cap B(0,T)$ will be exactly the number of points a_i' of $\mathscr{A}' \cap B(0,T)$ except perhaps within distance 1 from the boundary $\partial(B(0,T))$ of $B(0,T)$.

(i) first class of pairings (a_i,a_i') : those for which simultaneously a_i+B and $a_i'+B$ lie within $B(0,T)$. Their contributions cancel each other in the difference

$$|\delta_R(\mathscr{B}(\mathscr{A})) - \delta_R(\mathscr{B}(\mathscr{A}'))|$$

(ii) second class of pairings (a_i,a_i') : those for which either $(a_i + B) \notin B(0,T)$ or $(a_i' + B) \notin B(0,T)$. The elements a_i and a_i' both lie within $\partial(B(0,T)) + B(0,1)$. Then the maximal volume fraction occupied by the points $a_i \in \partial(B(0,T)) + B(0,1)$, resp. $a_i' \in \partial(B(0,T)) + B(0,1)$, is

$$\frac{\mathrm{vol}(\partial(B(0,T)) + B(0,1))}{\mathrm{vol}(B(0,T))}$$

which clearly tends to zero when T tends to infinity. Therefore there exists η_0 such that

$$\eta < \eta_0 \implies \frac{\mathrm{vol}(\partial(B(0,T)) + B(0,1))}{\mathrm{vol}(B(0,T))} < \epsilon/6$$

For all $\eta < \min\{\eta_0, \frac{1}{2R_0+3}\}$ we obtain

$$|\delta_R(\mathscr{B}(\mathscr{A})) - \delta_R(\mathscr{B}(\mathscr{A}'))| < 2\frac{\mathrm{vol}(\partial(B(0,T)) + B(0,1))}{\mathrm{vol}(B(0,T))} < \epsilon/3 \qquad (4)$$

From the inequalities (3), (4), we deduce (2), that is the continuity of the restriction of the density function δ to $\mathscr{C}$. □

This proof does not work in general on SS since a generic $\mathscr{UD}$-set has a density which is presumably not given by a true limit (such that lim inf = lim sup). The question is now: which Delone sets of constants $(1,1)$ have a density given by a true limit?

DEFINITION 2.6. — *The subset*

$$H_n := \delta^{-1}(\{\delta_n^+\}) \subset SS$$

is called the locus of densest systems of spheres (or sphere packings) of $\mathbb{R}^n$. *We will denote by* $H_{1,n}$ *the set of systems of spheres of* H_n *arising from Delone sets of constants* $(1,1)$.

The loci $H_n,H_{1,n}$ of densest packings of $\mathbb{R}^n$ may be empty.

3. Voronoi polyhedra and local densities

We will focus our attention to systems of spheres obtained from X_R with $R \geqslant R_{\min}$ and particularly from X_1 giving rise to the densest sphere packings of $\mathbb{R}^n$. Let $\mathscr{A} = (a_i)_{i\in\mathbb{Z}} \in X_R$ be a Delone set of constant $R \geqslant R_{\min}$ and $\mathscr{B}(\mathscr{A})$ its associated sphere packing of $\mathbb{R}^n$. To each sphere $a_i + B$ in $\mathscr{B}(\mathscr{A})$ are associated its local cell $C(a_i,\mathscr{B}(\mathscr{A}))$ defined by the closed convex polyhedron, called Voronoi cell or Voronoi polyhedron at a_i

$$C(a_i,\mathscr{B}(\mathscr{A})) = \{x \in \mathbb{R}^n \mid \|x - a_i\| \leqslant \|x - a_j\| \text{ for all } j \neq i\}$$

and its local density $\Delta(a_i,\mathscr{B}(\mathscr{A}))$ at a_i

$$\Delta(a_i,\mathscr{B}(\mathscr{A})) = v_n(1/2)/\mathrm{vol}(C(a_i,\mathscr{B}(\mathscr{A})))$$

The decomposition into Voronoi polyhedra of the sphere packing $\mathscr{B}(\mathscr{A})$ forms a tiling of $\mathbb{R}^n$. Each local cell has bounded volume. The density of $\mathscr{B}(\mathscr{A})$ is then the weighted average of the local densities $\Delta(a_i,\mathscr{B}(\mathscr{A}))$ where the weights are $\mathrm{vol}(C(a_i,\mathscr{B}(\mathscr{A})))$, all strictly positive. An upper bound of the local densities is therefore an upper bound of the density of the tiling (see lemma 3.2).

