THE STRUCTURE OF DELONE SETS

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Abstract. This article proposes a review of the mathematical structure of Delone sets in the context of metric spaces. After a reminder of the definition, the main series of results are established in finite dimensional Euclidean Spaces. Few words are dedicated to the applications in coding theory and in material sciences.

Contents

1. Motivations

This article is a contribution to the special issue published in Journal of Mathematical Physics dedicated to the Memory of Jean Bourgain. The author never met Jean Bourgain in person. However, he is familiar with some of his contributions in the field of Mathematical Physics, especially the ones concerning the small divisor problem that was introduced in the study of the Schrödinger Operator first in the seminal foundation paper of Dinaburg and Sinai [39] and used by the authors in various problems of Quantum Physics after 1981 (see for instance [9] and references therein).

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This article proposes a review of the most fundamental properties of Delone sets in finite dimensional Euclidean spaces. Delone sets are known under the name of Delaunay [38] in other communities.[1]. Considering the length of the paper allocated for this review, many aspects developed recently have been omitted, hoping to be published elsewhere in the near future.

Delone sets have a long history. Many important steps, those by Voronoi [98, 99], Delaunay-Delone [38] and Bernal [21, 22, 23] for instance, are described in this review. But they appeared in several forms in deep problems of mathematics. One of the most famous is the *densest sphere packing problem* solved in three dimension [51]. As it turns out, such a sphere packing problem occurs in *Coding Theory*, as was explained by Shannon in his proof of the *Channel Capacity Theorem* [91, 37]. This led John Leech [72] to propose in 1967 the most efficient code for codewords of 24 binary digit letters in the form of the *Leech lattice* in dimension 24. The proof that it was the densest sphere packing lattice was provided in [33], building upon a new method proposed in [96] where the densest sphere packing in dimension 8 was proved to be realized by the E_8-lattice. As it turns out, the sphere packing problem puts some restrictions on the existence of Delone sets as explained in this review (see Section 2.4, Remark 3).

However, the original motivation of the author in using Delone sets came from Physics. After the end of the 1980's, the author's research went to deepen the formalism he promoted by using Noncommutative Geometry to describe electronic properties of aperiodic media. All along this fascinating path, he was joined in the mid-1990's by a group of brilliant young mathematicians who had significants contributions in the direction of solids like quasicrystal, in terms of atomic structures and topological properties (see for instance [58, 1, 87] and references therein). By the end of the 1990's Lagarias came in to explain the structure in terms of Delone sets of *finite local complexity* (FLC) [61, 62, 63]. During the two previous decades the influence of the background, on the electrons of a solid, was described through the *Hull*, namely an unknown compact metrizable space endowed with an action of the translation group and a translation invariant probability distribution [10]. That was sufficient to account for the most important properties of the electrons in a solid, like the *Gap Labeling Theorem* [11], the *Quantum Hall Effect* [12] or the electronic transport [90, 14]. However with the intrusion of this new formalism, it became possible to describe more precisely this background in the form of atoms distributed in space [13].

In real materials, the temperature is never zero, so that the atomic thermal motion makes the atomic position unpredictable. A probability space is the right framework for their description. This was what a mathematically rigorous approach to Statistical Mechanic did in the 1960's and 1970's with the works by Sinai [93, 94], Dobrushin [26], Lanford [64, 65, 66] and Ruelle [84] for instance. It gave a lot of important results for spin systems and gas. However, the transition to liquids and solids was hardly understood this way. Indeed, daily experience with solids hardly backs up the prediction of the randomness approach by Statistical Mechanics: ergodicity of the probability distribution under the translation group, predicts that with probability one there are big holes in the solid and some clustering of atoms somewhere in space. Such holes or clusters are never really observed in practice. Why ? Because the lifetime of these configurations is

[1]Delaunay (1890-1980) is the French spelling version under which the author Boris Delaunay [38], called Delone in English speaking countries, is known. He was a Russian Mathematical Physicist who was descending from a Napoleon soldier who married and stayed in Russia after the defeat of the French Army in 1812. It seems that the cyrillic spelling of the French name was phonetically correct using correctly the cyrillic Э to translate the "ay", which sounds more like the English "a" like in "cake" or the English "ay" like in "say" at the end of the name. However, the translator of Russian to English did not distinguished between the cyrillic "e" and "Э", leading to Delone instead of Delonay as it should have been.

so short that they cannot be really observed. So the random description proposed by rigorous Statistical Mechanics is impractical (see the *Ergodicity Paradox* in [16]). Delone sets cures this problem by

(D1)- forcing atom to stay away from each other (there is a minimum distance between them),
(D2)- limiting uniformly in space the size of the holes. .

Actually it was proved rigorously, using the framework of rigorous Statistical Mechanics [15] that for spherical atoms interacting through an attractive hard core potential that the zero temperature limit Gibbs states are supported by a space of Delone sets. Replacing a hard core by some strong repulsion should, in principle, be sufficient, but the problem is *still open*. From this point of view, a Delone set approach is more appropriate to describe solids. The atomic motion is usually introduced as a small perturbation in the form of phonons. The author suspected for a long time that it could also serve to describe other media like liquids. This is actually what Bernal proposed to do [21, 22, 23] as he discovered later, after his meeting with T. Egami in 2012 who encoraged him to pursue along this path. And indeed liquids can be described by Delone sets, provided another type of atomic motion is included, the possibility of atomic jumps of larger amplitude. This new degree of freedom was called *anankeon* [40, 42, 16]. It was shown that the main difference between solid and liquid phases is that solids are dominated by the phonon degrees of freedom, while liquids are dominated by the anankeon ones. The most powerful application of this idea came recently by proposing a formula for the *viscosity of liquid* that fits quantitatively with the experimental data [17, 18] and permits to account for various temperature behaviors called *hard* or *soft* glasses near the solid-liquid transition. Anankeons are also the key to understand *plasticity* of solids under external stress [68, 69, 70, 71, 85].

Given a Delone set, atoms are caged in a convex polyhedron called the *Voronoi tile*. This concept of atomic cage has been used for a long time in numerical computations of the energy spectrum for electron in a crystal. These cages are the locus of phonon vibrations leading to *Theory of Elasticity*. Delaunay-Delone showed [38] that such a *Voronoi tesselation* can be replaced by a *triangulation* which represents the Poincaré-dual lattice in such a case. He defined it through the concept of *Empty Sphere Property*. Within this framework, a large atomic jump, an anankeon then, can be described by a local change of the Delaunay triangulation, the so-called *Pachner moves* [81]. Therefore the structure of Delone sets in the usual space $\mathbb{R}^3$ opens the door to a potential synthetic treatment of both Continuous Mechanics of Solids and Fluid Mechanics from the atomic scale point of view.

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2. Delone Sets

This Section provides the most elementary properties of Delone sets in metric spaces, inspired by [61, 62, 13]. It is worth noticing though, that Delone sets are related to the concepts of ϵ-packing and ϵ-covering, which are heavily used in Computational Geometry, Combinatorial Theory and Data Sciences (see for instance [57, 30, 52, 31, 53]). This definition has also been extended to locally compact groups [6]. The formal definition given here is motivated by Properties (D1-D2) given in Section 1.

In the following, (X, d) denotes a metric space equipped with its metric topology. The concept of metric was formally introduced by Hausdorff in his founding textbook [54, 55, 56]. It is worth noticing that he had been inspired by a work of Fréchet [46, 95], who, in his PhD Thesis introduced, among others, the concept of metric space. The name *"metric space"*, however, was proposed by Hausdorff. In its basic principle, a metric space is a natural framework for *geometry*, since this terms means literally *to measure the Earth*. Since the term geometry was developed in several directions, the restriction to metric spaces is called *Metric Geometry* in modern literature. A good more recent textbook for metric spaces is [27]. In his 1914 book on topology, Hausdorff also defined a metric on the space $\mathcal{C}(X)$ of closed subsets of a metric spaces.

Notations: The open ball of radius r centered at $x \in X$ will be denoted $\mathrm{B}(x; r)$, while $\overline{\mathrm{B}}(x; r)$ coincides with the closed ball $\{y \in X\,;\, d(x, y) \leq r\}$. In general $\overline{\mathrm{B}(x; r)} \subset \overline{\mathrm{B}}(x; r)$ but the closed ball might not coincide with the closure.

2.1. ϵ-nets.

Definition 1. *A subset $L \subset X$ is called ϵ-separated if, given any pair $x \neq y$ of points in L, $d(x, y) \geq \epsilon$. An ϵ-net in X is a maximum ϵ-separated subset of X.*

Proposition 1. *For any $\epsilon > 0$, any metric space (X, d) with diameter larger than ϵ contains an ϵ-net. In addition, an ϵ-separated set $N \subset X$ is an ϵ-net if and only if the family of open balls $\{B(x; \epsilon)\,;\, x \in N\}$ is an open cover of X. In particular, if X is compact, any ϵ-net is finite.*

Proof: (i) Since the diameter of X is larger than ϵ, there are at least two points x, y in X such that $d(x, y) \geq \epsilon$. Hence, the set of ϵ-separated subsets of X is not empty. Moreover, it is ordered by inclusion. A chain is a totally ordered family $(L_i)_{i \in I}$ of such subsets. Namely if $i \neq j$ then either $L_i \subset L_j$ or $L_j \subset L_i$. Let then L be the union of the L_i's. If $x \neq y$ are two distinct points of L, then there are i, j such that $x \in L_i$ and $y \in L_j$. Assuming, without loss of generality, that $L_i \subset L_j$, it follows that both x, y belong to L_j, so that $d(x, y) \geq \epsilon$. Hence L is itself ϵ-separated. Thanks to the Zorn Lemma, it follows that there is a maximum ϵ-separated subset of X.

(ii) Let N be an ϵ-net. If the family of open balls $\{B(x; \epsilon)\,;\, x \in N\}$ does not cover X, let y be a point in X outside of any ball $B(x; \epsilon)$ for $x \in N$. Then $d(x, y) \geq \epsilon$ for any $x \in N$. Hence $N \cup \{y\}$ is ϵ-separated and contains strictly N. Therefore N is not maximal, a contradiction.

(iii) Let now N be ϵ-separated and let the family of open balls $\{B(x; \epsilon)\,;\, x \in N\}$ cover X. If $y \in X$ is not in N, it belongs to at least one ball $B(x; \epsilon)$. Hence $d(x, y) < \epsilon$. Therefore $N \cup \{y\}$ is not ϵ-separated. Consequently N is maximal.

(iv) If N is an ϵ-net, the family of open balls $\{B(x; \epsilon)\,;\, x \in N\}$ covers X. By compactness a finite subcover of the form $\{B(x; \epsilon)\,;\, x \in L\}$ can be extracted. Namely $L \subset N$ is ϵ-separated and finite. By (ii) it must be maximal so that $N = L$. □

2.2. Delone Sets in Metric spaces.

Definition 2. *Let $\mathcal{L} \subset X$ be a discrete subset. Then*
(i) it is called uniformly discrete *whenever there is $\check{r} > 0$ such that any open ball of radius $\check{r}$ contains* at most *one point of $\mathcal{L}$;*
(ii) it is called relatively dense *whenever there is $\widehat{r} > 0$ such that any closed ball of radius $\widehat{r}$ contains* at least *one point of $\mathcal{L}$;*

(iii) it is called a Delone set if it is both uniformly discrete and relatively dense. A point $x \in \mathcal{L}$ will be called an atom.
Then, $\mathrm{UD}_X(\check{r})$ *(resp.* $\mathrm{RD}_X(\widehat{r})$*) will denote the uniformly discrete (resp. closed relatively dense) subsets of X, with parameters $\check{r}$ (resp. $\widehat{r}$). Similarly* $\mathrm{Del}_X(\check{r}, \widehat{r}) = \mathrm{UD}_X(\check{r}) \cap \mathrm{RD}_X(\widehat{r})$ *will denote the set of Delone sets with parameters $\check{r}, \widehat{r}$.*

From these definition it follows obviously that $\check{r} \leq \widehat{r}$ is a necessary condition for the set of Delone sets to not be reduced to one point only. Another immediate remark is that if the diameter of X be smaller than $2\check{r}$ then any Delone set is also reduced to one point. Hence this concept is useful only for "large" enough metric spaces. In addition, if $\check{r}_1 \leq \check{r}$ and $\widehat{r}_1 \geq \widehat{r}$ then $\mathrm{Del}_X(\check{r}, \widehat{r}) \subset \mathrm{Del}_X(\check{r}_1, \widehat{r}_1)$. Whether the space $\mathrm{Del}_X(\check{r}, \widehat{r})$ is nonempty or not is actually a nontrivial problem and the answer may depend on the space (X, d) itself. This leads to the following definition

Definition 3. *Let (X, d) be a metric space. Then the critical ratio* $\mathrm{CR}(X)$ *of X is the minimum of the ratio $\widehat{r}/\check{r}$ such that* $\mathrm{Del}_X(\check{r}, \widehat{r}) \neq \emptyset$.

The following result gives us upper and lower bounds on the critical ratio.

Theorem 1. *Let (X, d) be a metric space. Then* $1 \leq \mathrm{CR}(X) \leq 2$.

Proof: It is sufficient to prove that if $\epsilon > 0$ is smaller then the diameter of X, any ϵ-net is a Delone set in $\mathrm{Del}_X(\epsilon/2, \epsilon)$. Thanks to Proposition 1, given an ϵ-net $N \subset X$ for any point $y \in X$ there is $x \in N$ such that $y \in \mathrm{B}(x; \epsilon)$. Consequently $x \in \mathrm{B}(y; \epsilon) \subset \overline{\mathrm{B}}(y; \epsilon)$. In particular N is ϵ-relatively dense. In addition, an open ball $\mathrm{B}(y; \epsilon/2)$ cannot contain more than one element of N. For, if not, let $x, x' \in N \cap \mathrm{B}(y; \epsilon/2)$. Then $d(x, x') \leq d(x, y) + d(y, x') < \epsilon$, a contradiction since N is a ϵ-separated. Hence $N \in \mathrm{Del}_X(\epsilon/2, \epsilon)$ □

Example 1. As it turns out, in the Euclidean plane, the critical ratio is reached for the triangular lattice, corresponding to the densest packing of identical spheres, and is $\mathrm{CR}(\mathbb{R}^2) = 2/\sqrt{3}$. In the three dimensional Euclidean space, the densest packing of sphere is given by a Kepler lattice [51], for which $\widehat{r}/\check{r} = \sqrt{2}$. Whether $\mathrm{CR}(\mathbb{R}^3) = \sqrt{2}$ or not is not known to the author, even if it should be so. These two examples illustrate the difficulty of computing the critical ratio for a given metric space. □

Proposition 2. *(i) If $\mathcal{L} \in \mathrm{UD}_X(\check{r})$ then given $x \neq x'$ in $\mathcal{L}$ the balls $\mathrm{B}(x; \check{r})$ and $\mathrm{B}(x'; \check{r})$ do not intersect.*
(ii) If $\mathcal{L} \in \mathrm{RD}_X(\widehat{r})$ the balls $\{\overline{\mathrm{B}}(x; \widehat{r})\,;\, x \in \mathcal{L}\}$ cover X.

Proof: (i) If there were such $x, y \in \mathcal{L}$, let $z \in \mathrm{B}(x; \check{r}) \cap \mathrm{B}(y; \check{r})$, then both x, y would belong to the ball $\mathrm{B}(z; \check{r})$, which is excluded by the very definition of $\mathrm{UD}(\check{r})$.

(ii) If the closed balls of radius $\widehat{r}$ centered on atoms of $\mathcal{L}$ would not cover X, there would be a point $y \in X$ at distance strictly bigger than $\widehat{r}$ from any atom. Therefore the closed ball $\overline{\mathrm{B}}(y; \widehat{r})$ would not intersect $\mathcal{L}$, a contradiction since $\mathcal{L} \in \mathrm{RD}_X(\widehat{r})$. □

The name *atom* is suggested by the fact that Delone sets are modeling conveniently the atomic positions in a condensed material, be it a solid, a crystal or a glass, or a liquid [38, 42, 16]. In addition, it is worth noticing that the use of balls explains why the radius, and not the diameter, is preferred. In particular, at least for many metrics, the minimum distance between two points in $\mathcal{L}$ is at least $2r$. Similarly, any ball without any point of $\mathcal{L}$ in its interior has a diameter at most $2R$.

Lemma 1. *Any $\mathcal{L} \in \mathrm{UD}_X(\check{r})$ is a closed subset of X.*

Proof: Let $x \in X$ belong to the closure of $\mathcal{L}$. Then for any $\epsilon > 0$ there is $x_\epsilon \in \mathcal{L}$ with $d(x, x_\epsilon) < \epsilon$. If $\epsilon < \check{r}/2$ it follows that $x \in \mathrm{B}(x_\epsilon; \check{r})$. Similarly, if $\eta < \check{r}/2$, the triangle inequality gives $d(x_\eta, x_\epsilon) < \check{r}$ while both x_ϵ and x_η are in $\mathcal{L}$. Since $\mathcal{L} \in \mathrm{UD}_X(\check{r})$, it follows that $x_\epsilon = x_\eta$ and by taking the limit, $x = x_\epsilon$ proving that $x \in \mathcal{L}$. □

It is worth remarking that a relatively dense discrete subset of X might not be closed in X. This is why, in Definition 2, elements $\mathcal{L} \in \mathrm{RD}_X(\widehat{r})$ are required to be closed. However

Lemma 2. *If $\mathcal{L}$ is relatively dense, its closure is also relatively dense.*

Proof: Suppose not, then for all $\widehat{r} > 0$ there is a closed ball $\overline{\mathrm{B}}(x; \widehat{r}) \subset X$ such that $\overline{\mathrm{B}}(x; \widehat{r}) \cap \overline{\mathcal{L}} = \emptyset$. But since $\mathcal{L} \subset \overline{\mathcal{L}}$, the same property would hold for $\mathcal{L}$, a contradiction. □

2.3. **Topologies on the Space of Delone Sets.** What kind of topology should be used the space of Delone sets ? Thanks to S. Beckus' contributions [5, 7], it has been recognized that the Fell topology [45] is the most appropriate for various purposes related to physics. However, in the present study the Hausdorff topology will be of interest as well. The definition of the Hausdorff metric is now standard, but for convenience of the reader it is given as follows

Definition 4. *Given (X, d) a metric space, and if $A \subset X$, let A^ρ denote the union of balls $\{\mathrm{B}(x; \rho)\,;\, x \in A\}$. Then, the Hausdorff distance $d_H(A, B)$ between two subsets A, B of X is the infimum of the set of $\rho > 0$ such that $A \subset B^\rho$ and $B \subset A^\rho$*

It is easy to check that $d_H(A, B) = d_H(\overline{A}, \overline{B})$, so that $d_H(A, B) = 0$ if and only if the closures of A and B coincide. Hence the natural space on which this distance is defines is rather $\mathcal{C}(X)$ the space of closed subsets of X.