Denote by

$$\mathscr{V}_{R,n} := \{C(a_i,\mathscr{B}(\mathscr{A})) - a_i \mid i \in \mathbb{Z}, a_i \in \mathscr{A}, \mathscr{A} \in X_R\}$$

the set of all possible Voronoi cells (refered to the same origin, say 0) existing in systems of spheres arising from Delone sets of $\mathbb{R}^n$ of constant $(1,R)$. The number of vertices of a Voronoi cell $C(a_i,\mathscr{B}(\mathscr{A})) - a_i \in \mathscr{V}_{R,n}$ is uniformly bounded by construction and a Voronoi cell $C(a_i,\mathscr{B}(\mathscr{A}))$ is uniquely determined by a finite number of points of $\mathscr{B}(\mathscr{A}))$ which are close to a_i. More precisely, Rogers has shown in chapter 7 of [R] that $C(a_i,\mathscr{B}(\mathscr{A}))$ is entirely defined by the finite $\mathscr{UD}$-set made of the points of $\mathscr{B}(\mathscr{A})$ which are within the interior of the ball $B(a_i,2R)$. Therefore we can transport the d-topology existing on the space of clusters lying inside the closed ball $B(0,2R)$ to the set $\mathscr{V}_{R,n}$ of Voronoi cells associated with X_R and will still speak of the d-topology on this space. Since $R_{\min} \leqslant R' \leqslant R$ implies $X_{R'} \subset X_R$, then $\mathscr{V}_{R',n} \subset \mathscr{V}_{R,n}$. Let us define

$$\mathscr{V}_n := \bigcup_{R>0} \mathscr{V}_{R,n}$$

as the set of all possible Voronoi cells (refered to the same origin, say 0) existing in systems of spheres arising from Delone sets of $\mathbb{R}^n$.

PROPOSITION 3.1. — *Let $R \geqslant R_{\min}$. The space of Voronoi cells $\mathscr{V}_{R,n}$ is a compact space in the d-topology. The space $\mathscr{V}_n$ is locally compact in the d-topology.*

Proof. — In [MVG], it was shown that, on the space of clusters lying inside the closed ball $B(0,2R)$, the d-topology was exactly the topology given by the Hausdorff metric.

Since the ball $B(0,2R)$ is compact, the set of $\mathcal{UD}$-sets lying inside it is compact in the Hausdorff topology, therefore in the d-topology. By transport to $\mathcal{V}_{R,n}$ we deduce the result. □

Since the local density application $C(a_i,\mathcal{B}(\mathcal{A})) \to \Delta(a_i,\mathcal{B}(\mathcal{A}))$ is continuous in the d-topology, there exists at least one Voronoi cell of minimal local density, resp. maximal local density. Let us define, for all $R \geqslant R_{\min}$:

$$\Delta^+_{R,n} = \sup_{\mathcal{A}\in X_R} \sup_{a_i\in\mathcal{A}} \Delta(a_i,\mathcal{B}(\mathcal{A}))$$

$$\Delta^-_{R,n} = \inf_{\mathcal{A}\in X_R} \inf_{a_i\in\mathcal{A}} \Delta(a_i,\mathcal{B}(\mathcal{A}))$$

LEMMA 3.2. — *For all $R \geqslant 1$ we have:*

$$\Delta^-_{R,n} \leqslant \Delta^-_{1,n} \leqslant \delta^-_n \leqslant \delta^+_n \leqslant \Delta^+_{1,n} = \Delta^+_{R,n}$$

Proof. — Indeed, the equality comes from the fact that any $\mathcal{UD}$-set belonging to X_1 also belongs to X_R so that the densest local cells are equally produced by systems of sphere from one or the other set of Delone sets. As for the inequalities, they are obvious. □

The main questions we can ask are the following:

(Q3) Given the integer $n \geqslant 2$, does there exists only one minimal Voronoi cell in $\mathbb{R}^n$ up to rotation and symmetry? What is/are its/their geometry?