Theorem 2 (Hausdorff [54, 27])**.** *The Hausdorff distance d_H, defined on the space $\mathcal{C}(X)$ of closed subsets of the metric space (X, d), defines a metric. If (X, d) is complete, so is $(\mathcal{C}(X), d_H)$. If in addition (X, d) is compact, so is $(\mathcal{C}(X), d_H)$.*

In 1922 [97], Vietoris gave the definition of a topology on the set of closed subsets of a topological space (see also [76] where it is called the finite-topology), that was an extension of the one provided by the Hausdorff metric on metric spaces. In 1950, Chabauty [29] redefined it as a topology on closed subgroups of a locally compact group to study approximations of groups. Finally, Fell in 1962 [45], motivated by continuous fields of C^*-algebras, gave a different version of the Vietoris topology, extending Chabauty's work, that turns out to be more convenient in the present case to study Delone sets. Let $\mathcal{C}(X)$ denote the set of all closed subsets of X, including the empty set. The Fell topology is generated by a basis of open sets $\mathcal{U}(K, \mathcal{F})$ where $K \subset X$ is compact and $\mathcal{F}$ is a *finite* family of open subsets of X, and defined as the set of closed subsets $F \subset X$ intersecting each open set in $\mathcal{F}$ but not K. Sometimes such a topology is called "hit-and-run". More formally:

$$\mathcal{U}(K, \mathcal{F}) = \{F \in \mathcal{C}(X)\,;\, F \cap K = \emptyset\,,\, F \cap U \neq \emptyset \ \ \forall U \in \mathcal{F}\}$$

For the record, the Vietoris topology is defined exactly as the Fell topology with the difference that K is closed without being necessarily compact.

Theorem 3 (Fell [45], Th. 1)**.** *If X is locally compact (not necessarily Hausdorff), then $\mathcal{C}(X)$ is compact Hausdorff for the Fell topology.*

From now on, it will be assumed that (X, d) is *proper*. As a reminder, a map between topological spaces is called proper whenever the inverse image of compact sets are compact. For a metric space, the term *proper* means that given any $x \in X$, the map $d_x : y \in X \to d(x, y) \in [0, \infty) \subset \mathbb{R}$ is proper. It follows that every closed ball is compact and that X is locally compact for the topology induced by the metric. Conversely if any ball in (X, d) has a compact closure, then it is proper. Hence proper metric spaces are locally compact, but the converse is not true in general. Compact metric spaces are automatically proper. It follows that proper metric spaces are automatically complete.

Theorem 4. *Let (X, d) be a proper metric space. The subsets $\mathrm{UD}_X(\check{r})$, $\mathrm{RD}_X(\widehat{r})$ and $\mathrm{Del}_X(\check{r}, hr)$ are closed in $\mathcal{C}(X)$ for the Fell topology. In particular they are compact Hausdorff.*

Proof: (i) Let $F \in \overline{\mathrm{RD}_X(\widehat{r})}$. If $F \notin \mathrm{RD}_X(\widehat{r})$ there is $z \in X$ such that $\overline{\mathrm{B}}(z; \widehat{r}) \cap F = \emptyset$. Since X is proper, $K = \overline{\mathrm{B}}(z; \widehat{r})$ is compact so that $F \in \mathcal{U}(K, \emptyset)$. Since the later is an open neighborhood of F in the Fell topology, it follows that there is an $\mathcal{L} \in \mathrm{RD}(\widehat{r}) \cap \mathcal{U}(K, \emptyset)$. But as a uniformly dense set with parameter $\widehat{r}$, $\mathcal{L}$ must intersect the compact ball $\overline{\mathrm{B}}(z; \widehat{r})$, so $\mathcal{L}$ cannot belong to $\mathcal{U}(K, \emptyset)$ a contradiction. Hence $F \in \mathrm{RD}_X(\widehat{r})$.

(ii) Let $F \in \overline{\mathrm{UD}_X(\check{r})}$. If $F \notin \mathrm{UD}_X(\check{r})$ there is $z \in X$ such that $F \cap \mathrm{B}(z; \check{r})$ contains at least two points $x \neq y$, so that $d(x, y) > 0$. Since $\mathrm{B}(z; \check{r})$ is open in X its complement $\mathrm{B}(z; \check{r})^c$ is closed and neither x nor y belong to it. Thus $\rho_x = \mathrm{dist}(x, \mathrm{B}(z; \check{r})^c) > 0$. Similarly $\rho_y = \mathrm{dist}(y, \mathrm{B}(z; \check{r})^c) > 0$. Let now $0 < \rho < \min(\rho_x, \rho_y, d(x, y)/2)$. It follows that $U_x = \mathrm{B}(x; \rho) \subset \mathrm{B}(z, \check{r})$ and similarly for U_y replacing x by y. In addition, $2\rho < d(x, y)$ implies $U_x \cap U_y = \emptyset$. In particular, $F \in \mathcal{U}(\emptyset, \{U_x, U_y\})$. Thus there is $\mathcal{L} \in \mathrm{UD}_X(\check{r})$ in this neighborhood. Consequently, $\mathcal{L} \cap U_x$ contains a point x' while $\mathcal{L} \cap U_y$ contains a point y'. But this is a contradiction since then $x' \neq y'$ while they are both inside $\mathrm{B}(z; \check{r})$. Thus $F \in \mathrm{UD}_X(\check{r})$. □

In order to understand more concretely the Fell topology on Del, few properties will be provided here. First, if $z \in X$ and $A \subset X$ it is convenient to introduce

$$\beta(z, A) = \sup\{d_X(z, y)\,;\, y \in A\} = \mathrm{diam}(A \cup \{z\})\,, \qquad \mathrm{dist}(z, A) = \inf\{d_X(z, y)\,;\, y \in A\}\,.$$

Then if $\overline{A}$ denotes the closure of A, $\beta(z, A) = \beta(z, \overline{A})$ and similarly for $\mathrm{dist}(z, A) = \mathrm{dist}(z, \overline{A})$. It follows that $\mathrm{dist}(z, A) = 0$ if and only if $z \in \overline{A}$. Now let F, G be two closed subsets of X. Then, using the Definition 4 it can be checked that

$$\delta(F, H) = \sup_{x \in F} \mathrm{dist}(x, H)\,, \qquad d_H(F, H) = \max\{\delta(F, H), \delta(H, F)\}\,.$$

However, whenever X is locally compact, the Hausdorff metric defines a topology strictly finer than the Fell one, unless X itself is compact. But first if $R > 0$, since X is proper, the closed ball $\overline{\mathrm{B}}(z; R)$ is compact for any $z \in X$, hence $\overline{\mathrm{B}(z; R)}$ is compact as well. Thus the set $\mathcal{L} \cap \overline{\mathrm{B}(z; R)}$ is finite whenever $\mathcal{L}$ is discrete and closed. Since the corresponding open ball $\mathrm{B}(z, R)$ is open, if $\mathcal{L} \in \mathrm{Del}_X(\check{r}, \widehat{r})$, then $\mathcal{L} \cap \mathrm{B}(z; R)$ is finite and for each $x \in \mathcal{L} \cap \mathrm{B}(z; R)$, there is $\epsilon_x > 0$ such that $\mathrm{B}(x; \epsilon_x) \subset \mathrm{B}(z; R)$. Thus $\epsilon = \min\{\epsilon_x\,;\, x \in \mathcal{L} \cap \mathrm{B}(z; R)\} > 0$. Let then

$$\mathcal{W}(\mathcal{L}, \epsilon; z, R) = \{\mathcal{L}' \in \mathrm{Del}_X(\check{r}, \widehat{r})\,;\, d_H(\mathcal{L} \cap \mathrm{B}(z; R), \mathcal{L}' \cap \mathrm{B}(z; R)) < \epsilon\}$$

More intuitively, a Delone set $\mathcal{L}'$ is "close" to $\mathcal{L}$, in the sense of the $\mathcal{W}$'s above, if and only if in any "large" open ball, the elements of $\mathcal{L}'$ it contains are uniformly close to the elements of $\mathcal{L}$ in the same ball. The Hausdorff metric is such that if $\epsilon < \check{r}$ each ball $\mathrm{B}(x; \epsilon)$ with $x \in \mathcal{L} \cap \mathrm{B}(z; R)$

contains one and only one point in $\mathcal{L}'$ and no other point of $\mathcal{L}'$ are in the large ball $\mathrm{B}(z;R)$. However, at this points nothing prevents $\mathcal{L}'$ nor $\mathcal{L}$ to have points on the boundary of $\mathrm{B}(z;R)$.

Proposition 3. *The topology on* $\mathrm{Del}_X(\check{r},\widehat{r})$ *generated by the family of sets* $\mathcal{W}(\mathcal{L},\epsilon;z,R)$*, whenever* $\mathcal{L}\in\mathrm{Del}_X(\check{r},\widehat{r})$*,* $z\in X$*,* $R>0$ *and* $\epsilon>0$*, coincides with the Fell topology.*

Proof: (i) First it is shown that $\mathcal{W}(\mathcal{L},\epsilon;z,R)$ is Fell-open whenever $0<\epsilon<\check{r}$. Indeed, let $\mathcal{F}$ denotes the set of open balls $\mathrm{B}(x;\epsilon)$, with $x\in\mathcal{L}\cap\mathrm{B}(z;R)$. It is a finite set of open subsets of X, each contained in the open ball $\mathrm{B}(z;R)$ provided $\epsilon\leq\rho_x$ where ρ denotes the distance of x to the complement of $\mathrm{B}(z;R)$, each such ball containing a point in $\mathcal{L}$. In addition, since X is proper, the "large" ball $\overline{\mathrm{B}(z;R)}$ is compact. Then let $\mathcal{L}^{\epsilon}_{z,R}$ denotes the union of the balls in $\mathcal{F}$, which is open and included in $\mathrm{B}(z;R)$. So that $K=\overline{\mathrm{B}(z;R)}\setminus\mathcal{L}^{\epsilon}_{z,R}$ is compact as well and $\mathcal{L}\cap K=\emptyset$. Hence $\mathcal{U}(K,\mathcal{F})$ is a Fell neighborhood of $\mathcal{L}$. Hence $\mathcal{W}(\mathcal{L},\epsilon;z,R)=\mathcal{U}(K,\mathcal{F})$ is Fell-open.

(ii) (a) Let now $\mathcal{U}(G,\mathcal{G})$ be a Fell neighborhood of $\mathcal{L}$. Namely G is compact in X, and does not intersect $\mathcal{L}$, while $\mathcal{G}$ is a finite family of open sets each having with $\mathcal{L}$ a point in common. If $V\in\mathcal{G}$, V is open but it might be unbounded. However, if $x\in\mathcal{L}\cap V$, there is $\check{r}>\epsilon_x>0$ so that $W_V=\mathrm{B}(x;\epsilon_x)\subset V$. Consequently, if $\mathcal{G}_b=\{W_V\,;\,V\in\mathcal{G}\}$, $\mathcal{L}\in\mathcal{U}(G,\mathcal{G}_b)\subset\mathcal{U}(G,\mathcal{G})$. Hence, the Fell open sets $\mathcal{U}(G,\mathcal{G})$, with all elements of $\mathcal{G}$ bounded open, make up a basis for the Fell topology.

(ii) (b) Let $z\in X$ and let $R>0$ be chosen such that $R>\beta(z,G)$ so that $G\subset\mathrm{B}(z;R)$. By increasing R if necessary, it can be chosen so that $\beta(z,V)<R$ for $V\in\mathcal{G}$. Since V is assumed to be bounded, such a finite $R\in\mathbb{R}$ exists. Then $\mathcal{L}_{z,R}=\mathcal{L}\cap\mathrm{B}(z;R)$ is finite and does not intersect G. Thus there is $\check{r}>\epsilon>0$ such that the balls $\mathrm{B}(x;\epsilon)$, for $x\in\mathcal{L}_{z,R}$, are all included in $\mathrm{B}(z;R)$ and none intersects G. Therefore setting $\mathcal{F}=\{\mathrm{B}(x;\epsilon)\,;\,x\in\mathcal{L}(z,R)\}$ gives a finite family of open sets such that $\mathcal{L}$ intersects each of its element, and $F=\overline{\mathrm{B}}(z;R)\setminus\left(\bigcup_{x\in\mathcal{L}(y,R)}\mathrm{B}(x;\epsilon)\right)$ is compact, with $G\subset F$ and $\mathcal{L}\cap F=\emptyset$. Thus $\mathcal{L}\in\mathcal{U}(F,\mathcal{F})\subset\mathcal{U}(G,\mathcal{G})$. Now, it suffices to remark that $\mathcal{W}(\mathcal{L};\epsilon,R)=\mathcal{U}(F,\mathcal{F})$, by construction. Consequently any Fell-open set contains a $\mathcal{W}$ neighborhood of some Delone set $\mathcal{L}$. □

Proposition 4. *Let* (X,d) *denote a proper metric space with critical ratio* $\mathrm{CR}(X)$*. If its diameter is larger than* $\check{r}$*, the space* $\mathrm{Del}_X(\check{r},\mathrm{CR}(X)\check{r})$ *is not empty.*

Proof: By Definition 3 of the critical ratio, for any $\lambda>\mathrm{CR}(X)$ and any $\check{r}<\mathrm{diam}(X,d)$, the set $\mathcal{K}_\lambda=\mathrm{Del}_X(\check{r},\lambda\check{r})\neq\emptyset$. Thanks to Theorem 4 it is a Fell-compact subset of $\mathcal{C}(X)$. Moreover, if $\lambda<\mu$ then $\mathcal{K}_\lambda\subset\mathcal{K}_\mu$. It follows from the finite intersection property that $\mathcal{K}=\bigcap_{\lambda>\mathrm{CR}(X)}\mathcal{K}_\lambda$ is not empty. And clearly $\mathcal{K}=\mathrm{Del}_X(\check{r},\mathrm{CR}(X)\check{r})$, as can be checked by inspection. □

Remark 1. In the case $X=\mathbb{R}^2$, equipped with the Euclidean metric, the triangular lattice gives the densest packing of isometric disks. If the minimal distance between the disk centers is chosen to be 1, then it belongs to $\mathrm{Del}_{\mathbb{R}^2}(1,2/\sqrt{3})$. It is surmised here that $\mathrm{CR}(\mathbb{R}^2)=2/\sqrt{3}$. However it is reasonable to guess that $\mathrm{Del}_{\mathbb{R}^2}(1,2/\sqrt{3})$ contains only isometric images of this lattice, namely that $\mathrm{Del}_{\mathbb{R}^2}(1,2/\sqrt{3})$ is homeomorphic to the isometry group of $\mathbb{R}^2$, modulo the period group of this lattice. □

2.4. **Welding.** It is common in Material Science to glue together various materials like welding two pieces of metal. It always implies the matching between atomic arrangement along the separation lines of the gluing. The present Section will investigate this problem in the present mathematical setup.

These results lead to a solution of the *welding problem* for ϵ-nets. Let L and N denote two ϵ-nets in X. Given a closed set $F \subset X$ let $L_F = L \cap F$ denote the set of points of L that are contained in F. Clearly in order to weld L_F with the points of N outside, only those points in N located at least ϵ apart from L_F are needed. Therefore let $G_\epsilon = (L \cap F)^\epsilon$ denotes the union of open balls of radius ϵ centered at L_F. Then $N_F = N \setminus G_\epsilon$. Welding should start from the union of these two pieces $L_F \cup N_F$. At least this is an ϵ-separated set. Using again the Zorn Lemma, there is a maximum ϵ-separated set $L \lhd_F N$ containing $L_F \cup N_F$. This maximum element might not be unique but it is a weld.

Definition 5. *Let (X, d) be a metric space and let $F \subset X$ be a closed subset. Given two ϵ-nets L, N, a weld of L inside F with N outside is any maximal ϵ-separated set $L \lhd_F N$ containing $L_F \cup N_F$, where $L_F = L \cap F$ and N_F denotes the set of points in N at distance at least ϵ from L_F.*

Proposition 5. *Let (X, d) be a metric space and let $F \subset X$ be a closed subset. A weld of two ϵ-nets inside F is an ϵ-net.*

Proof: By construction, if L, N are ϵ-nets, any weld $L \lhd_F N$ over F is ϵ-separated. Thanks to Proposition 1 it is sufficient to prove that the open balls of radius ϵ center at the point of the weld cover the space. If not, indeed the same argument used above in proof of Proposition 1 (ii), is used to show that $L \lhd_F N$ would not be maximum. □

Remark 2. In order to extend that to other types of metric spaces, the concept of *Assouad dimension* [2, 3] might turn out to be relevant eventually. Such a dimension characterizes whether bi-Lipshitz embeddings of a metric space in some Euclidean space exist. □

Remark 3. It ought to be remarked that in order to model a liquid or a glass, physicists work in the Euclidean space $\mathbb{R}^3$. Then, they argue that the ratio $\widehat{r}/\check{r}$ ought to be smaller than or equal to $\sqrt{2}$. Indeed, if not, a configuration of 4 atoms located on the vertices of a square of size $2\check{r}$ becomes possible. But, as the argument goes, such a configuration is unstable under shear (at least in the plane). In such an argument, physicists have in mind the existence of interactions between atoms. However, if the atomic configuration is represented by a Delone set, this raises the question of whether such Delone sets exists. In the Euclidean space $\mathbb{R}^3$ the Kepler lattice which was proved to be a densest packing of balls of identical radii [51], satisfies this criterion exactly. This lattice can be built in two ways called *fcc* (face centered cubic) and *hcp* (hexagonal closed packed). The difference is only how the various layers are arranged. Metals like cobalt (hcp) and copper (hcp) choose one of these two lattices depending only upon tiny differences in the potential energy between them. Hence, geometrically they are similar. Actually both contained stable square configurations as can be seen in Fig. 2 at the very end of this review (for the hcp lattice), contradicting the standard argument. Moreover, since the Kepler lattice has densest packing [51], it questions whether Delone sets other than rescaling an isometric images of the hcp, fcc lattices with $\widehat{r}/\check{r} \leq \sqrt{2}$ do exist in $\mathbb{R}^3$. It seems likely that the $\sqrt{2}$-constraint should be relaxed to fit with the geometrical constraints of $\mathbb{R}^3$. □

Remark 4. Material scientists interested in understanding glasses and liquids have investigated such a question in a more practical way. They related the dense sphere packing in the Euclidean space to evaluating the family of possible densest atomic clusters made of one atom and its nearest neighbors, that can be found in a given solid compound [41, 77, 78]. They surmised that for monoatomic materials with hard sphere atoms the average number of neighbor is 4π, namely nearly 12. In particular a regular icosahedron could be such a cluster, apart that they cannot tiles the space. However, a slight deformation of it leads to the Kepler lattice, namely six balls on a regular hexagon surrounding the central atom in a median plane, and 3 balls on a triangle once on the upper and once on the lower level of lattice planes. Such packings are too tight to allow for atomic motion as it should in order to explain plasticity [68, 69, 70, 71]. But it explains why both the fcc and hcp are so commonly chosen for monoatomic solids. As explained in [16], this formalism is only an effective and realistic instantaneous representation of the atomic distribution of atoms in solids or liquids. The physical reality though requires to take the potential energy into account, responsible for pressure and mechanical stress, permitting to violate this model at positive temperature, but in a way that is amenable to computation [17, 18]. □

2.5. **Isometries and Delone Sets.** Since (X, d) is a metric space, there is a natural symmetry group, namely the group of isometries

Definition 6. *Let (X, d_X) and (Y, d_Y) denote a pair of metric spaces.*
(i) A map $\phi : X \to Y$ is isometric whenever it preserves the metric, namely $d_Y(\phi(x), \phi(x')) = d_X(x, x')$ for any $x, x' \in X$.
(ii) A isometric map is an isometry whenever it is onto, namely whenever $\phi(X) = Y$.
(iii) The set of isometries from X into itself is denoted by $\mathrm{Iso}(X, d_X)$ or by $\mathrm{Iso}(X)$ if there is no ambiguity on the metric.
(iv) An isometry $\phi : X \to X$ is called bounded whenever there is a finite positive real number $C > 0$ such that $d_X(x, \phi(x)) \leq C$ for all $x \in X$. The set of bounded isometries will be denoted by $\mathrm{Iso}_b(X)$.

It is clear from this definition that an isometric map is continuous and one-to-one. But it might not be onto, namely the image $\phi(X) \subset Y$ might not coincide with Y. An isometry is therefore a bijection with an isometric inverse. In addition, if both X, Y are complete, then the set $\phi(X)$ is automatically closed in Y. The set $\mathrm{Iso}(X)$ always contains the identity map of X. But in most cases it contains nothing more. So, metric spaces with a non trivial set of isometries are usually remarkable. If X is not compact, then

Proposition 6. *Let (X, d) be a complete metric space. Then*
(i) the set $\mathrm{Iso}(X)$ is a group.
(ii) The set $\mathrm{Del}_X(\check{r}, \widehat{r})$ is invariant by isometries.
(iii) The group $\mathrm{Iso}(X)$ acts by homeomorphisms on $\mathrm{Del}_X(\check{r}, \widehat{r})$.
(iv) If (X, d) is compact, then equipped with the uniform topology, $\mathrm{Iso}(X)$ is compact.
(v) If (X, d) is a proper metric space, then equipped with the uniform topology, the subspace $\mathrm{Iso}_b(X)$ of bounded isometries is also proper, thus locally compact.

Proof: (i) It is clear that the identity map is an isometry of X. If ϕ, ψ are both isometries of X, their composition $\psi \circ \phi : X \to X$ is well defined and is also an isometry. Indeed, $d(\psi(\phi(x)), \psi(\phi(x'))) = d(\phi(x), \phi(x')) = d(x, x')$. Since each isometry is invertible and its inverse is an isometry, it follows that $\mathrm{Iso}(X)$ is a group.

(ii) Let $\mathcal{L} \in \mathrm{Del}_X(\check{r}, \widehat{r})$ and let $\phi \in \mathrm{Iso}(X, d)$. Then the image $\phi(\mathcal{L})$ is a Delone set. This is because the image of an open (*resp.* closed) ball $B = \mathrm{B}(x; R)$ is any open (*resp.* closed) ball is $\phi(B) = \mathrm{B}(\phi(x); R)$ (*resp.* $\overline{\mathrm{B}}(\phi(x); R)$) as can be checked by inspection. In particular if $y_1, y_2 \in \phi(\mathcal{L}) \cap \mathrm{B}(y; \check{r})$ are two points then $x_j = \phi^{-1}(y_j)$ with $j = 1, 2$ are both in $\mathcal{L} \cap \mathrm{B}(\phi^1(y); \check{r})$ and therefore $x_1 = x_2$ so that $y_1 = y_2$. The same argument shows that, given any $y \in X$, $\phi(\mathcal{L}) \cap \overline{\mathrm{B}}(y; \widehat{r})$ is not empty. Hence $\phi(\mathcal{L}) \in \mathrm{Del}_X(\check{r}, \widehat{r})$.

(iii) It is sufficient to show that the map $\phi_* : \mathcal{L} \in \mathrm{Del}_X(\check{r}, \widehat{r}) \to \phi(\mathcal{L}) \in \mathrm{Del}_X(\check{r}, \widehat{r})$ is Fell-continuous. For indeed, $(\phi^{-1})_*$ is nothing but the inverse of ϕ_* in such a case, since $\mathrm{Del}_X(\check{r}, \widehat{r})$ is Fell-compact, the inverse ϕ_*^{-1} is also continuous. Let $K \subset X$ be compact and let $\mathcal{F}$ be a finite family of open subsets of X. Then $\mathcal{U}(K, \mathcal{F})$ be a Fell-open set. Moreover, $\phi^{-1}(K)$ is compact since ϕ is an homeomorphism of X. Similarly, if $U \in \mathcal{F}$ then $\phi^{-1}(U)$ is open in X since ϕ is continuous. Hence $\phi^{-1}(\mathcal{F}) = \{\phi^{-1}(U)\,;\, U \in \mathcal{F}\}$ is itself a finite family of open sets. Hence $\phi_*^{-1}\left(\mathcal{U}(K, \mathcal{F})\right) = \mathcal{U}(\phi^{-1}(K), \phi^{-1}(\mathcal{F}))$ as can be checked by inspection. Hence ϕ_* is Fell continuous.

(iv) Let (X, d) be compact for the metric topology. Let ϕ, ψ denote two isometries of X. Then, the map $x \in X \to d(\phi(x), \psi(x))$ is continuous, so it is bounded. The uniform distance is defined by

$$\delta_X(\phi, \psi) = \sup_{x \in X} d(\phi(x), \psi(x))\,.$$

It is easy to check by inspection that it defines a metric on $\mathrm{Iso}(X)$ which is left and right invariant by group multiplication. A standard 3-ϵ argument shows that endowed with this uniform metric, $\mathrm{Iso}(X)$ is a complete metric space. The first important remark is that $\mathrm{Iso}(X)$ is uniformly equicontinuous: indeed, given $\epsilon > 0$ then, for any pair x, y of points in X such that $d(x, y) < \epsilon$ the distance $d(\phi(x), \phi(y)) = d(x, y) < \epsilon$ for any $\phi \in \mathrm{Iso}(X, d)$. The other remark is that the set $\{\phi(x) \in X\,;\, \phi \in \mathrm{Iso}(X, d)\}$ is contained in the compact metric space (X, d) so it is bounded uniformly with respect to both $x \in X$ and $\phi \in \mathrm{Iso}(X, d)$. By the Arzelà-Ascoli Theorem, $\mathrm{Iso}(X)$ is uniformly compact.

(v) Let δ_X denote the uniform metric on $\mathrm{Iso}_b(X)$ defined as for the compact case in (iv). For $C > 0$ let $\mathcal{B}_C \subset \mathrm{Iso}_b(X)$ denote the set of isometries such that $\sup_{x \in X} d(x, \phi(x)) = \delta_X(\mathbf{1}_X, \phi) \leq C$. This is a closed ball centered at the origin of the metric group $\mathrm{Iso}_b(X)$. By similar arguments, $\mathrm{Iso}_b(X)$ is complete and since δ_X is left and right invariant by the group multiplication, any neighborhood is obtained by translation in the group from neighborhood of the identity. The closed ball $\mathcal{B}_C$ is compact. Indeed, it is equicontinuous (same argument as in (iv), in addition the set $B_x = \{\phi(x)\,;\, \phi \in \mathcal{B}_C\}$ is contained in the closed ball $\overline{\mathrm{B}}(x; C)$ in (X, d). Since (X, d) is proper, it follows that this ball is compact. Thanks to the Arzelà-Ascoli Theorem, it follows that $\mathcal{B}_C$ is compact for the uniform topology. □

3. Delone Sets in $\mathbb{R}^d$

At this point, in order to get more properties, several additional assumptions on X should be made. One is to add a locally compact group G acting by isometries on X. Another one would be to have a G-invariant positive Borel measure λ that satisfies $\lambda(\mathrm{B}(x; \rho)) = \rho^d \lambda(\mathrm{B}(x; 1))$ for some $d > 0$ and all $\rho > 0$. Such locally compact metric spaces exist, for example finite dimensional Euclidean spaces, but more singular spaces could be considered. However, at this point, in order to go forwards, in view of applications to material sciences, it is definitively simpler to consider Euclidean spaces of finite dimensions.

3.1. **Euclidean Bounded Geometry.** In what follows, $d \in \mathbb{N}$ is a natural integer and $X = \mathbb{R}^d$ will be endowed with its usual real vector space structure. In particular, $\mathbb{R}^d$ is an Abelian group for the vector addition and it acts on itself by translation. In addition, $\mathbb{R}^d$ is endowed with its usual Euclidean metric $d_E(x, y) = \|y - x\|$, where

$$\|u\| = \left(\sum_{i=1}^{d} u_i^2\right)^{1/2}, \qquad u = (u_1, \cdots, u_d) \in \mathbb{R}^d .$$

As a well-known reminder, the following properties hold:

(i) the metric space $(\mathbb{R}^d, d_E)$ is Hausdorff and proper;

(ii) the Hausdorff dimension of the metric space $(\mathbb{R}^d, d_E)$ is precisely d;

(iii) The Hausdorff measure associated with the dimension d is precisely the Lebesgue measure λ (It is coming from the fact that the volume of a rectangle is given by the product of the lengths of its sides);

(iv) the metric is translation invariant, in particular the translation group acts by isometries; consequently λ is translation invariant as well; by the Haar theorem, it follows that this measure is unique up to a normalization (which conventionally consists in giving volume 1 to the unit cube);

(v) the metric defines a norm on the vector space $\mathbb{R}^d$, so it is dilation invariant, namely for $s \in \mathbb{R}, s \geq 0$, $d_E(sx, sy) = s d_E(x, y)$. Consequently

$$\frac{\lambda(\mathrm{B}(x;R))}{\lambda(\mathrm{B}(y;r))} = \left(\frac{R}{r}\right)^d \tag{1}$$

It is worth remarking that in $\mathbb{R}^d$, as a consequence of *convexity*, a closed ball $\overline{\mathrm{B}}(z;R)$ coincides with the closure $\overline{\mathrm{B}(z;R)}$ of the corresponding open ball (this is not true in general in metric spaces). In addition, since $\mathbb{R}^d$ is separable any uniformly discrete subset is countable. In the following d_H will denote the Hausdorff metric for compact subsets of $\mathbb{R}^d$.

Warning: *In what follows, whenever there is no ambiguity on X, the notation* $\mathrm{UD}(\check{r})$ *will be used instead of* $\mathrm{UD}_X(\check{r})$*, and similarly for* $\mathrm{RD}, \mathrm{Del}$. In this Section $X = \mathbb{R}^d$.

Proposition 7. *(i) Let $\mathcal{L} \in \mathrm{UD}(\check{r})$. Then the number of points of $\mathcal{L}$ contained in a closed ball $B = \overline{\mathrm{B}}(z;R)$ is at most*

$$N = |\mathcal{L} \cap \overline{\mathrm{B}}(z;R)| \leq \left(\frac{R}{\check{r}} + 1\right)^d .$$

(ii) If in addition $\mathcal{L} \in Del(\check{r}, \widehat{r})$ then

$$\left(\frac{R}{\widehat{r}} - 1\right)^d \leq N \leq \left(\frac{R}{\check{r}} + 1\right)^d .$$

Remark 5. It is remarkable that an extension of such bounds on the number of points of a Delone set in a ball, was used by Gromov [50] to define the concept of *bounded geometry* on a non compact proper metric space. It actually addresses the question of whether or not the concept of Delone set, its topological Hull, and its C^*-algebra may be defined for proper metric spaces with bounded geometry [8]. □

Proof: (i) Since the balls $\mathrm{B}(x;\check{r})$, with $x \in \mathcal{L} \cap \overline{\mathrm{B}}(z;R)$, cannot intersect, the union of these balls are included in the ball $\mathrm{B}(z;R+\check{r})$. The volume of this union is $N\lambda\left(\overline{\mathrm{B}}(0;\check{r})\right) \leq \lambda\left(\overline{\mathrm{B}}(y;R+\check{r})\right)$ giving the upper bound thanks to eq. 1.

(ii) Assume now that any closed ball of radius at least $\widehat{r}$ contains at least one point of $\mathcal{L}$. Hence, if $R \geq \widehat{r}$ the union of the Balls $\overline{\mathrm{B}}(x;\widehat{r})$, with $x \in \mathcal{L} \cap \overline{\mathrm{B}}(z;R)$, should cover the ball $\overline{\mathrm{B}}(y;R-\widehat{r})$.

Indeed if not, there would be $y \in \overline{\mathrm{B}}(z; R - \widehat{r})$ such that $d_E(y, x) \geq \widehat{r}$ for $x \in \mathcal{L} \cap \overline{\mathrm{B}}(z; R)$. Now if $x' \in \mathcal{L} \setminus \overline{\mathrm{B}}(z; R)$, $d_E(y, x') > \widehat{r}$ as well by definition. Hence this would get $d_E(y, x) > \widehat{r}$ for all $x \in \mathcal{L}$, a contradiction. Therefore

$$N\lambda\left(\overline{\mathrm{B}}(0; \widehat{r})\right) \geq \lambda\left(\overline{\mathrm{B}}(0; R - \widehat{r})\right) ,$$

giving the lower bound thanks to eq. 1. $\square$

Definition 7. *Let $\mathcal{L}$ be a Delone set.*
(i) a patch of radius $\ell \geq 0$ is a finite set of the form $p = (\mathcal{L} - x) \cap \overline{\mathrm{B}}(0; \ell)$ for some atom $x \in \mathcal{L}$.
(ii) The set of all patches of $\mathcal{L}$ with radius ℓ will be denoted by $\mathcal{P}_\ell(\mathcal{L})$.

It follows that $\mathcal{P}_\ell(\mathcal{L})$ is a countable subset of $X = \mathcal{C}(\overline{\mathrm{B}}(0; \ell))$. Equipped with its Fell topology X is compact. Since $\overline{\mathrm{B}}(0; \ell)$ is compact, it follows that the Fell topology coincides with the Hausdorff topology induced by the Hausdorff distance.

Definition 8. *Let $\mathcal{L}$ be a Delone set. Then $\mathcal{Q}_\ell(\mathcal{L})$ will denote the Fell closure of $\mathcal{P}_\ell(\mathcal{L})$ in X. Then $(\mathcal{Q}_\ell(\mathcal{L}), d_H)$ is a compact metric separable space, called the quasi-patch space.*

Definition 9. *A Delone set $\mathcal{L}$ is called repetitive whenever for each patch p of finite radius and each $\epsilon > 0$ there is $R > 0$, depending of p and ϵ, such that in any ball of radius R, there is a point $x \in \mathcal{L}$ such that $d_H(p, (\mathcal{L} - x) \cap \overline{\mathrm{B}}(0; \ell)) < \epsilon$ where ℓ is the radius of p.*

3.2. **The Dynamical Hull and its Transversal.** Before going further, it is worth reminding that a topological dynamical system (see for instance [49] as the original reference for this topics) is a triple (Ω, G, ϕ), such that Ω is a compact Hausdorff space, G is a locally compact group and ϕ is an *action* of g on Ω. By action, it is meant a pointwise continuous group homomorphism $\phi : g \in G \to \phi_g \in \mathrm{Homeo}(\Omega)$ where $\mathrm{Homeo}(\Omega)$ is the group of homeomorphism of Ω onto itself. The pointwise continuity means that the map ϕ is continuous when seen as a function $\phi : (\omega, g) \in \Omega \times G \to \phi_g(\omega) \in \Omega$. The orbit of a point $\omega \in \Omega$, is the set $Orb(\omega) = \{\phi_g(\omega) \in \Omega\,;\, g \in G\} \subset \Omega$. The orbit closure will be called here the *Hull* namely $Hull_d(\omega) = \overline{Orb(\omega)}$. A topological dynamical system or the group action are called *topologically transitive* whenever one orbit at least is dense in Ω. A closed subset $F \subset \Omega$ is called *G-invariant* whenever the orbit of any point in F is contained in F. In particular F is compact and defines a dynamical system $(F, G, \phi\restriction_F)$. For example $Hull_d(\omega)$ is G-invariant by construction. Ordered by inclusion, and using the Zorn Lemma, it can be proved that every topological dynamical system admits *minimal* closed G-invariant subsets. Equivalently a system is minimal if and only each of its point admits a dense orbit [24, 49].