(Q4) In a densest sphere packing in $\mathbb{R}^n$, are necessarily minimal Voronoi cells present? does there exist densest sphere packings of $\mathbb{R}^n$ containing none of the minimal Voronoi cells?

(Q5) if a densest sphere packing of $\mathbb{R}^n$ contains minimal Voronoi cells, what is their distribution in space?

Partial answers exist nowadays. If $n = 2$ or $n = 3$, (Q3) is answered by yes and the geometry of the minimal Vornoi cells is given by the following results (theorem 3.4 is cited in [H]).

THEOREM 3.3 (Thue, Fejes-Tóth). — *The densest packing of identical discs (of radius 1/2) in the plane is obtained from a lattice packing, which is the hexagonal packing. The maximal local density of any disc packing is the packing constant, namely*

$$\delta^+_2 = \max_{\mathcal{B}=(a_i)\in SS, a_i\in\mathcal{B}} \Delta(a_i,\mathcal{B}) = \pi/\sqrt{12}$$

It is reached at one disc centre if and only if the Voronoi cell at this disc centre is a regular hexagon (of inradius 1/2).

Geometrically, the plane can be tiled with regular triangles. The minimal Voronoi cell tiles the plane.

THEOREM 3.4 (McLaughlin). — *The maximal local density*

$$\frac{2\pi}{15\sqrt{130-58\sqrt{5}}} = 0.7546974\ldots$$

over all packings of identical spheres (of radius 1/2) in $\mathbb{R}^3$ *is reached at one sphere centre if and only if the Voronoi cell at this sphere centre is a regular dodecahedron (of inradius 1/2).*

Let us remark two facts which are at the origin of Kepler's conjecture. First, the minimal Voronoi cell does not tile space in dimension 3. Indeed, it is impossible to make a lattice packing of dodecahedra in $\mathbb{R}^3$ without leaving some remaining part of space unoccupied. Second, the maximal local density is strictly greater than the Kepler bound $\pi/\sqrt{18} = 0.74048\ldots$.

When a Voronoi cell is minimal at a sphere centre, that is a regular dodecahedron, the first-neighbour spheres constitute the vertices of a regular icosahedron about the central one. This is an answer to the problem of 13 spheres around a central sphere and a solution to the controversy between Newton and Gregory (see [O]).

The observation that the minimal Voronoi cells are unique and highly symmetrical for $n = 2$ and 3 by Verger-Gaugry [VG] led this author to investigate quasiperiodic sphere packings in $\mathbb{R}^n$ from their symmetry group using the formalism of cut-and-project schemes.

If $n \geqslant 4$ then (Q3) seems to be an open problem nowadays. The question is now: does a suitable set of minimal Voronoi cells tile the n-dimensional euclidean space?

4. Lattice sphere packings

Let $\mathscr{L}_n$ be the set of lattices of the affine space $\mathbb{R}^n$ (they all contain the origin). The space $\mathscr{L}_n$ is parametrized by the locally compact group $GL(n,\mathbb{R})/GL(n,\mathbb{Z})$ and therefore endowed with the quotient topology arising from this homogeneous space (Oesterlé [O1], Martinet [M]). In [MVG] it is also shown that this topology coincides on $\mathscr{L}_n \cap \mathscr{UD}$ with the restriction of the d-topology and that corollary 2.3 is a key result as aperiodic generalization of Mahler's selection theorem for lattices (see section 4 in [MVG]).