Here a specific Delone set $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ is chosen. Then, since d_E is translation invariant, it follows that $\mathbb{R}^d$ acts on itself by isometries, which are homeomorphisms. It acts as well on the set of subsets of $\mathbb{R}^d$ by

$$\mathrm{T}^a\Lambda = \Lambda + a = \{y + a\,;\, y \in \Lambda\} \qquad\qquad a \in \mathbb{R}^d ,$$

From this definition it follows immediately that $\mathrm{T}^a \circ \mathrm{T}^b = \mathrm{T}^{a+b}$ and that $\mathrm{T}^0 = \mathbf{1}$ is the identity map. In particular T^a is invertible with inverse T^{-a}. Since these are isometries, the image of a closed (*resp.* compact, open) set is closed (*resp.* compact, open). In particular it acts on $\mathcal{C}(\mathbb{R}^d)$ in such a way that the inverse image of a basic Fell-open set $\mathcal{U}(K, \mathcal{F})$ by T^a is $\mathcal{U}(K - a, \mathcal{F} - a)$. Here $\mathcal{F} - a$ denotes the set of $U - a$ for $U \in \mathcal{F}$. Thus it induces a group of homeomorphisms on the Fell-compact space $\mathcal{C}(\mathbb{R}^d)$. Similarly, the various Fell-closed subspaces $\mathrm{UD}(\check{r}), \mathrm{RD}(\widehat{r}), \mathrm{Del}(\check{r}, \widehat{r})$

are also translation invariant since their definition depends only on the metric. This leads to the following definition

Definition 10. *If* $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ *its Hull is the Fell-closure of its orbit,*

$$Hull_d(\mathcal{L}) = \overline{Orb(\mathcal{L})} = \overline{\{\mathcal{L} + a\,;\, a \in \mathbb{R}^d\}} \subset \mathrm{Del}(\check{r}, \widehat{r})\,.$$

The concept of Hull has been used under various names in many situation involving topological dynamical systems. But it was named and used to describe the electronic properties of aperiodic media in [10, 11]. It was then realized that the previous concept could be used for tilings of $\mathbb{R}^d$ [58].

It follows from the definition and from Theorem 4, that each element $\omega \in Hull_d(\mathcal{L})$ defines a unique $\mathcal{L}_\omega \in \mathrm{Del}(\check{r}, \widehat{r})$. At the notational level, it will be convenient to distinguish between ω as a point in $\Omega = Hull_d\mathcal{L}$ and the Delone set $\mathcal{L}_\omega$, even if, according to the definition of the Hull, both represent the same object. But in the first case, it is viewed just as a point in some "abstract" compact space, while in the other case this point is viewed as a Delone subset of $\mathbb{R}^d$. In this notation system the translation group acts covariantly as $\mathcal{L}_{\mathrm{T}^a\omega} = \mathcal{L}_\omega + a$. In addition, the translation group leaves the Hull invariant, so that $(Hull_d(\mathcal{L}), \mathbb{R}^d, \mathrm{T})$ defines a topological dynamical system on the compact space $Hull_d(\mathcal{L})$.

Clearly Ω is foliated by the $\mathbb{R}^d$ orbits. It is not necessarily a smooth foliation if Ω is not a manifold, but each leave is a copy of $\mathbb{R}^d$ so it can be endowed with a smooth structure.

Definition 11. *Given a Delone set* $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$*, the set of* $\xi \in Hull_d(\mathcal{L})$ *such that* $0 \in \mathcal{L}_\xi$ *is called the canonical dynamical transversal and is denoted by* $Trans_d(\mathcal{L})$*.*

Remark 6. In the literature, $Trans_d(\mathcal{L})$ is sometimes called the Hull or the discrete Hull, while $Hull_d(\mathcal{L})$ is called the continuous Hull. The transversal plays for $\mathbb{R}^d$ the role of the Poincaré section for dynamical systems on $\mathbb{R}$. The name transversal was suggested by the definition of such a concept in the groupoid theory (see for instance [35, 10, 36]). □

Proposition 8. *(i) If* $\xi \in Trans_d(\mathcal{L})$ *then* $\mathrm{T}^a\xi \neq Trans_d(\mathcal{L})$ *as long as* $\|a\| < \check{r}$*. Hence* $Trans_d(\mathcal{L})$ *is transverse to all orbits within* $Hull_d(\mathcal{L})$*.*
(ii) $Trans_d(\mathcal{L})$ *is a closed and compact subset of its Hull.*

Proof: (i) Let $\xi \in Trans_d(\mathcal{L})$. Then the Delone set $\mathcal{L}_\xi$ contains the origin. Therefore is $\|a\| < \check{r}$, the open ball $\mathrm{B}(0; \check{r})$ contains the point $a \in \mathcal{L}_{\mathrm{T}^a\xi} = \mathcal{L}_\xi + a$. Since $\mathcal{L}_\xi$ is a Delone set it follows that no other point in this ball can belong to $\mathcal{L}_\xi + a$, in particular $0 \notin \mathcal{L}_\xi + a$, namely $\mathrm{T}^a\xi \notin Trans_d(\mathcal{L})$.

(ii) Let $\xi \in \overline{Trans_d(\mathcal{L})}$. If ξ were not in $Trans_d(\mathcal{L})$ then $0 \notin \mathcal{L}_\xi$. Since $\mathcal{L}_\xi$ is a Delone set, it is a closed subset of $\mathbb{R}^d$ (see Lemma 1). Hence the distance ρ from 0 to $\mathcal{L}_\xi$ is positive, $\rho > 0$. Given any $0 < \epsilon < \rho$, it follows that $\overline{\mathrm{B}}(0; \epsilon) \cap \mathcal{L}_\xi = \emptyset$. Let then $\mathcal{U}_\epsilon = \mathcal{U}(\overline{\mathrm{B}}(0; \epsilon), \emptyset)$. It is a Fell open set that contains $\mathcal{L}_\xi$. Since $\mathcal{L}_\xi$ belongs to the closure of $Trans_d(\mathcal{L})$, $\mathcal{U}_\epsilon$ must contains an element $\omega \in Trans_d(\mathcal{L})$. But this is a contradiction since it would implies $0 \in \mathcal{L}_\omega \cap \overline{\mathrm{B}}(0; \epsilon) = \emptyset$. □

The following Theorem uses the concept of minimality, the terminology of which was fixed in [24] for dynamical systems. Its relation with what is called repetitivity here, was understood early in the context of dynamical systems by Gottschalk [48] under the name of weak almost periodicity. It was formulated in a way closer to the language of Delone sets in the context of substitutions [82], and later in the context of Ergodic Theory [83]. Its extension to Delone sets, through tiling were proposed later by various author. For a partial review, centered on tilings, see [47], for instance and references therein. A full proof is provided for the sake of clarity.

Theorem 5. *The compact set $Hull_d(\mathcal{L})$ is always topologically transitive. In addition the dynamical system $(Hull_d(\mathcal{L}), \mathbb{R}^d)$ is minimal if and only if $\mathcal{L}$ is repetitive.*

Proof: (i) by construction the orbit of $\mathcal{L}$ is dense in $Hull_d(\mathcal{L})$, making the Hull topologically transitive.

(ii) Let assume $\mathcal{L}$ is not repetitive. Then, using Definition 9, there is $\ell \geq 0$, a patch $p \in \mathcal{P}_\ell(\mathcal{L})$ and some $\eta > 0$ such that, for any $R > 0$ there is a closed ball $\overline{\mathrm{B}}_R$ of radius R, such that for any $z_R \in \mathcal{L} \cap \overline{\mathrm{B}}_R$, $d_H\left((\mathcal{L} - z_R) \cap \overline{\mathrm{B}}(0;\ell), p\right) \geq \eta$.

(a) Let $x_p \in \mathcal{L}$ be such that $p = (\mathcal{L} - x_p) \cap \overline{\mathrm{B}}(0;\ell)$. Since p is finite, let $\ell_p = \max\{d_E(0,y)\,;\, y \in p\}$. In addition, any other point in $\mathcal{L} - x_p$ outside the ball $\overline{\mathrm{B}}(0;\ell_p)$ are at a minimal distance ℓ^p from the origin so that $\ell_p < \ell^p$. Let $0 < \delta \leq \min\{\eta, \check{r}\}$ be chosen so that $\delta < \ell^p - \ell_p$. Then for any $y \in p$ let $U_y = \mathrm{B}(y;\delta/2)$. This is an open ball and the family $\mathcal{F} = \{U_y\,;\, y \in p\}$ is a finite family of open balls. In addition each such ball is contained in the closed ball $\overline{\mathrm{B}}(0;\ell_p + \delta)$. Consequently, the complement K of these balls in $\overline{\mathrm{B}}(0;\ell_p + \delta)$ is compact and $(\mathcal{L} - x_p) \cap K = \emptyset$. In addition, $(\mathcal{L} - x_p) \cap U_y$ contains exactly one point of p, namely y, since $\delta \leq \check{r}$. This means $\mathcal{L} - x_p \in \mathcal{U}(K, \mathcal{F})$. It is worth remarking that, by definition, any patch contains the origin $0 \in \mathbb{R}^d$, so that U_0 is among the open balls in $\mathcal{F}$.

(b) Let now $\omega \in Hull_d(\mathcal{L})$ belong to the closure of the family $\mathcal{L} - z_R$ as defined above. Then since $\mathcal{L}$ is not repetitive, it follows that the orbit of ω cannot be dense. For if it were, there would be an $z_\omega \in \mathbb{R}^d$ such that $\mathcal{L}_\omega - z_\omega \in \mathcal{U}(K, \mathcal{F})$. If so, it would mean that $(\mathcal{L}_\omega - z_\omega) \cap K = \emptyset$ while $(\mathcal{L}_\omega - z_\omega) \cap U_y \neq \emptyset$ for all $y \in p$. Again, since $\omega \in \mathrm{Del}(\check{r}, \widehat{r})$, there is exactly one point of $(\mathcal{L}_\omega - z_\omega)$ in each ball U_y. In particular $\mathcal{L}_\omega - z_\omega$ contains exactly one point x_ω in the ball $U_0 = \mathrm{B}(0;\delta/2)$. Thus $\mathcal{L}_\omega - z_\omega - x_\omega$ contains the origin. On the other hand, the intersection of the ball $\overline{\mathrm{B}}(0;\ell_p + \delta)$ with its translated by $\pm x_\omega$ contains the ball $\overline{\mathrm{B}}(0;\ell_p + \delta/2)$. Hence $q = (\mathcal{L}_\omega - z_\omega - x_\omega) \cap \overline{\mathrm{B}}(0, \ell_p + \delta/2)$ is a patch of $\mathcal{L}_\omega$ with radius $\ell_p + \delta/2$ such that $d_H(p,q) < \delta/2 < \eta$, a contradiction. Hence the orbit of ω cannot be dense, so that $(Hull_d(\mathcal{L}), \mathbb{R}^d, \mathrm{T})$ is not a minimal dynamical system.

(iii) Conversely, let $\mathcal{L}$ be repetitive. Let ω, ξ be two points in $\Omega = Hull_d(\mathcal{L})$. The goal is to prove that the orbit of ω is dense, namely, given any Fell open neighborhood $\mathcal{W}$ of ξ, there is a point $\mathrm{T}^b\omega \in \mathcal{W}$.

(iii-a) By construction of the Fell topology, it is sufficient to choose $\mathcal{W}$ of the form $\mathcal{U}(K, \mathcal{F})$. Here K is a compact subset of $\mathbb{R}^d$ and $\mathcal{F}$ is a finite family of open subsets of $\mathbb{R}^d$. If $\mathcal{L}' \in \mathcal{U}(K, \mathcal{F}) \subset \mathrm{Del}(\check{r}, \widehat{r})$, it follows that for any $U \in \mathcal{F}$, there is a point $x_U \in \mathcal{L}_\xi \cap U$. Moreover since K is compact there is a positive real number ℓ large enough so that, given any $x_0 \in \mathcal{L}'$, the set K and the family $\{x_u\,;\, U \in \mathcal{F}\}$ are included in the open ball $\mathrm{B}(x_0;\ell)$. Let then $q_0 = \mathcal{L}' \cap \overline{\mathrm{B}}(x_0;\ell)$. Here, by changing ℓ a bit if necessary, it can be assumed that no $y \in q$ belongs to the boundary of the closed ball. By hypothesis q is a finite set with none of his points in K. In addition, the points x_U's are all in q. Therefore there is $\epsilon > 0$ such that $\epsilon < \check{r}$ and that, for any $y \in q$, each open ball $V_y = \mathrm{B}(y;\epsilon) \subset \overline{\mathrm{B}}(x_0;\ell)$, and $V_y \cap K = \emptyset$. By construction, thanks to the Delone property, y is the only point in V_y. Let then $\mathcal{F}' = \{V_y\,;\, y \in q\}$. Moreover let $K' = \overline{\mathrm{B}}(x_0;\ell) \setminus \bigcup_{y \in q} V_y$. Then $K \subset K'$ and are compact subset of $\mathbb{R}^d$ and $\mathcal{L}' \in \mathcal{U}(K', \mathcal{F}') \subset \mathcal{U}(K, \mathcal{F}) \subset \mathcal{W}$. Let $\mathcal{V}(\mathcal{L}', x_0, ; \ell, \epsilon)$ denote the Fell open set $\mathcal{U}(K', \mathcal{F}')$, constructed here, a neighborhood of $\mathcal{L}'$ contained in $\mathcal{W}$.

(iii-b) Following the previous construction, let $\mathcal{W}_\xi$ be a Fell open neighborhood of ξ. Then, let $\ell > 0$ and let $\epsilon > 0$ be chosen such as to define $\mathcal{V}(\xi, x_\xi; \ell, \delta) \subset \mathcal{V}(\xi, x_\xi; \ell, \epsilon) \subset \mathcal{W}_\xi$ where ξ

denotes actually $\mathcal{L}_\xi$ and $0 < \delta < \epsilon$ be chosen. Since the orbit of $\mathcal{L}$ is dense in Ω, there is $a_\xi \in \mathbb{R}^d$ such that $\mathcal{L} + a_\xi \in \mathcal{V}(\xi, x_\xi; \ell, \delta)$. By construction $p_\xi = (\mathcal{L} + a_\xi) \cap \overline{\mathrm{B}}(0;\ell))$ contains a point in each ball $U_y = \mathrm{B}(y;\delta)$ for $y \in q_\xi$, and this point is unique by the Delone property, while it has no other point in $\overline{\mathrm{B}}(x_\xi;\ell)$. Equivalently $d_H(p_\xi, q_\xi) < \delta < \check{r}$. In particular there is a unique point $z_\xi \in \mathcal{L} + a_\xi$ at distance less than δ from x_ξ. Thus $p_\xi - z_\xi - a_\xi = p \in \mathcal{P}_\ell(\mathcal{L})$ is a patch of $\mathcal{L}$ of radius ℓ.

(iii-c) Thanks to the repetitive character of $\mathcal{L}$, for any $\eta > 0$ there is $R_p > 0$ (large enough) such that in the ball $\mathrm{B}(x_\xi; R_p)$ there is a point of $x_p \in \mathcal{L}$ such that $p_\xi = (\mathcal{L} - x_p) \cap \overline{\mathrm{B}}(0;\ell))$, which is a patch of $\mathcal{L}$ of radius ℓ, satisfies $d_H(p, p_\xi) < \eta$. In particular the finite set $p_\xi + x_p$ is contained in the ball $\overline{\mathrm{B}}(x_\xi; R)$ for any $R > R_p + \ell$. Therefore, the Delone set $\mathcal{L} + x_\xi - x_p \in \mathcal{V}(\xi, x_\xi; \ell, \eta)$. In particular if $\eta < \delta$ then $\mathcal{V}(\xi, x_\xi; \ell, \eta) \subset \mathcal{V}(\xi, x_\xi; \ell, \delta)$.

(iii-d) Using the previous constructions with $\eta < \delta$, if $x_\omega \in \mathcal{L}_\omega$, let $\mathcal{V}(\omega, x_\omega; R, \eta)$ be the corresponding Fell open neighborhood of $\mathcal{L}_\omega$ where $R > R_p + \ell$. Then there is a point $a_\omega \in \mathbb{R}^d$ such that $\mathcal{L} + a_\omega \in \mathcal{V}(\omega, x_\omega; R, \eta)$, since the orbit of $\mathcal{L}$ is dense in Ω. In addition, there is $x_p \in (\mathcal{L} + a_\omega) \cap \overline{\mathrm{B}}(x_\omega; R_p)$ such that $p_\omega = (\mathcal{L} + a_\omega - x_p) \cap \overline{\mathrm{B}}(0;\ell)$ is a patch of $\mathcal{L}$ of radius ℓ with $d_H(p, p_\omega) < \eta$. By construction it follows that there is a unique $y_\omega \in \mathcal{L}_\omega$ such that $d_E(x_p, y_\omega) < \eta$. Therefore $q_\omega = (\mathcal{L}_\omega - y_\omega + x_\xi) \cap \overline{\mathrm{B}}(x_\xi;\ell)$ satisfies $d_H(q_\omega, q_\xi) < d_H(q_\omega, p + x_\xi) + d_H(p + x_\xi, q_\xi) < \eta + \delta$. If $\eta < \delta$ are chosen so that $\eta + \delta < \epsilon < \check{r}$ then this implies $(\mathcal{L}_\omega - y_\omega + x_\xi) \in \mathcal{V}(\xi, x_\xi; \ell, \eta + \delta) \subset \mathcal{V}(\xi, x_\xi; \ell, \epsilon) \subset \mathcal{W}$. In particular, since $\xi, x_\xi, \mathcal{W}$ are arbitrary, it follows that ω has a dense orbit. $\Box$

3.3. **Finite Local Complexity, Topological Hull.**

Definition 12. *(i) A Delone set $\mathcal{L}$ has* finite type *or* finite local complexity *(FLC) whenever the set of vectors $\mathcal{L} - \mathcal{L} = \{x - y\,;\, x, y \in \mathcal{L}\}$ is a discrete in $\mathbb{R}^d$ and closed (no accumulation points).*
(ii) A Meyer set *is an FLC Delone set $\mathcal{L}$ such that $\mathcal{L} - \mathcal{L}$ is Delone.*
(iii) The (free) Abelian group generated by $\mathcal{L} - \mathcal{L}$ is called the Lagarias group of $\mathcal{L}$ and will be denoted by $\mathbb{L}_{\mathcal{L}}$ or $\mathbb{L}$ if there is no ambiguity.

Meyer sets were defined in Meyer [73, 74] in the context of Harmonic Analysis and Number Theory. He developed a definition called *model sets* nowadays [75, 60, 79, 80] characterized by the pure point nature of the Fourier transform of the sum of Dirac measures on points of $\mathcal{L}$ (Poisson formula). It was realized after the discovery of quasicrystals [92], that Meyer's work was exactly the concept required to describe quasicrystals, exhibiting a point-like diffraction pattern. Lagarias [60, 61, 62, 63] introduced the language of Delone set unifying tiling theory, the so-called *cut-and-project* method also called *model sets*, the Meyer approach of Meyer sets through harmonic analysis. He defined the group called here the Lagarias group and showed that all FLC Delone sets have a finitely generated such group (see Theorem 6 (ii) below)). It seems that the converse should be true, opening the way to a classification of FLC tilings having a given Lagarias group.

The following results summarize the characteristics of FLC Delone sets

Theorem 6 (Dynamical and Topological Hulls coincide)**.** *Let $\mathcal{L} \in \mathrm{Del}(\check{r}, \hat{r})$ be FLC. Then*
(i) for any $\ell \geq 0$ its set $\mathcal{P}_\ell(\mathcal{L})$ of patches of radius ℓ is finite.
(ii) The Lagarias group is a finitely generated free Abelian group. If N is its rank, it is isomorphic to $\mathbb{Z}^N$.

(iii) In addition, its canonical dynamical transversal is completely disconnected and can be identified modulo homeomorphism with the canonical topological transversal defined as the inverse limit $Trans_t = \lim_{\leftarrow}(\mathcal{P}_\ell, \pi)$ *where* $\pi : \mathcal{P}_{\ell'}(\mathcal{L}) \to \mathcal{P}_\ell(\mathcal{L})$ *is the restriction map* $\pi(p') = p' \cap \overline{\mathrm{B}}(0;\ell)$ *for* $\ell' \geq \ell$.

Remark 7. The statement (i) and its proof can be found in [61]. The proof that the transversal of FLC Delone sets is completely disconnected can be found in [58]. The equivalence of topological and dynamical Hull was known from the earliest times of the quasicrystal era in the mid 1980's. The formal proof for Meyer sets or model sets, can be found in [89]. The adjustment to FLC was an exercice (see for instance [86]). □

Definition 13. *Let* $\mathcal{L}$ *be an FLC Delone set. Then*
(i) Its topological Hull is the set $Hull_t(\mathcal{L})$ *defined, modulo homeomorphism, as the closure of the union of translated of the topological transversal, namely as the set of all Delone sets sharing with* $\mathcal{L}$ *the family of all its patches.*
(ii) The symbol $Hull(\mathcal{L})$ *(*resp. *$Trans(\mathcal{L})$) will denote both the dynamical and topological Hull (*resp. *transversal)$Trans(\mathcal{L})$) of* $\mathcal{L}$.

Proof of Theorem 6: (i) Given $\ell \geq 0$ (thus finite), and given any $x \in \mathcal{L}$ the set of vectors $\{y - x\,;\, y \in \mathcal{L}, d_E(x, y) \leq \ell\}$ belong to the set $\mathcal{E}_\ell = (\mathcal{L} - \mathcal{L}) \cap \overline{\mathrm{B}}(0;\ell)$. Since $\mathcal{L} - \mathcal{L}$ is closed discrete, $\mathcal{E}_\ell$ is finite. Then the set of such patches is a set of subsets of $\mathcal{E}_\ell$ and so it is finite.

(ii) Given any pair of atoms $x, y \in \mathcal{L}$, the segment joining them is the sets $[x, y] = \{z_t \in \mathbb{R}^d\,;\, \exists\, 0 \leq t \leq 1\,,\, z_t = ty+(1-t)x\}$. Clearly this segment is compact as the continuous image of the interval $[0, 1] \subset \mathbb{R}$. It is covered by the balls $\mathrm{B}(z_t;\widehat{r})$, so it is possible to extract a finite subcover by balls $B_i = \mathrm{B}(z_i;\widehat{r})$ where $z_i = z_{t_i}$ and $t_0 = 0 < t_1 < \cdots < t_{n-1} < t_n = 1$. If two such balls intersect, their center are less than $2\widehat{r}$ apart. By definition of a Delone set, it is relative dense, so that the closure of each such ball contains at least one point $x_i \in \mathcal{L}$. The distance between two consecutive point satisfies $d_E(x_i, x_{i+1}) \leq d_E(x_i, z_i) + d_E(z_i, z_{i+1}) + d_E(z_{i+1}, x_{i+1}) < 4\widehat{r}$. Thus the vectors $u_i = x_i - x_{i-1}$ belongs to the set $\mathcal{E}_{4\widehat{r}}$ thus to a finite set and $y - x = u_1 + \cdots + u_n$. By definition, the vectors of the form $y - x$ with $x, y \in \mathcal{L}$ generate the Lagarias group so that the finite set $\mathcal{E}_{4\widehat{r}}$ generates it. Since any subgroup of the additive group $\mathbb{R}^d$ is free Abelian (see for instance [67], Chap. 1.8), there is a unique integer N such that $\mathbb{L}_{\mathcal{L}}$ is isomorphic to $\mathbb{Z}^N$.

(iii) Since $\mathcal{L}-\mathcal{L}$ is closed and discrete, it follows that the countable set $\mathcal{L} = \{d_E(x, y) = d_E(0, y-x)\,;\, x, y \in \mathcal{L}\}$ is actually discrete and contained in $[0,\infty)$. This is because the subset $\mathcal{L} \cap [0, \ell]$ is finite for any $0 \leq \ell < \infty$ by (i). In particular denoting $\lambda(p) = \max\{d_E(0, y)\,;\, y \in p\} \subset \mathcal{L} \cap [O, \ell]$ for $p \in \mathcal{P}_\ell(\mathcal{L})$. Therefore $\ell_m = \max\{\lambda(p)\,;\, p \in \mathcal{P}_\ell(\mathcal{L})\} \in \mathcal{L} \cap [O, \ell]$. In particular given $\ell \geq 0$ there are $\ell_m \leq \ell < \ell^m$ where $\ell_m, \ell^m \in \mathcal{L}$ such that $\mathcal{P}_{\ell_m}(\mathcal{L}) = \mathcal{P}_\ell(\mathcal{L}) \neq \mathcal{P}_{\ell^m}$. This implies the existence of an increasing sequence $(\ell_n)_{n\in\mathbb{N}}$ with $\ell_0 = 0$, such that $\ell_n \to \infty$ as $n \to \infty$ and that if $\mathcal{P}_n$ denotes $\mathcal{P}_{\ell_n}(\mathcal{L})$ any patch of $\mathcal{L}$ belongs to one of the $\mathcal{P}_n$'s. In particular the infinite product space $\prod_{n\in\mathbb{N}} \mathcal{P}_n$ is compact and completely disconnected. Then the restriction map is defined by the maps $\pi_n : \mathcal{P}_{n+1} \to \mathcal{P}_n$ defined by $p \in \mathcal{P}_{n+1} \Rightarrow \pi_n(p) = p \cap \overline{\mathrm{B}}(0;\ell_n) \in \mathcal{P}_n$. By definition, π_n is onto. Then, the inverse limit $\Xi = \lim_{\leftarrow}(\mathcal{P}_n, \pi_n)$ is defined as the subset of $\prod_{n\in\mathbb{N}} \mathcal{P}_n$ made of sequences $(p_n)_{n\in\mathbb{N}}$ such that $\pi_n(p_{n+1}) = p_n$. Such sequences are called *compatible*. In particular Ξ is closed thus compact and completely disconnected as well.

(iv) That there is an homeomorphism between Ξ and $Trans_d(\mathcal{L})$ goes as follows. Given a compatible sequence $\xi = (p_n)_{n\in\mathbb{N}}$ of patches of $\mathcal{L}$, each patch being a finite subset of $\mathbb{R}^d$ containing the origin, the union $\mathcal{L}_\xi = \bigcup_{n\in\mathbb{N}} p_n$ is a discrete subset of $\mathbb{R}^d$, containing the origin, which is closed as well, since its restriction to any ball centered at the origin is one of the p_n's. By construction in any open ball $\mathrm{B}(z;\check{r})$, with $z \in \mathbb{R}^d$, there is at most one point of $\mathcal{L}_\xi$ since this is already true for any patch. Moreover given any closed ball $\overline{\mathrm{B}}(z;\widehat{r})$ there is $n \in \mathbb{N}$ such that $\overline{\mathrm{B}}(z;\widehat{r}) \subset \mathrm{B}(0;\ell_n) \subset \overline{\mathrm{B}}(0;\ell_n)$. Therefore its intersection with $\mathcal{L}_\xi$ coincides with its intersection with p_n which, by construction contains at least one point. Therefore $\mathcal{L}_\xi \in \mathrm{Del}(\check{r},\widehat{r})$. In addition, by the same argument $\mathcal{L}_\xi - \mathcal{L}_\xi \subset \mathcal{L} - \mathcal{L}$. In particular any patch in $\mathcal{L}_\xi$ is a patch of $\mathcal{L}$. At last, for each $n \in \mathbb{N}$ there is $x_n \in \mathcal{L}$ such that $p_n = (\mathcal{L} - x_n) \cap \overline{\mathrm{B}}(0;\ell_n)$. In particular $\lim_{n\to\infty} \mathrm{T}^{-x_n}\mathcal{L} = \mathcal{L}_\xi$. Therefore, denoting by $\phi(\xi)$ the corresponding point of the Hull, $\phi(\xi) \in \mathit{Trans}_d(\mathcal{L})$ since $\mathcal{L}_\xi$ contains the origin. By definition of Ξ, if $\xi = (p_n)_{n\in\mathbb{N}}, \eta = (q_n)_{n\in\mathbb{N}}$ are close in the product topology means that there is an $n \in \mathbb{N}$ such that $p_m = q_m$ for $m \leq n$. Thus $\mathcal{L}_\xi \cap \overline{\mathrm{B}}(0;\ell_n) = \mathcal{L}_\eta \cap \overline{\mathrm{B}}(0;\ell_n)$, namely both Delone set are close to each other in the Fell topology. Thus ϕ is continuous. In particular, since Ξ is compact, this map is proper. By construction it is one-to-one as can be checked by inspection. It remains to prove that it is invertible. Given $\omega \in \mathit{Trans}_d(\mathcal{L})$, the Delone set $\mathcal{L}_\omega$ can be approximated in the Fell topology by a translated $\mathcal{L}-z$ for some $z \in \mathbb{R}^d$. Using the arguments used in Section 3.2, there is no loss of generality in assuming that $z \in \mathcal{L}$ and then for any $R > 0$ and $\epsilon > 0$ there is such a $z \in \mathcal{L}$ for which the Hausdorff distance $d_H\left(\mathcal{L}_\omega \cap \overline{\mathrm{B}}(0;R)\,,\,(\mathcal{L}-z) \cap \overline{\mathrm{B}}(0;R)\right) < \epsilon$. In particular, choosing $\epsilon = \epsilon_k = \check{r}/(k+1)$, with $k \in \mathbb{N}$, leads to a sequence $z_k \in \mathbb{R}^d$ so that the family $p_k = (\mathcal{L} - z_k) \cap \overline{\mathrm{B}}(0;R)$ is stationary, namely $p_k = p_1$ implying that the Fell limit $\mathcal{L}_\omega \cap \overline{\mathrm{B}}(0;R) = p_1$. Consequently, in each ball centered at the origin, $\mathcal{L}_\omega$ coincides with some patch of $\mathcal{L}$. In particular choosing $\ell_n \leq R < \ell_{n+1}$ implies that this patch is $p_n \in \mathcal{P}_n$. This sequence of patches is compatible under the restriction map. Therefore it follows that there is $\xi \in \Xi$ such that $\mathcal{L}_\omega = \mathcal{L}_\xi$, namely $\omega = \phi(\xi)$, showing ϕ is onto. Since ϕ is one-to-one, onto, continuous and proper, its inverse is continuous so that ϕ is an homeomorphism. □

Definition 14. *Let $\mathcal{L}$ be an FLC Delone set with Lagarias group $\mathbb{L}_\mathcal{L}$. If $\mathbb{L}_\mathcal{L}$ has rank N an address map is any group isomorphism $\phi : \mathbb{L}_\mathcal{L} \to \mathbb{Z}^N$.*

When an address map is restricted to $\mathcal{L} \subset \mathcal{L} - \mathcal{L} \subset \mathbb{L}_\mathcal{L}$ the image of $\mathcal{L}$ is a subset of $\mathbb{Z}^N$ the shape of which is unknown yet. This lead to the following open problem

Problem 1. Classify all FLC Delone set with Lagarias group of rank $N > d$ modulo an address map. □

4. Voronoi Tesselation and Bernal Graph

In 1908, Voronoi, then a Professor at Warsaw, published two articles on quadratic forms [98, 99], leading to the concept of Voronoi tessellation. And Voronoi passed away the same year. In 1934 Delaunay (Delone) published another work [38] in memory of Voronoi, where he considered a distribution of atoms, represented by what was called here a Delone set. He focussed his paper on the size of balls in the space, which are empty of atoms. From then was derived the concept of *Delaunay triangulation*. Finally, in the late 1950's, J.D. Bernal [20], an expert of X-ray crystallography who developed the technique to investigate biological molecules in the 1930's, published, at the end of his career, a series of papers [21, 22, 23] in which he rediscovered the Voronoi and Delone constructions with no knowledge of these earlier references, obviously, and adding to it a graph construction in order to describe the structure of the atomic arrangement in a liquid and the nature of their interaction using the graph edges to represent them. These structures actually were already guessed earlier, as Bernal remind his readers in [23], and these ideas are still in the mind of many experts today. The author of this review indeed used this construction spontaneously after Takeshi Egami had explained him what he thought being important to understand the atomic structure of liquid and glasses, as well as the nature of the forces between atoms that should be essential to understand the dynamics and the macroscopic consequences. This is actually why the author proposes to assign the name of Bernal to these graphs, which will be the case in this review.

In this Section, these mathematical concepts will be described in detail. They can be considered as a convenient way of encoding the information contained in the atomic distribution. However, while it would be possible to define many of the concepts used in this Section in a much larger class of metric spaces, some of the results obtained by Voronoi, Delone, and Bernal, require this space to be Euclidean and equipped with the Euclidean metric d_E. In particular the concept of convexity plays a role in the three authors construction. In order to generalize these constructions to complete metric spaces, the Bernal graph must be extended to a looser concept of nearest neighbor, which still catch the essence of the idea, but are not as precise when it comes to study real materials in the common space.

For instance the following reminder will be useful

Lemma 3. *Let x, y be two distinct points in the Euclidean metric space $(\mathbb{R}^d, d_E)$. Then*
(i) the set $H_{x,y}$ made of points $z \in \mathbb{R}^d$ at equal distance from both x and y is the affine hyperplane perpendicular to $y - x$ and passing through $(x + y)/2$.
(ii) The set $H_x(y)$ of points in $\mathbb{R}^d$ located at a shorter distance from x than from y is the open half-space bounded by $H_{x,y}$ and containing x. This open set is convex. Its closure is $\overline{H_x(y)} = H_x(y) \cup H_{x,y}$ and $H_{x,y}$ is a face.

Proof: Let $f : \mathbb{R}^d \to \mathbb{R}_+$ be defined by $2f(z) = \|y - z\|^2 - \|x - z\|^2$. Then, the equation defining $H_{x,y}$ is $f(z) = 0$ while $H_x(y)$ is defined by $f(z) > 0$. Since this function is continuous, it follows that $H_x(y)$ is open while $H_{x,y}$ is closed and it proves that the closure of $H_x(y)$ is obtained by adding $H_{x,y}$. Moreover, a simple algebra gives $f(z) = \|y - x\|^2/2 - \langle z - x|y - x\rangle = \langle (x + y)/2 - z|y - x\rangle$. In particular $f(z) = 0$ if and only if the vector $\zeta = z - (x + y)/2$ is perpendicular to $y - x$ proving (i). In addition, $z_0, z_1 \in H_x(y)$ if and only if, for $i = 0, 1$, $f(z_i) > 0$, namely if and only if $\|y - x\|^2/2 > \langle z_i - x|y - x\rangle$. Then for any $0 \leq s \leq 1$ the point $z_s = sz_1 + (1 - s)z_0$ satisfies $\langle z_s - x|y - x\rangle = s\langle z_1 - x|y - x\rangle = (1 - s)\langle z_0 - x|y - x\rangle < \|y - x\|^2/2$ proving that $z_s \in H_x(y)$. Namely $H_x(y)$ is convex open. At last, this argument shows that if $z \in H_{x,y}$ is a convex combination of two points z_0, z_1 in $\overline{H_x(y)}$, one of these points, at least, must belong to $H_{x,y}$. If one of them, say z_0, is not in the hyperplane then z_s can be in $H_{x,y}$ only if $s = 1$ and $z = z_1$. □

4.1. **The Voronoi Tesselation.**

In this Section, a specific Delone set $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ will be chosen.

Definition 15. *Let $x \in \mathcal{L}$: (i) its Voronoi cell is the open set of points in $\mathbb{R}^d$ closer to x than to any other atom in $\mathcal{L}$. (ii) its Voronoi tile T_x is the closure of its Voroinoi cell.*

Out of the most important result of Voronoi the following can be drawn

Theorem 7 ([98, 99])**.** *Given any atom x in $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$, its Voronoi tile T_x is a convex polyhedron, contained in the ball $\overline{\mathrm{B}}(x; \widehat{r})$. Its Voronoi cell V_x contains the open ball $\mathrm{B}(x; \check{r})$.*

Proof: (i) given two atoms $x, y \in \mathcal{L}$, and using the notations and the results of Lemma 3, the half-spaces $H_x(y)$ containing x and bounded by $H_{x,y}$ is open and convex. By construction $V_x = \bigcap_{y \in \mathcal{L}; y \neq x} H_x(y)$ is convex. Similarly $T_x = \bigcap_{y \in \mathcal{L}; y \neq x} \overline{H_x(y)}$ is both closed and convex.

(ii) If now $z \in T_x$. By definition, the closed ball $\overline{\mathrm{B}}(z;\hat{r})$ contains at least one atom say $y \in \mathcal{L}$. This implies $d_E(x,z) \leq d_E(y,z) \leq \hat{r}$. Hence the closed ball $\overline{\mathrm{B}}(x;\hat{r})$ contains T_x. This implies that if z is at equal distance from both x and y, then $d_E(x,y) \leq 2\hat{r}$. In particular only a finite number of such atoms contribute to the building of T_x since a closed ball is compact and $\mathcal{L}$ is discrete. Consequently, the intersection $\bigcap_{y\in\mathcal{L};y\neq x} \overline{H_x(y)}$ is reduced to a finite number of half-spaces so it is a convex polyhedron. Therefore $V_x = \bigcap_{y\in\mathcal{L};y\neq x} H_x(y)$ is open and convex as a finite intersection of open half spaces.