Let $L \in \mathscr{L}_n$ be a lattice of $\mathbb{R}^n$. We will denote by $m(L) = \inf\left\{\|l\|^2 \mid l \in L, l \neq 0\right\}$ the minimal square distance between two distinct elements of L. We will consider the packing of identical spheres obtained from L by putting a sphere centred at each element of L of radius equal to $\sqrt{m(L)}/2$. Let us denote by $\langle .,. \rangle$ the standard scalar product over $\mathbb{R}^n$. If $\{e_1, e_2, \ldots, e_n\}$ is an arbitrary basis of L, let us define the discriminant of L by

$$\mathrm{disc}(L) = \det(\langle e_i, e_j \rangle)$$

It is independent of the basis of L and is the square of the volume of the compact space $\mathbb{R}^n/L$. It is usual to define the lattice function γ on the quotient space $GL(n,\mathbb{R})/GL(n,\mathbb{Z})$

by

$$\gamma(L) = \frac{m(L)}{\mathrm{disc}(L)^{1/n}}$$

This function is continuous and satisfies $\gamma(tL) = \gamma(L)$ for all $t > 0$. Therefore, to know it on lattices which are $\mathcal{UD}$-sets of constant 1, it is sufficient to study it on the space of unimodular lattices which identifies to $SL(n,\mathbb{R})/SL(n,\mathbb{Z})$.

PROPOSITION 4.1. — *The application* $\gamma : SL(n,\mathbb{R})/SL(n,\mathbb{Z}) \to]0,+\infty[$ *is proper. The closed set* $\mathcal{R}_n := \gamma^{-1}(\{\gamma_n\})$ *is finite.*

Proof. — See Oesterlé [O1], Martinet [M] and Gruber and Lekkerkerker [GL]. □

The supremum $\gamma_n = \sup_{L\in\mathcal{L}_n} \gamma(L)$ is reached at at least one unimodular lattice of $\mathbb{R}^n$ and consequently at at least one lattice which is a $\mathcal{UD}$-set of $\mathbb{R}^n$. This constant γ_n is called the Hermite constant; it is a function of n.

For any lattice $L \in \mathcal{L}_n \cap \mathcal{UD}$, the density of the lattice sphere packing $\mathcal{B}(L) = \{a_i + B(0,m(L)/2) \mid a_i \in L\}$ is given by

$$\delta(\mathcal{B}(L)) = 2^{-n} v_n(1) \gamma(L)^{n/2} = \frac{\pi^{n/2}}{2^n \Gamma(\frac{n+2}{2})} \gamma(L)^{n/2}$$

DEFINITION 4.2. — *The lattice packing constant* $\delta^+_{L,n}$ *is by definition the maximal density of a lattice sphere packing:*

$$\delta^+_{L,n} := \sup_{L\in\mathcal{L}_n} \delta(\mathcal{B}(L)) = \sup_{L\in\mathcal{L}_n\cap\mathcal{UD}} \delta(\mathcal{B}(L)) = \sup_{L\in\mathcal{L}_n, det(L)=1} \delta(\mathcal{B}(L))$$

Let us define in a similar way:

$$\delta^-_{L,n} := \inf_{L\in\mathcal{L}_n\cap X_1} \delta(\mathcal{B}(L))$$

COROLLARY 4.3. — *For all integer* $n \geqslant 1$, *there exist lattices* L *in* $\mathbb{R}^n$ *of maximal, resp. minimal, density which are uniformly discrete sets of constant 1, i.e. such that*

$$\delta(\mathcal{B}(L)) = \delta^+_{L,n} = \sup_{L\in\mathcal{L}_n\cap\mathcal{UD}} \delta(\mathcal{B}(L)) = \frac{\pi^{n/2}}{2^n \Gamma(\frac{n+2}{2})} \gamma_n^{n/2}, \quad \textit{resp. } \delta(\mathcal{B}(L)) = \delta^-_{L,n}$$

Lattices $L \in \mathcal{L}_n$ such that $\delta(\mathcal{B}(L))$ is a local maximum are called extreme lattices. The study of extreme lattices was done in particular by Voronoi and was considerably developed since then (chapter III in Martinet [M]) and generalized in the theory of systoles by Bavard [B] and Akrout [A].