(iii) Let now $z \in \mathbb{R}^d \backslash V_x$. If it were belonging to the open ball $\mathrm{B}(x;\check{r})$ then there would be another atom $y \in \mathcal{L}$ and $y \neq x$ from which z is closer to than to x namely $d_E(z,y) \leq d_E(z,x) < \check{r}$. That would imply that both atoms x and y would belong to the open ball $\mathrm{B}(z;\check{r})$, a contradiction. Hence $\mathrm{B}(x;\check{r}) \subset V_x$. $\Box$

Theorem 8 ([98, 99])**.** *The family of all Voronoi tiles covers the space $\mathbb{R}^d$. Moreover two distinct Voronoi cells do not intersect. At last, if two tiles intersect, their intersection is a face of each of them (they touch face-to-face). In particular, the Voronoi tiles makes a tessellation or a tiling of $\mathbb{R}^d$ by convex polyhedra.*

Proof: (i) If $z \in \mathbb{R}^d$, then there is at least one atom of $\mathcal{L}$ within the closed ball $\overline{\mathrm{B}}(z;\hat{r})$. Since $\mathcal{L}$ is discrete, such atoms can only be in finite number. Then one at least, say x is closer to z than the other. Therefore $z \in T_x$. Hence the Voronoi tiles cover the space.

(ii) Let $x \neq y$ be two distinct points in $\mathcal{L}$. If $z \in V_x \cap V_y$ then by definition of V_x, $d_E(z,x) < d_E(z,y)$ and by definition of V_y, $d_E(z,y) < d_E(z,x)$, a contradiction. Consequently $V_x \cap V_y = \emptyset$.

(iii) Since two distinct Voronoi cells do not intersect, if $F = T_x \cap T_y \neq \emptyset$ then F is made of boundary points of both cells and $F \subset H_{x,y}$. Either F is reduced to one point and it is indeed a face. Or if not, there are $z_0 \neq z_1$ in F. By convexity of T_x and of T_y it follows that any point $z_s = (1-s)z_0 + sz_1$ if $0 \leq s \leq 1$ belong to both T_x and T_y thus to F. Hence F is convex. To prove that it is a face, let $z \in F$ be a convex combination of two points $z_0, z_1 \in T_x$. Then there is $0 \leq s \leq 1$ such that $z = z_s \in F$. If both z_i are in the interior $V_x \subset H_x(y)$, it follows by convexity (see Lemma 3) that $z = z_s \in V_x$, a contradiction. If one of the two point, say z_0 does not belong to F, then $z_0 \in H_x(y)$, it follows from the proof of Lemma 3 that z can only be equal to z_1 and $s = 1$. This is exactly a definition of a face for T_x. Similarly F is a face of T_y. $\Box$

4.2. **The Bernal Graph.** The definitions of graph theory, used here, follow the textbook of [19]. On a connected graph, the graph distance between two vertices is the minimal number of edges required to make a walk joining them. The Bernal Graph is defined as follows

Definition 16. *Let $\mathcal{L} \in \mathrm{Del}(\check{r},\hat{r})$ be a Delone set.*
(i) A pair $\{x,y\} \in \mathfrak{P}_2(\mathcal{L})$ of distinct atoms are called nearest neighbors if and only if the intersection of their Voronoi tiles is a facet, namely a face of minimal co-dimension 1*. Let $\mathcal{E}$ denote the set of pairs of nearest neighbors.*
(ii) An element of $\mathcal{E}$ will be called an edge*. The pair $\mathcal{G} = (\mathcal{L},\mathcal{E})$ defines a simple graph where atoms become* vertices*. $\mathcal{G}$ will be called the* Bernal Graph *of $\mathcal{L}$.*

The Bernal Graph as a countably infinite number of vertices and edges.

Theorem 9. *Given $\mathcal{L} \in \mathrm{Del}(\check{r},\hat{r})$, its Bernal Graph is connected. Its graph distance $d_{\mathcal{L}}$ is equivalent to the Euclidean distance on $\mathcal{L}$.*

Proof: (i) given two atoms $x \neq y \in \mathcal{L}$, the interval $[x,y] \subset \mathbb{R}^d$ is the convex hull of the two atoms, namely it is the set $[x,y] = \{x_s \in \mathbb{R}^d\,;\, x_s = sy + (1-s)x\,,\, 0 \leq s \leq 1\}$. Then, given any $\epsilon > 0$, let $\eta : s \in [0,1] \to \mathbb{R}^d$ be a path such that (a) η is continuously differentiable, (b) $\eta(0) = x$ and $\eta(1) = y$, (c) $\|\eta(s) - x_s\| + \|d\eta/ds - (y-x)\| < \epsilon$ for all $s \in [0,1]$, (d) if $b \in \mathcal{L}$ is an atom such that η intersects the tile T_b, then this tile intersects also $[x,y]$ and η intersects its boundary ∂T_b at isolated points in the relative interior of some of its facets. Such a path will be called *generic* in this proof. If such a generic path exists then the set of atoms $b \in \mathcal{L}$ such that η meets the tile T_b defines a unique sequence $\gamma = (a_0 = x_0, a_1, \cdots, a_{n-1}, a_n = x_1)$ of atoms in $\mathcal{L}$ such that $\{a_{k-1}, a_k\}$ is an edge or the Bernal Graph. Hence γ is a walk in the Bernal Graph joining the two points x_0 to x_1 (if ϵ is small enough, it is actually a path, but it does not really matter at this point). The order of this sequence is defined by the order of $[0,1]$ namely the "times of visit" of each such tile. In particular the existence of a generic path proves that the Bernal Graph is connected.

(ii) To prove the existence of a generic path η, let $W(x,y)$ be the set of atoms a the tile of which intersect the interval $[x,y]$ namely $I_a = T_a \cap [x,y] \neq \emptyset$. This implies $\mathrm{dist}(a,[x,y]) \leq \widehat{r}$ so that $W(x,y)$ is finite. Since the Voronoi tiles cover the space, the subfamily $\{T_a\,;\, a \in W(x,y)\}$ cover $[x,y]$, so that the sets I_a, for $a \in W(x,y)$, are also covering $[x,y]$. It must be remarked at this point that as the intersection of two closed and convex sets, I_a is closed and convex, so it is a closed interval in the line generated by x,y. Moreover, if an end ξ of I_a is neither x nor y, then ξ is interior to $[x,y]$ and therefore its must belong to the boundary of T_a. Similarly let $J_a = V_a \cap [x,y]$. Then, using the inverse map of $s \to x_s$, J_a defines in $[0,1]$ an open interval $\widehat{J}_a$ which might be empty even if $a \in W(x,y)$. Let then $J = \bigcup_a \widehat{J}_a$. This is a open subset of $[0,1]$. Let then $K = [0,1] \setminus J$. Then K is compact and if $s \in K$, then x_s belongs to a face of one of the T_a's with $a \in W(x,y)$. Let then x_K denote the image of K inside $[x,y] \subset \mathbb{R}^d$. If x_K does not intersect a tile T_b then $\mathrm{dist}(x_K, T_b) = \rho_b > 0$. In addition if $\mathrm{dist}(b,[x,y]) > \widehat{r}$ then $T_b \cap [x,y] = \emptyset$. Then $\rho = \min\{\rho_b\,;\, b \notin W(x,y)\}$ exists. The let $0 < \epsilon < \rho$. The open set $\widehat{K}^\epsilon = \{z \in \mathbb{R}^d\,;\, 0 < \mathrm{dist}(z, x_K) < \epsilon\}$ then intersects each Voronoi cell V_a for $a \in W(x,y)$ and none of the others. To complete the picture let H be the set of points belonging to a face of codimension at least 2 of one of the T_a's with $a \in W(x,y)$. This set is a finite union of compact sets, so H is actually closed and compact. In addition, because of the codimension 2, its complement in $K^\epsilon = \widehat{K}^\epsilon \setminus H$ is a path connected open set. Let then η be defined by $\eta(s) = x_s + \phi(s)$, where $\phi : [0,1] \to \mathbb{R}^d$ is C^1 and satisfies: (a) $\phi(s) \in x_J \cup K^\epsilon$, (b) $\sup_{s\in[0,1]} \|d\phi/ds(s)\| < \epsilon$ and $\min_{s\in[0,1]} (\|\phi(s)\| + \|d\phi(s)/ds\|) > 0$ (c) at each value of s such that $\eta(s)$ belongs to a facet of a Voronoi tile, $d\eta/ds$ is transversal to this facet. Then η is generic.

(iii) Then comes the first comparison between metrics. First let $\gamma : x \to y$ be a path in the Bernal Graph defined by the vertices $\gamma = \{x_0 = x, x_1, \cdots, x_{n-1}, x_n = y\}$. Then its graph length is $\ell(\gamma) = n$. Thanks to the triangle inequality it follows that $d_E(x,y) \leq \sum_{k=1}^n \|x_k - x_{k-1}\| \leq 2\widehat{r}\ell(\gamma)$. Minimizing over the length of γ gives

$$\frac{d_E(x,y)}{\check{r}} \leq d_{\mathcal{L}}(x,y)\,.$$

(iv) To prove an opposite inequality, the vertices of the path γ defined in (i) & (ii) are all contained in the closed set $S_{\widehat{r}} = \{z \in \mathbb{R}^d\,;\, \mathrm{dist}(z,[x,y] \leq \widehat{r}\}$. Thus the length of γ is bounded from above by the number of points $N_{x,y}$ of $W(x,y)$. In other words $d_{\mathcal{L}}(x,y) \leq \ell(\gamma) \leq N_{x,y}$. To estimate $N_{x,y}$, it is enough to remark that, if $a \in W(x,y)$, the open ball $\mathrm{B}(a;\check{r})$ is contained in the interior of $S_{\widehat{r}+\check{r}}$ and that these balls are disjoint. Consequently the volume of their union $B = \bigcup_{a\in W(x,y)} \mathrm{B}(a;\check{r})$ is bounded by

$$\mathrm{Vol}(B) = N_{x,y}\omega_d \check{r}^d \leq \mathrm{Vol}(S_{\widehat{r}+\check{r}})\,,$$

where ω_d is the volume of the unit ball $\overline{\mathrm{B}}(0;1) \in \mathbb{R}^d$. It should be remarked that the volume of $S_{\widehat{r}+\check{r}}$ is the sum of the volume of the ball $\overline{\mathrm{B}}(0;\widehat{r}+\check{r})$ and of the cylinder $C_{\widehat{r}+\check{r}}(x,y) = [x,y] \times \overline{\mathrm{B}}^{\perp}(0;\widehat{r}+\check{r})$ where $\overline{\mathrm{B}}^{\perp}(0;R)$ denotes the ball centered at the origin with radius R in the hyperplane $(y-x)^{\perp}$ orthogonal to the vector $y-x$. This gives

$$\mathrm{Vol}(S_{\widehat{r}+\check{r}}) \leq \omega_d(\widehat{r}+\check{r})^d + \|y-x\|\omega_{d-1}(\widehat{r}+\check{r})^{d-1}\,.$$

It should also be remarked that since both $x, y \in \mathcal{L}$, $2\check{r} \leq \|x-y\| = d_E(x,y)$. Factorizing $\check{r}$ gives

$$d_{\mathcal{L}}(x,y) \leq N_{x,y} \leq \frac{3c_d}{2}\left(1+\frac{\widehat{r}}{\check{r}}\right)^{d-1} \frac{d_E(x,y)}{\check{r}}\,, \qquad\qquad c_d = \max\left\{1, \frac{\omega_{d-1}}{\omega_d}\right\}\,.$$

□

Proposition 9. *Let $\mathcal{L} \in \mathrm{Del}(\check{r},\widehat{r})$ be a Delone set and let $x \in \mathcal{L}$ one of its atoms. Then the number n_x of its nearest neighbors satisfies*

$$d+1 \leq n_x \leq \left(2\frac{\widehat{r}}{\check{r}}+1\right)^d - 1$$

Proof: (i) To prove the lower bound, let $m = n_x$ and denote by $\{x_1, x_2, \cdots, x_m\}$ the nearest neighbors of x. By construction, for each $1 \leq j \leq m$, the hyperplane

$$H_j = \left\{ y \in \mathbb{R}^d\,;\, \left\langle \left(y - \frac{x+x_j}{2}\right) \middle| x_j - x \right\rangle = 0 \right\}\,, \tag{2}$$

is the set of vectors at equal distance from x and x_j. Let M be the $d \times m$ matrix with j-th column given by the coordinates of $x_j - x$. Let also $a \in \mathbb{R}^m$ be the vector with coordinates $a_j = 1/2(\|x_j\|^2 - \|x\|^2)$. The equation (2) can be rewritten in the matrix form $M^t y = a$ as can be checked by inspection. Then there is a point at equal distance from x and all of the x_j's if and only if the linear equation $M^t y = a$ has a solution for y. As long as $m \leq d$, the rank of M is at most m, so that either $\mathrm{Ker}(M^t) = \mathrm{Im}(M)^{\perp}$ is not empty or M is invertible. In both cases, there is a solution, which means that $F = \bigcap_{j=1}^m H_j \neq \emptyset$. In addition, substituting x for y gives $\langle x - (x+x_j)/2 \big| x_j - x\rangle = -\|x_j - x_0\|^2 < 0$. In particular, if $m \leq d$ and if $y_0 \in F$, any point of $\mathbb{R}^d$ of the half-line $L = \{y(s) = (1-s)y_0 + sx\,;\, s > 0\}$, starting from y_0 and passing through x, satisfies $\langle y(s) - (x+x_j)/2 | x_j - x\rangle = -s\|x_j - x_0\|^2 < 0$. Consequently this half line, which is unbounded, never meets any of the hyperplanes H_j. Since the Voronoi tile of x is bounded, convex and since L pass through x for $s = 1$, it must intersect a face for some $s > 1$, namely one of the H_j's, leading to a contradiction. Hence $m = n_x > d$.

(ii) To establish the upper bound, all the nearest neighbors of x are contained in the closed ball $\overline{\mathrm{B}}(x;2\widehat{r})$. Since the number of points of $\mathcal{L}$ contained in this ball is bounded by the maximum number N of nonintersecting balls of radius $\check{r}$ it contains, as in Proposition 7. Since x is the center of such a ball, it follows that $n_x \leq N - 1$ giving the upper bound. □

A better bound is provided by the following estimate

Proposition 10. *Let $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ be a Delone set and let $x \in \mathcal{L}$ one of its atoms. Then the number n_x of its nearest neighbors satisfies*

$$n_x \leq \frac{\sqrt{\pi}\,\Gamma\{(d-1)/2\}}{\Gamma(d/2)\ \int_0^{\theta_m} \sin^{d-2}(\theta)\,d\theta}\,, \qquad\qquad \sin\theta_m = \frac{\check{r}}{2\widehat{r}}\,.$$

Proof: If x' is a nearest neighbor to x, it is located at a distance at most $2\widehat{r}$ from x. Moreover the ball $\mathrm{B}(x'; \check{r})$ does not touch any other such balls centered at an atom of $\mathcal{L}$. So the maximum number of nearest neighbors is certainly smaller than or equal to the maximum number of non intersecting open balls B of radius $\widehat{r}$ centered on the sphere $S = \partial\overline{\mathrm{B}}(x; 2\widehat{r})$. Such a ball B is seen from x at the angle θ_m, as a simple geometric picture can show. This angle define a spherical cap A of spherical volume independent of the position of B on that sphere. Standard formulae for the volume of this spherical cap give both $\mathrm{Vol}(S)$ and $\mathrm{Vol}(A)$, leading to this formula. □

Remark 8. The proposition 10 applied to the limiting case of hard sphere atoms, corresponding to $\widehat{r} = \check{r}$, given for $d = 3$ the bound $n_x \leq 4(1 - \sqrt{3}/2)^{-1} \simeq 14.93$, a much better estimate that in Proposition 9 predicting $n_x \leq 26$. This is because the counting in the latter does not restricts itself to only the nearest neighbors. In [41] the author gives a more accurate estimate in dimension 3 taking into account the nature of various possible clusters of atoms. As a result he surmises that the average number of neighbors in this case should be $4\pi \simeq 12.57$ instead. Indeed cluster of 13 atoms are possible in a hard sphere packing without creating holes that are too big [77, 78], so without violating the Delone property of being relatively dense. □

5. The Delaunay Triangulation

The main seminal result obtained by Delaunay-Delone [38], concerns the empty sphere property. Namely the atoms of a Delone set and its closed neighbors, can be grouped on a common sphere the interior of which has no atoms. In the generic case (meant in a sense of a dense G_δ- set in Del), the number of these atoms are exactly $d+1$. Their convex hull is therefore a simplex in $\mathbb{R}^d$. These simplexes are tiling the Euclidean space so as to produce a triangulation. The latter can also be viewed as a simplicial complex the homology of which is trivial since $\mathbb{R}^d$ is contractible (Poincaré Theorem). Each graph ball induce a simplicial sub-complex. But the useful property of this complex comes from the possibility to identify graph balls modulo homotopy inducing complex isomorphisms.

5.1. **Interlude: Geometry and Algebra.**

Before going further, some technical results will be useful. In what follows S will denote a finite subset of $\mathbb{R}^d$ (with $d \geq 1$) with exactly $n+1$ elements, and $n \geq 1$. Choosing an order on S, it can be written as $S = \{x_0, \cdots, x_n\}$. Then M_S will denote the $d \times n$ matrix the k-th column of which is the vector $x_k - x_0$, for $1 \leq k \leq n$, namely $(M_S)_{ik} = (x_k)_i - (x_0)_i$ where $(x_k)_i$ is the i-th coordinate of the vector $x_k \in \mathbb{R}^d$. In particular the image $\mathrm{Im}(M_S)$ is the linear subspace of $\mathbb{R}^d$ generated by the vectors $(x_k - x_0)$. Let M_S^t denote the transposed matrix so that $\mathrm{Im}(M_S)^\perp = \mathrm{Ker}(M_S^t)$. Let then a denotes the vector in $\mathbb{R}^n$ with components $a_k = (\|x_k\|^2 - \|x_0\|^2)/2$. Then

Lemma 4. *(i) The points of S lie on a sphere if and only if the equation $M_S^t y = a$ admits at least one solution y in $\mathbb{R}^d$.*
(ii) The set of solutions is the set of points in $\mathbb{R}^d$ at equal distance from each of the elements of S. Two solutions differ by an element in $\mathrm{Ker}(M_S^t) = \mathrm{Im}(M_S)^\perp$ namely by a vector perpendicular to the affine space generated by S.

(iii) If the vectors $(x_k - x_0)$ are linearly independent and if $n \leq d$ the set of solutions is not empty.
(iv) If the solution exists and is unique then $n \geq d$, namely S has at least $(d+1)$ elements.

Proof: (i) It is just an elementary calculation to show that the equation $M_S^t y = a$ admits a solution $y \in \mathbb{R}^d$ if and only if $\|x_k - y\|^2 = \|x_0 - y\|^2$ for $1 \leq k \leq n$.
(ii) Clearly, y, y_0 are solutions if and only if $M_S^t(y - y_0) = 0$, if and only if $(y - y_0) \in \mathrm{Ker}(M_S^t)$.
(iii) The rank m of M_S is always less than or equal to the minimum of n and d. If $n \leq d$ then $m = n$ if and only if the columns of M_S are linearly independent. In such a case the $n \times n$ matrix $M_S^T M_S$ has the same rank n as M_S, so that it is invertible. Therefore the vector $b = (M_S^T M_S)^{-1} a \in \mathbb{R}^n$ is well defined so that $y_0 = M_S b$ is a special solution of $M_S^T y = a$.
(iv) To get a unique solution, then M_S^t must have a trivial kernel, meaning that $\mathrm{Im}(M_S) = \mathbb{R}^d$, namely the $(x_k - x_0)$ generate $\mathbb{R}^d$ implying that $n \geq d$. □

The following results is a direct consequence of the previous proof and will be left to the reader

Corollary 1. *Let $\mathcal{O}_n$ denotes the set of ordered subset $S = (x_0, \cdots, x_n) \in (\mathbb{R}^d)^{n+1}$ such that the vectors $(x_k - x_0)$ are linearly independent. Then $\mathcal{O}_n$ is a dense (algebraic) open set. The set C_S of points at equal distance from all points in S varies smoothly with S. In particular if $S \in \mathcal{O}_d$ the unique center y_S of the sphere containing S is a smooth (algebraic) function of S.*

Another way to express algebraically these result consists in introducing the following $(d+2) \times (n+1)$ matrix N_S defined by

$$N_S = \begin{bmatrix} 1 & 1 & \cdots & 1 & 1 \\ x_0 & x_1 & \cdots & x_{n-1} & x_n \\ |x_0|^2 & |x_2|^2 & \cdots & |x_{n-1}|^2 & |x_n|^2 \end{bmatrix}. \tag{3}$$

The symbol $\mathrm{S}(y; \rho)$ denotes the sphere in some $\mathbb{R}^n$ centered at y with radius ρ. If a set A is contained in some sphere, this sphere is not necessarily unique, for instance if A is contained in an affine subspace of positive codimension.

Lemma 5. *(i) The kernel of N_S^t is non trivial either if S is contained in some hyperplane of $\mathbb{R}^d$ or if the elements of S lie in some sphere.*
(ii) If S has $n+1$ points, if N_S^t has non trivial kernel, and if S lies in the sphere $\mathrm{S}(y; \rho)$, then $N_S^T \eta(y) = \rho^2 f$ where $\eta(y) = (\|y\|^2, -2y, 1) \in \mathbb{R}^{d+2}$ and $f = (1, 1, \cdots, 1) \in \mathbb{R}^{n+1}$. In particular the map $(S, y) \to \rho$ is smooth on a dense open set.
(iii) if S lies in a unique sphere, then S generates $\mathbb{R}^d$ as an affine space, in particular S admits at least $d+1$ elements.
(iv) If S generates $\mathbb{R}^d$ and lies in the sphere $\mathrm{S}(y; \rho)$ centered at y with radius ρ, let $B \subset S$ be a minimal set generating $\mathbb{R}^d$ as an affine space and let $x \notin B$ be a vector, then the matrix $N_{B \cup \{x\}}$ is a square matrix of size $(d+2)$ such that

$$\det(N_{B \cup \{x\}}) = (\|x - y\|^2 - \rho^2) \det(M_B)$$

The set of x's for which $\det(N_{B \cup \{x\}}) = 0$ is the compact set $\mathrm{S}(y; \rho)$ the complement of which is a dense open set.

Proof: (i) Let $b \in \mathrm{Ker}(N_S^t) \subset \mathbb{R}^{d+2}$ be written as $(b_0, -2\beta, b_\infty)$ where $b_0, b_\infty \in \mathbb{R}$ and $\beta \in \mathbb{R}^d$. Then the equation $0 = N_S^t b$ is nothing but $b_0 - 2\langle \beta | x_k \rangle + b_\infty \|x_k\|^2 = 0$ for $0 \leq k \leq n$. If

$b_\infty = 0$ then either $\beta = 0$ and the solution is trivial, or $\beta \neq 0$ and then these equations define an hyperplane perpendicular to β and passing though $b_0\beta/2\|\beta\|^2$ in which the set S lies. If $b_\infty \neq 0$, then by dividing b by b_∞ if necessary, there is a solution with $b_\infty = 1$. In such a case the equation gives $\|x_k - \beta\|^2 = \|\beta\|^2 - b_0$ which admits a solution provided $b_0 \leq \|\beta\|^2$ and S lies on the sphere $\mathrm{S}\left(\beta; (\|\beta\|^2 - b_0)^{1/2}\right)$.

(ii) Let S have $n+1$ points with the equation $\|x_k - y\|^2 = \rho^2$ for $0 \leq k \leq n$ is equivalent to the equation $N_S^T \eta(y) = \rho^2 f$ as can be checked by inspection. Thanks to the Corollary 1, the smoothness follows.

(iii) If S lies in a unique sphere $\mathrm{S}(y;\rho)$, then the set of points at equal distance from the elements of S is reduced to the center of the sphere and, by Lemma 4, S must generate $\mathbb{R}^d$ as an affine space so that it has at least $d+1$ elements. Moreover, from (i), the kernel equation $N_S^t b = 0$ admits only one solution with $b_\infty = 1$, with $\beta = y$ and $b_0 = \|y\|^2 - \rho^2$. All other solution is proportional to this one.

(iv) If N is a $(d+2)\times(d+2)$ matrix with real coefficients, let R_i, with $0 \leq i \leq d+1$ denote the i-th row of N (counted from top to bottom in eq. 3). Similarly let C_k, for $0 \leq k \leq d_1$ denotes the k-th column of N counted from left to right. Let also $y \in \mathbb{R}^d$ have coordinates $y = (y_i)_{i=1}^d$. Then the following algorithm of row and column operations is applied to $N_{B\cup\{x\}}$, in the order from (a) to (d), to get another matrix $N^{(f)}_{B\cup\{x\}}$ with the same determinant:

(a) add to the row R_{d+1} the linear combination $(|y|^2 - \rho^2)\, R_0 - 2\sum_{i=1}^d y_i\, R_i$,
(b) subtract from the row R_i $(1 \leq i \leq d)$ the expression $(x_0)_i\, R_0$.
(c) subtract from C_k the column C_0 for $1 \leq k \leq d+1$.
(d) since B generates $\mathbb{R}^d$ as an affine space, the family $\{x_k - x_0\,;\, 1 \leq k \leq d\}$ is a linear basis. Thus $x - x_0$ can be written as $x - x_0 = \sum_{k=1}^d \sigma_k (x_k - x_0)$ for some real σ_k's. Then subtract from the column C_{d+1} the linear combination $\sum_{k=1}^d \sigma_k\, C_k$.
Therefore

$$N^{(f)}_{B\cup\{x\}} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & x_1 - x_0 & \cdots & x_d - x_0 & x - x_0 \\ 0 & 0 & \cdots & 0 & |x-y|^2 - \rho^2 \end{bmatrix}.$$

This gives the determinant and the rest is elementary. □

5.2. **The Delaunay Empty Sphere Property.** The main topic of the original Delone paper [38] is precisely the topic of this Section. It should be noted, however, that this property was rediscovered as a conjecture by the physicist Bernal [22] in his study of liquids at the atomic scale. In order to organize the various concept the following definition will be useful

Definition 17. *Let $\mathcal{L} \in \mathrm{Del}(\check{r}, \hat{r})$ be a Delone set. Then*

(i) a Voronoi point for $\mathcal{L}$ is an extreme point of a Voronoi tile namely a vertex or a face of zero dimension. The set of Voronoi points will be denoted by $\mathcal{L}^*$.

(ii) a dual edge will be any face of dimension 1 of a Voronoi tile. Let $\mathcal{E}^*$ denote the set of dual edges.

(iii) A dual edge e has exactly two distinct extreme points $\phi(e) = \{y_0, y_1\} \in \mathfrak{P}_2(\mathcal{L}^*)$ which are also Voronoi points. This defines the dual Bernal graph $\mathcal{G}^* = (\mathcal{L}^*, \mathcal{E}^*, \phi)$ with vertices $\mathcal{L}^*$ and edges $\mathcal{E}^*$ and boundary map ϕ. This graph is simple.

Since a tile is a compact convex polyhedron in $\mathbb{R}^d$, it can be seen as the convex hull of its extremal points. Such points are faces of zero dimension and are in finite numbers. Similarly, the dual edges in a Voronoi tile are in finite numbers. The remarkable fact is the following *empty sphere property* emphasized by Delaunay (Delone) in his original paper.

Theorem 10 (Empty Sphere Property [38])**.** *Let $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ be a Delone set. Then*

(i) any Voronoi point y is the center of a sphere on which lie the atoms with Voronoi tile containing this point as a vertex, called atomic neighbors or neighboring atoms, and with no atoms in its interior. Then $\mathrm{AN}(y)$ will denote the set of atomic neighbors of y. In particular the radius ρ of this "empty sphere" satisfies

$$\check{r} \leq \rho \leq \widehat{r}\,.$$

(ii) The set $\mathrm{AN}(y)$ of atomic neighbors of a Voronoi point $y \in \mathcal{L}^*$ generates $\mathbb{R}^d$ as an affine space. Its number of points satisfies

$$d+1 \leq \#\mathrm{AN}(y) \leq \frac{\sqrt{\pi}\,\Gamma\{(d-1)/2\}}{\Gamma(d/2)\ \int_0^{\theta_n} \sin^{d-2}(\theta)\,d\theta}\,, \qquad\qquad \sin\theta_n = \frac{\check{r}}{\widehat{r}}\,.$$

The set of Delone sets $\mathcal{L} \in \mathrm{Del}(\check{r}, \widehat{r})$ for which all its Voronoi points have exactly $d+1$ neighboring atoms is generic, namely it is a dense G_δ set for the Fell topology.

(iii) If $\mathcal{L}$ is generic, then the atoms neighboring a Voronoi point y form a simplex of dimension d. The family of such simplexes defines a simplicial complex of $\mathbb{R}^d$ called the Delaunay triangulation.

Proof of Theorem 10: (i) Let $y \in \mathcal{L}^*$ be a Voronoi point for $\mathcal{L}$. By definition, if $x \in \mathrm{AN}(y)$ then y is an extreme point of the tile T_x. By definition of Voronoi tiles, $d_E(x, y) \leq d_E(x', y)$ for all $x' \in \mathcal{L}$. In particular if both x and x' are atomic neighbors of y, $d_E(x, y) = d_E(x', y) = \rho$ for some $\rho \geq 0$ and since $\mathrm{B}(x; \check{r}) \subset V_x \subset T_x$ it follows that $\check{r} \leq \rho$. Similarly, since $y \in T_x$ it follows that $\rho = d_E(x, y) \leq \widehat{r}$. In addition, since y does not belong to any other Voronoi tile, $d_E(x", y) > \rho$ for $x" \notin \mathrm{AN}(y)$. Hence all the atomic neighbors of y belong to the sphere centered at y of radius ρ and the interior of which is the open ball $\mathrm{B}(y; \rho)$ which, by the previous argument contains no atom. In addition the convexity of the polyhedral Voronoi tiles prevent the equality $\rho = \check{r}$ unless $d = 1$.

(ii) Thanks to Lemma 4, the set of points at the same distance from elements of $\mathrm{AN}(y)$ is an affine subspace or $\mathbb{R}^d$. By construction this set is made of the Voronoi point y, namely the intersection $\bigcap_{x\in\mathrm{AN}(y)} T_x$ which is compact. The only way to accommodate both constraints is that $\mathrm{AN}(y)$ contains at least $d+1$ atoms and generates affinely the whole space $\mathbb{R}^d$. On the other hand the argument given in the proof of Proposition 10 applies here, provided $2\widehat{r}$ is replaced by $\widehat{r}$, leading to the upper bound on the number of atomic neighbors.

(a) Let the number of atomic neighbors be exactly $(d+1)$. Then, thanks to Lemma 5, there is $\check{r} > \epsilon > 0$ such that if B is a finite set of points with $d_H(B, \mathrm{AN}(y)) < \epsilon$ there is still a unique point y_B at the center of a sphere containing B. Therefore, the smoothness (differentiability) of the matrices N_B as a function of the elements of B, it follows that there is a constant $\kappa_y > 0$ such that $\|y_B - y\| < \kappa_y \epsilon$ for ϵ small.

(b) Let then $\mathcal{F}$ denotes the family of open balls $\mathcal{F} = \{\mathrm{B}(x; \epsilon)\,;\, x \in \mathrm{AN}(y)\}$ and let $O_{\mathcal{F}}$ be the union of these balls. By construction $\mathrm{B}(x; \epsilon) \subset V_x \subset T_x$. In particular if P_y denotes the *local patch* around y, namely the union of the tiles T_x for $x \in \mathrm{AN}(y)$, it is a compact subset of $\mathbb{R}^d$, so that $K = P_y \setminus O_{\mathcal{F}}$ is also compact. Then $\mathcal{L} \in \mathcal{U}(K, \mathcal{F})$ as can be checked easily. In addition, if $\mathcal{L}' \in \mathcal{U}(K, \mathcal{F})$, then, thanks for the Delone property, the set $B = \mathcal{L}' \cap P_y$ has still exactly $d+1$

atoms admitting a unique Voronoi point y_B such that $\|y - y_B\| < \kappa_y \epsilon$. Hence the set of Delone sets admitting a generic Voronoi point near a point $y \in \mathcal{L}^*$ is Fell-open.

(c) If $\mathrm{AN}(y)$ has $n > (d+1)$ elements, the Lemma 5 shows that in any Hausdorff neighbourhood of $\mathrm{AN}(y)$ there is a set which admits only generic Voroni points. To see this, let $B = \{x_0, \cdots, x_d\}$ be a minimal generating subset of $\mathrm{AN}(y)$, namely generating $\mathbb{R}^d$ as an affine space. Let also ρ denote the radius of the empty sphere containing $\mathrm{AN}(y)$. Then, the set $U_x = \mathrm{B}(x;\epsilon) \setminus \overline{\mathrm{B}}(y;\rho)$ is open. Then the family $\mathcal{G}$ made of the open balls $\mathrm{B}(x_k;\epsilon)$ and of the open sets U_x for $x \in \mathrm{AN}(y) \setminus B$ is a finite family of open sets. By construction, and thanks to Lemma 5, any finite subset A containing B and intersecting each open set in $\mathcal{G}$ at only one point, still admits y as the center of the ball containing B but no other point of $\mathrm{AN}(y) \setminus B$ belong to that sphere. Proceeding by induction on $m = n - d - 1$ and modifying the U_x accordingly, the centers of the sphere of each subset with $d+1$ element of $\mathrm{AN}(y)$ are pairwise distinct. It is worth remarking here that these centers may not be all Voronoi point of a perturbation of $\mathcal{L}$ (see Section 5.3 for this). In particular this gives a family $\mathcal{G}'$ of nonempty open subsets of the balls $\mathrm{B}(x;\epsilon)$ for $x \in \mathrm{AN}(y)$ and a compact set K' obtained from $\widehat{K}$ by removing the union of open sets in $\mathcal{G}'$. Thus any Delone set $\mathcal{L}' \in \mathcal{U}(K', \mathcal{G}') \subset \mathcal{U}(K, \mathcal{F})$ admits only generic Voronoi points in the vicinity of y. And since $\epsilon > 0$ can be chosen arbitrary small, it follows that any Fell-neighborhood of $\mathcal{L}$ contains an open Fell-neighborhood of the form $\mathcal{U}(K', \mathcal{G}')$, namely contained a generic Delone set near y.

(d) Given $n \in \mathbb{N}$, let $\mathcal{W}_n$ denote a Fell-open subset of all Delone sets which are generic in the ball $\overline{\mathrm{B}}(0;n)$. the previous arguments show that it is a dense Fell-open subset. Therefore, thanks to the Baire Category Theorem, the set $\mathcal{W}_\infty = \bigcap_{N\in\mathbb{N}} \mathcal{W}_n$ is a dense G_δ-setin $\mathrm{Del}(\check{r}, \widehat{r})$. An element $\mathcal{L} \in \mathcal{W}_\infty$ is generic in any ball around the origin, so that all its Voronoi points are simple.

(iii) If $\mathcal{L}$ is generic, then any Voronoi point $y \in \mathcal{L}^*$ is the center of a sphere containing the exactly $(d+1)$ atomic neighbors of y. Using the previous results in this proof, these atoms generate $\mathbb{R}^d$ as an affine space. So, choosing an order so that $\mathrm{AN}(y) = \{x_0, \cdots, x_d\}$, the vectors $(x_k - x_0)$ makes a linear basis for $\mathbb{R}^d$. In particular their convex hull is the simplex $\mathcal{S}_y = \{\sum_{k=0}^d \sigma_k x_k\,;\, 0 \leq \sigma_k \leq 1\,,\, \sum_{k=0} \sigma_k = 1\}$ and this simplex has a non empty interior. Following [43] (see Chapter II, Section 8), the family $\mathcal{K}(\mathcal{L}) = \{\mathcal{S}_y\,;\, y \in \mathcal{L}^*\}$ defines a simplicial complex, also called, in geometry, a *triangulation*. Since this triangulation covers $\mathbb{R}^d$ the singular cohomology of this simplex is trivial. Hence each generic Delone set defines a unique non ambiguous triangulation, through this construction and is called the *Delaunay triangulation* given by $\mathcal{L}$. □

Corollary 2. *Let $\mathcal{L}$ be a generic Delone set. Then, given any open ball $B = \mathrm{B}(z;R) \subset \mathbb{R}^d$ with no atoms nor Voronoi points of $\mathcal{L}$ in its boundary, and given $0 < \eta < \check{r}$, there is a Fell-open neighborhood $\mathcal{U}$ of $\mathcal{L}$ such that if $\mathcal{L}' \in \mathcal{U}$ its Voronoi points contained in B are all simple and at distance at most η from a Voroinoi point of $\mathcal{L}$ in B. In addition, the restriction to B of the dual Bernal graph of $\mathcal{L}'$ is graph isomorphic to the one of $\mathcal{L}$ in the same ball.*

Proof: This is a direct consequence of the part (ii.b) of the proof of the previous Theorem 10 and checking the details will be left to the reader. □

Definition 18. *The V-degree of a Voronoi point y for the Delone set $\mathcal{L}$ is defined by $d_v(y) = \#\mathrm{AN}(y) - d$. A Voronoi point will be called simple whenever it has V-degree 1. A Voronoi point of V-degree m will be called m-generic whenever no subset of $\mathrm{AN}(y)$ with exactly $d+1$ atoms is contained in an affine hyperplane of $\mathbb{R}^d$.*

5.3. **Pachner Moves.** What happens when a Delone set $\mathcal{L}$ is not generic ? To investigate this problem, in view of the argument given in part (ii.c) of the Proof of Theorem 10, it is sufficient to consider one Voronoi point $y \in \mathcal{L}^*$ of V-degree 2. Namely such a point has exactly $d+2$ atomic neighbors. Indeed, if y has more atomic neighbors, the same procedure may be applied a finite number of times until all Voronoi points are simple.