It seems reasonable to say that densest systems of spheres do not arise in general from lattice systems of spheres since lattices are not in general Delone sets of constant

(1,1) (see proposition 2.1). Indeed, a lattice $L \in \mathscr{L}_n \cap \mathscr{UD}$ is naturally a Delone set of constant $(1,R(L))$ where $R(L)$ is the *covering radius* of L defined by

$$R(L) = \sup_{z \in \mathbb{R}^n} \inf_{\lambda \in L} \|z - \lambda\|$$

If L possesses so-called deep holes, the constant $R(L)$ may be very large. Recall that a *hole* in L is a point of $\mathbb{R}^n$ whose distance from L is a local maximum [CS] therefore a vertex of Voronoi cell of L. The greatest distance of any hole of L from L is the covering radius $R(L)$ of L. The covering radius $R(L)$ is also the circumradius of the Voronoi cell of L at the origin. The existence of possible deep holes in a lattice prevents it from being a good candidate for providing a very dense system of spheres. Let us define

$$R_{L,\min} := \inf\{R(L) \mid L \in \mathscr{L}_n \cap \mathscr{UD}\}$$

the infimum of all covering radii of all lattices in $\mathscr{L}_n \cap \mathscr{UD}$. We have

$$R_{\min} \leqslant R_{L,\min}$$

Is it true that for all integers $n \geqslant 2$ we have $R_{\min} = R_{L,\min}$? For $n = 2$ theorem 3.3 gives the equality. In the case $n = 3$ the minimal Voronoi cell over all lattices of $\mathscr{L}_3 \cap \mathscr{UD}$ is not a regular dodecahedron (of inradius 1/2) but a rhombic dodecahedron (with the same inradius 1/2) which is given by the Voronoi cell at the origin of the face centred cubic lattice (densest lattice sphere packing). Nevertheless, we still have equality.

Thue - Fejes-Toth theorem 3.3 and Hales - Ferguson theorem 1.1, i.e. Kepler conjecture (in dimension 3), can be reformulated as follows: for $n = 2,3$

$$d(\mathscr{L}_n \cap \mathscr{UD}, H_n) = \inf\{d(L,\Lambda) \mid L \in \mathscr{L}_n \cap \mathscr{UD}, \Lambda \in H_n\} = d(\mathscr{L}_n \cap \mathscr{UD}, H_{1,n}) = 0$$

Let us state a general conjecture.

CONJECTURE 1. — *For all integer* $n \geqslant 4$

$$d(\mathscr{L}_n \cap \mathscr{UD}, H_n) = d(\mathscr{L}_n \cap \mathscr{UD}, H_{1,n}) > 0$$

This conjecture calls for the subsidiary question: is the distance between the subset $H_{1,n}$ and the locally compact subspace $\mathscr{L}_n \cap \mathscr{UD}$ computable?

The main question is the proximity of $H_{1,n}$ to the subspace of lattices of $\mathscr{UD}$ which are of constant 1. Assume that there exists a Delone set Λ of $\mathbb{R}^n$ of constants (1,1) and a lattice L such that

$$L \in \mathscr{L}_n \cap \mathscr{UD},\ \Lambda \in H_{1,n} \quad \text{with} \quad d(\Lambda,L) = d(\mathscr{L}_n \cap \mathscr{UD}, H_{1,n}) > 0$$

By lemma 2.4 this implies that both point sets L and Λ resemble within a certain distance from the origin by the phenomenon of pairings of points whatever their distributions of points are at infinity. But by definition the density of Λ is an asymptotic measure of its points at infinity. This shows that the d-topology is not fine enough to deal with the problem of the continuity of density functions in general.

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