Remark 9. In $\mathbb{R}^3$ such a Voronoi point has 5 neighbors. This explains why in the numerical simulations of glasses and liquids using a molecular dynamics, the atomic jumps. detected through a statistically higher velocity of a particle, involves in the average 5 particles [44]. Actually the statistical plot shows that this number is likely to be a Poisson random variable of average 5. $\square$

Then, $\text{AN}(y)$ has exactly $d+2$ elements, all on the same sphere centered at y with radius ρ, with no other atom of $\mathcal{L}$ in its interior. Since y belongs to the Voronoi tile T_x for $x \in \text{AN}(y)$, it follows from Theorem 7 that $\check{r} \leq \rho \leq \widehat{r}$. What happens when only one of the atomic neighbors, say x, move slightly away from this sphere ? If x moves outside of this sphere and if $A_x = \text{AN}(y) \setminus \{x\}$ is not contained in an affine hyperplane of $\mathbb{R}^d$, then y still stays a Voronoi points. Indeed, the sphere is uniquely defined by A_x and its interior is still empty of atoms. However, if x moves in the interior of this sphere, by the same argument, y cannot be a Voronoi point anymore. This type of move will then change locally the Delaunay triangulation defined by $\mathcal{L}$.

How does a triangulation changes is a problem occurring also in the description of a Riemannian manifold. A triangulation is a convenient combinatoric description of such a manifold, amenable to computer calculation. These moves are a numerical way to describe continuous deformations leading to the field of Computational Geometry [4, 25, 28, 88]. This was the original motivation of Pachner in giving a general description of such moves [81]. However, the formalism used in the previous reference requires some background that would take too much space in this review. Working in the Euclidean space $\mathbb{R}^d$ and the algebraic formalism described in Section 5.1 allows to give a proof without it.

The main result of this Section is summarized as follows

Theorem 11 (Generic Pachner Moves)**.** *Let $\mathcal{L}$ be a Delone set. Let y be a 2-generic Voronoi point. Let $\mathcal{L}_x$ denote a small perturbation of $\mathcal{L}$ differing by one of the elements $x \in \text{AN}(y)$ in $\mathcal{L}$ moving out of the empty sphere defined by y in $\mathcal{L}$. Let $\text{AN}_x(y)$ denote the new set of atoms obtained this way. Then*
(i) there is a subset $V \subset \text{AN}_x(y)$ with $2 \leq \#V \leq d$ elements, such that for $v \in V$, the set $\text{AN}_x(y) \setminus \{v\}$ defines a simplex of the triangulation of $\mathcal{L}_x$. In particular this simplex is contained on an empty sphere and its center is a simple Voronoi point for $\mathcal{L}_x$
(ii) If instead x moves inside the empty sphere defined by y in $\mathcal{L}$, then the same holds provided V is replaced by its complement.

Proof: By assumption, y is a Voronoi point with exactly $\#\text{AN}(y) = d+2$ atomic neighbors. Moreover each subset of $\text{AN}(y)$ with exactly $d+1$ elements generates $\mathbb{R}^d$ affinely. Let ρ_y denote the radius of the empty sphere it defines.

1)- Let $x_0 \in \text{AN}(y)$ be chosen. Let H_0 denote the affine hyperplane passing though x_0 and orthogonal to $y - x_0$. Then the open half-space H_+ containing y and bounded by H_0, is the set of points $x \in \mathbb{R}^d$ such that $\langle x - x_0 | y - x_0 \rangle > 0$. Moreover, H_0 is the tangent space at x_0 to the sphere centered at y of radius $\|y - x_0\| = \rho_y$. The strict convexity of Euclidean balls implies that all points of that sphere but x_0 are contained in H_+. Let the other atomic neighbors be ordered as $x_1, \cdots, x_d, x_{d+1}$ so that the projection of $x_{d+1} - x_0$ on the oriented affine line generated by $y - x_0$ be the largest namely

$$\langle x_{d+1} - x_0 | y - x_0 \rangle \geq \langle x_k - x_0 | y - x_0 \rangle > 0\,, \qquad 1 \leq k \leq d\,. \tag{4}$$

The subset $A = \{x_0, x_1, \cdots, x_d\}$ has $d+1$ elements, so that by assumption, it generates affinely $\mathbb{R}^d$. Equivalently, the vectors $B = \{x_1 - x_0, \cdots, x_d - x_0\}$ make up a linear basis. Permuting the indices $\{1, \cdots, d\}$ if necessary, there is no loss of generality is assuming that $\det(M_A) > 0$. Thus, there are coordinates $(\xi_k)_{1 \leq k \leq d}$ uniquely defined by

$$x_{d+1} - x_0 = \sum_{k=1}^{d} \xi_k \,(x_k - x_0)\,.$$

It ought to be remarked that the only way for the inequalities in eq. (4) to be all equalities is to assume that the subset $\{x_1, \cdots, x_d, x_{d+1}\}$, which has $d+1$ elements, belong to the same affine hyperplane orthogonal to $y - x$. But this is excluded by the genericity assumption. Now comes some remark: the coordinates ξ_k are all positive if and only if x_{d+1} belongs to the cone with vertex x_0 and based on B. In such a case

$$0 < \langle x_{d+1} - x_0 | y - x_0 \rangle = \sum_{k=1}^{d} \xi_k \langle x_k - x_0 | y - x_0 \rangle < \left(\sum_{k=1}^{d} \xi_k \right) \langle x_{d+1} - x_0 | y - x_0 \rangle\,,$$

namely

$$\xi_k \geq 0\,,\ \ \forall 1 \leq k \leq d\,, \qquad \Longrightarrow \qquad \sum_{k=1}^{d} \xi_k > 1\,. \tag{5}$$

2)- This ordering of the element of $\mathrm{AN}(y)$ being made, let N_y denote the matrix $N_{\mathrm{AN}(y)}$. By construction $\det(N_y) = 0$ since all atomic neighbors are on the same sphere of radius ρ_y. Then let x be a point in a small neighborhood of x_{d+1} located *outside* the empty sphere. Let then $\mathcal{L}_x$ be a slight perturbation of the Delone set $\mathcal{L}$ obtained form keeping the elements in A but moving x_{d+1} towards x. This leads to keep y at equal distance of all other atomic neighbors in A without introducing any new atom inside the empty sphere. Since A generates affinely the whole space, it follows that y is uniquely defined by A. Therefore y is still a Voronoi point for $\mathcal{L}_x$. However now, $\det(N_{A\cup\{x\}}) = (\|y - x\|^2 - \rho_y^2)\det(M_A) > 0$. So y is a simple Voronoi point for $\mathcal{L}_x$ while the triangle it defines is the d-simplex built from A.

3)- Let now $0 \leq j \leq d$ and let $A_j = (A \cup \{x\}) \setminus \{x_j\}$. By construction $A_j \neq A$ but has still $d+1$ element so that, by genericity the same argument can be made provided $\|x - x_{d+1}\|$ is small enough. Namely there a unique empty sphere containing A_j, with center y_j and radius ρ_j. In order to compare with A, the matrix $N_{A\cup\{x\}}$ will be reordered following a sequence of row and column operations as indicated in the Proof (iv) of Lemma 5, to lead to the matrix $N^{(j)}_{A\cup\{x\}}$ with same determinant and defined by

$$N^{(j)}_{A\cup\{x\}} = \begin{bmatrix} 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 \\ x_0 - x & \cdots & x_{j-1} - x & 0 & x_{j+1} - x & \cdots & x_d - x & 0 \\ 0 & \cdots & 0 & (x_j - y_j)^2 - \rho_j^2 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

Expanding the determinant along the first row, then along the last, gives

$$\det\left(N_{A\cup\{x\}}\right) = \det\left(N^{(j)}_{A\cup\{x\}}\right) = (-1)^{j+1}\left((x_j-y_j)^2-\rho_j^2\right)\,\det(M_j)\,,$$

where M_j is the $d\times d$ matrix with columns

$$M_j = [x_0-x,\cdots,x_{j-1}-x,x_{j+1}-x,\cdots,x_d-x]$$

Let the case $j\neq 0$ be considered first. It is convenient to use the vectors $u_k = x_k - x_0$ and $v_k = x_k - x$ for $0\leq k\leq d+1$, with the convention that $u_{d+1} = x - x_0 = -v_0$ and $v_{d+1} = 0 = u_0$. It follows then that $v_k = u_k + v_0$. For convenience, the representation of the determinant by wedge product will be used, but, if the reader is uncomfortable, the same can be done with column operations. Consequently, the determinant of M_j becomes

$$\det(M_j) = v_0\wedge\cdots\wedge v_{j-1}\wedge v_{j+1}\wedge\cdots\wedge v_d\,.$$

Using multilinearity, the anticommutativity of the wedge product and the relation $v_k = u_k + v_0$, this gives

$$\det(M_j) = v_0\wedge u_1\wedge\cdots\wedge u_{j-1}\wedge u_{j+1}\wedge\cdots\wedge u_d\,.$$

Now since $B = \{u_1,\cdots,u_d\}$ is a linear basis, v_0 can be written as $v_0 = -(x-x_0) = -\sum_{k=1}^d \eta_k u_k$. On the other hand a wedge product of the form $u_k\wedge\cdots\wedge u_k\wedge\cdots$ always vanishes. Hence, using the change of sign by transposition of neighboring vectors in the wedge product this leads to

$$\det(M_j) = -\eta_j u_j\wedge u_1\wedge\cdots\wedge u_{j-1}\wedge u_{j+1}\wedge\cdots\wedge u_d = (-1)^j\eta_j\det\left(M_A\right).$$

Therefore

$$\det\left(N_{A\cup\{x\}}\right) = -\eta_j\left((x_j-y_j)^2-\rho_j^2\right)\det\left(M_A\right)\,.$$

Then y_j is a (simple) Voronoi point for $\mathcal{L}_x$ if and only if $(x_j-y_j)^2-\rho_j^2>0$, implying that $\eta_j<0$. In such a case y_j defines the simplex with vertices on A_j as one triangle of the triangulation defined by $\mathcal{L}_x$.

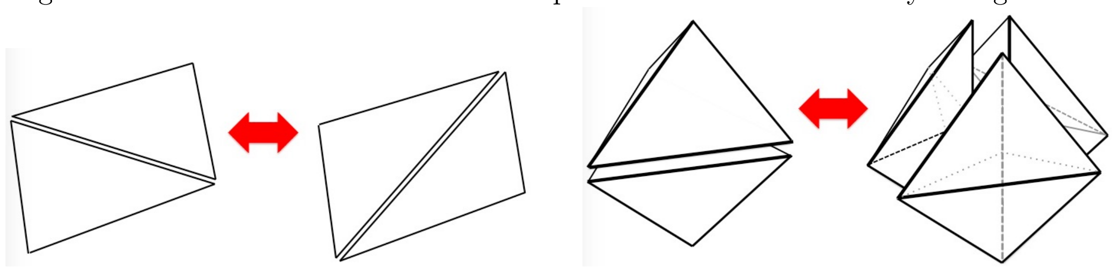
In the case $j=0$ the same argument leads to

$$\det(M_0) = \left(1-\sum_{k=1}^d \eta_k\right)\det\left(M_A\right)\,.$$

Therefore the point y_0 is a (simple) Voronoi point of $\mathcal{L}_x$ if and only if $\sum_{k=1}^d \eta_k > 1$.

4)- Let then V the set of indices $0\leq j\leq d+1$ such that y_j is a Voronoi point of $\mathcal{L}_x$. Equivalently it is the set of indices such that $\eta_j<0$. From the previous reasoning all these Voronoi points are simple. It ought to be remarked that , by construction $0\in V$. Now, if none of the indices $1\leq j\leq d$ belong to V, meaning $\eta_j\geq 0$, then eq. (5) implies $\sum_{k=1}^d \eta_k>1$, namely $d+1\in V$. Hence V has at least two elements. Moreover, the points $\{y_j; j\in V\}$ are simple Voronoi points for $\mathcal{L}_x$ and definie each one simplex of the Delaunay triangulation. At last, the same argument made whenever one of the atoms in $\mathrm{AN}(y)$ enters inside the empty sphere, instead, shows that V is transformed into its complement $V^c = [0,d+1]\setminus V$. In particular if $m=\#V$ then, since both V and V^c must contain at least two points, so that $2\leq m\leq d$. $\square$

Example 2. In order to illustrate the results of Theorem 11 above, here are a representation of the generic Pachner moves in $2D$ and $3D$ expressed in terms of Delaunay triangulation.



□

FIGURE 1. Left: generic Pachner moves in dimension 2; Right: generic Pachner moves in dimension 3

What happens if y be a non necessarily generic Voronoi point of $\mathcal{L}$ of higher V-degree ? This is a difficult combinatoric question in general which will not be investigated here. Only the few remarks below will give a hint of the variety of situations that may occur to describe the result of a Pachner move. If y has V-degree 2 but is non-generic, there is one subset $A \subset \text{AN}(y)$, having $d+1$ atoms, and contained in an affine hyperplane of $\mathbb{R}^d$. Such a situation appears in the Kepler lattice as shown in Fig. 2. This lattice corresponds to orange piles on a table at the market, assuming the oranges are perfect Euclidean balls of equal radius $\check{r}$. More precisely each

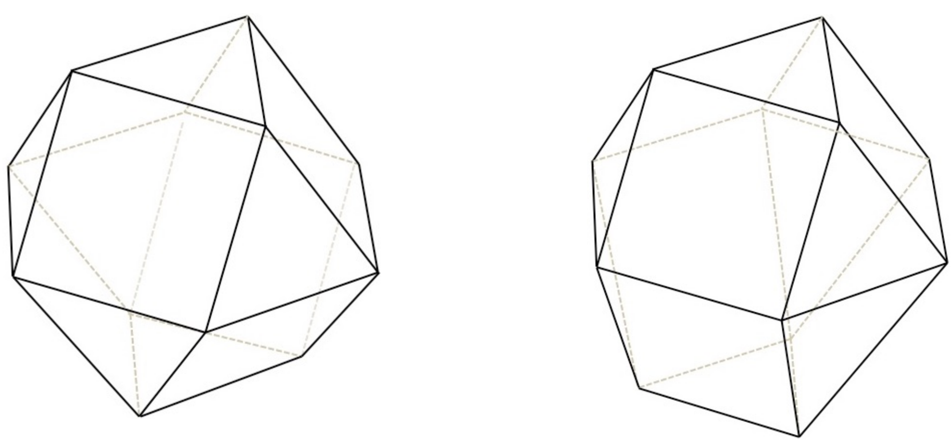


FIGURE 2. Nearest neighbors of an atom in the fcc (Left) and hcp (Right) lattices

horizontal layer L_n is given by a regular triangular lattice the sites of which labeling the centers of the oranges. In such a lattice tiles are staggered equilateral triangles with alternating orientations which will be labeled by $\uparrow$ or $\downarrow$. The next layer is staggered so that the centers of the balls at layer L_{n+1} are located vertically on top of the centers of the $\uparrow$-triangle of layer L_n. The difference between the *fcc* and *hcp* version of the orange stacking comes from the flip $\uparrow\rightarrow\downarrow$ on L_{n-1} in the fcc case while the hcp reproduces exactly L_{n+1}. As seen in Fig. 2, the family of nearest neighbors of a point is a polyhedron with 12 vertices, 14 facets, 24 edges so that the Euler-Poincaré caracteristic is 2 like for the sphere $\mathbb{S}^2$. Six facets are perfect squares, making with the center a pyramid with square base. It can be computed that the center of the square facet is a Voronoi point for this pyramid, with radius $\check{r}/\sqrt{2}$.

In general, if $A \subset \mathrm{AN}(y)$ has $d+1$ atoms and is contained into an affine hyperplane H_A, let then y_A denotes the center of the sphere in H_A defined by A. That this point is unique comes from the fact that it belongs to the intersection of tiles of atoms in A, so this intersection must be compact. If it where not unique it would be given by the kernel of a non invertible matrix, which excludes compactness. If $y_A \neq y$ then the vector $y - y_A$ is perpendicular to H_A. In addition the remaining point $x_A \in \mathrm{AN}(y) \setminus A$ cannot be contained in H_A, Thanks to Theorem 10. So the geometry of $\mathrm{AN}(y)$ is a tilted version of the square pyramid for the Kepler lattice. Moving x_A slightly would not move A, thus would not move y_A, so that y would move slightly along the line orthogonal to H_A passing through y_A. Hence such a move would not change the V-degree of y. It follows that the only way to breaks the degeneracy of y is to move one of the atoms in A either outside of the empty sphere or inside. This case can be reduced to the situation of generic case in dimension $d-1$ by considering locally the traces of the Voronoi tiles inside H_A. But this method is specific to this situation.

However, in view of the random character of thermal motion of atoms in real material, the non generic situation is practically irrelevant for Physics. Indeed such configurations have zero probabilities if the probability is locally absolutely continuous with respect t the Lebesgue measure. This is the main reason why the author never went beyond this point. Hopefully this argument will be investigated more thoroughly in a future publication.

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