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Uniqueness Theorem for Locally Antipodal Delaunay Sets

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Abstract—We prove theorems on locally antipodal Delaunay sets. The main result is the proof of a uniqueness theorem for locally antipodal Delaunay sets with a given $2R$-cluster. This theorem implies, in particular, a new proof of a theorem stating that a locally antipodal Delaunay set all of whose $2R$-clusters are equivalent is a regular system, i.e., a Delaunay set on which a crystallographic group acts transitively.

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INTRODUCTION

This paper is a continuation of the studies [8, 9] on the so-called locally antipodal Delaunay sets, i.e., sets in which every $2R$-cluster is centrally symmetric (antipodal) with respect to its center. In particular, it was proved that if all $2R$-clusters are equivalent, then the set is a regular system and, hence (by the Schoenflies–Bieberbach theorem), is periodic.

The study of locally antipodal sets has been motivated by the fact that atoms during crystallization often form centrally symmetric clusters for physical reasons. The theorem on regularity of locally antipodal Delaunay sets, just as the series of theorems on their crystallinity in the large, is a continuation of the local theory of regular and crystal structures that was laid down in [7]. As is well known, this theory is aimed at formulating and proving necessary and sufficient conditions for the regularity/crystallinity of a Delaunay set in terms of the congruence of its local fragments. The repetitiveness of local fragments in a crystal structure is attributed by physicists to the fact that "when the atoms of matter are not moving around very much, they get stuck together and arrange themselves in a configuration with as low an energy as possible. If the atoms in a certain place have found a pattern which seems to be of low energy, then the atoms somewhere else will probably make the same arrangement. For these reasons, we have in a solid material a repetitive pattern of atoms" (R. Feynman [10]).

If we recall the aphorism sometimes attributed to H. Poinaré ("science is a cemetery of hypotheses"), the local theory of crystal structures is a "grave" for the well-known postulate on the relationship between the repetitiveness of local fragments in the atomic structure of a crystal and its "global order," i.e., the existence of a spatial symmetry group of the crystal.

The distinguishing feature of the theorems for locally antipodal sets is that they require just the coincidence of clusters of radius $2R$ as a sufficient condition for regularity. To better appreciate the "modesty" of this requirement, recall[1] that in the class of all Delaunay sets, even in the case of the plane, for a set to be regular, one should require the coincidence of the $4R$-clusters. Indeed, for every $\varepsilon > 0$, one can construct a Delaunay set in which all $(4R - \varepsilon)$-clusters are equivalent, although the set is not a regular system.

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[1] M. I. Shtogrin, Private communication, 1980. See also [8].

It is useful to begin the presentation of the main results with the proof of Theorem 1 given in [8] as well as with the proof of a new theorem (Theorem 2). This order is motivated by the fact that both the idea of the proof of Theorem 1 and Theorem 2 itself are used in the proof of Theorem 3. Theorem 4 on regularity of locally antipodal Delaunay sets with equivalent $2R$-clusters follows from Theorem 3.

1. MAIN DEFINITIONS AND RESULTS

A set $X \subset \mathbb{R}^d$ is called a *Delaunay set* with parameters r and R, where $r, R > 0$ (or an (r,R)-*system*, see [6]), if it satisfies the following two conditions:

(1) the open d-ball $B_y^\circ(r)$ of radius r with center at an *arbitrary* point $y \in \mathbb{R}^d$ contains at most one point from X:
$$\#(B_y^\circ(r) \cap X) \le 1; \tag{r}$$

(2) any closed d-ball $B_y(R)$ of radius R contains at least one point from X:
$$\#(B_y(R) \cap X) \ge 1. \tag{R}$$

Note that in view of condition (r), the distance between any two points is at least $2r$.

For $x \in X$, we set $C_x(\rho) := X \cap B_x(\rho)$ and say that $C_x(\rho)$ is the ρ-*cluster* of the point x. In fact, by a ρ-cluster $C_x(\rho)$ one means a pair (center, set of points): $(x, C_x(\rho))$. Information on such a pair is contained in the very notation $C_x(\rho)$. We stress that we distinguish between the ρ-clusters $C_x(\rho)$ and $C_{x'}(\rho)$ of different points x and x' even if the sets of points that belong to these clusters coincide.

Two ρ-clusters $C_x(\rho)$ and $C_{x'}(\rho)$ are said to be *equivalent* if there exists an isometry $g \in O(d)$ such that
$$g\colon\ x \mapsto x' \qquad \text{and} \qquad g\colon\ C_x(\rho) \to C_{x'}(\rho).$$

Note that the requirement of equivalence of clusters is somewhat stronger than the requirement of congruence of the sets of points that belong to these clusters.

Let X be a Delaunay set. If for every $\rho > 0$ the number of classes of equivalent ρ-clusters is finite, then the set X is said to be of *finite type*. For a Delaunay set X of finite type, denote the number of classes of ρ-clusters by $N(\rho)$. The function $N(\rho)$ in such a Delaunay set is positive, integer-valued, nondecreasing, piecewise constant, and right-continuous. Important examples of Delaunay sets of finite type are given by regular systems and by a more general class of Delaunay sets, the so-called crystals.

A *regular system* is a Delaunay set whose symmetry group acts transitively; i.e., for any two points x and x' in X, there exists an isometry g of the space $\mathbb{R}^d$ such that
$$g\colon\ x \mapsto x' \qquad \text{and} \qquad g\colon\ X \to X.$$

A set $X \subset \mathbb{R}^d$ is a regular system if and only if it is an orbit of a point $x \in \mathbb{R}^d$ under some crystallographic group G acting in $\mathbb{R}^d$.

Recall that a subgroup $G \subset \mathrm{Iso}(d)$, where $\mathrm{Iso}(d)$ is the group of all isometries of the space $\mathbb{R}^d$, is called a *crystallographic group* if

(1) G acts discontinuously at every point $x \in \mathbb{R}^d$; i.e., the orbit $G \cdot x$ is discrete;

(2) G has a compact fundamental domain.

A *crystal* is a Delaunay set that is an orbit $G \cdot X_0$ of a *finite* set X_0 under some crystallographic group G.

Thus, a regular system is an important case of a crystal, with $\#(X_0) = 1$. In terms of the cluster-counting function $N(\rho)$, these sets are distinguished as follows. A Delaunay set is a regular system if and only if $N(\rho) \equiv 1$ on $\mathbb{R}_+$. A Delaunay set is a crystal if and only if the cluster-counting function is bounded:

$$N(\rho) \le m < \infty, \qquad \text{where} \quad m \le \#(X_0).$$

If $m = 1$, then the crystal is a regular system. The possible inequality $m < \#(X_0)$ is due to the fact that some points in the set X_0 may generally belong to the same G-orbit.

Regular systems were introduced and studied by Sohncke [2] and Fedorov [1].

Theorem (Schoenflies [3] for $d = 3$, Bieberbach [4, 5] for $d \ge 4$)**.** *Every crystallographic group $G \subset \mathrm{Iso}(\mathbb{R}^d)$ contains a finite-index subgroup T of parallel translations of the space*:

$$G = T \cup Tg_2 \cup \ldots \cup Tg_h,$$

where the index h is bounded by a constant depending on d: $h \le H(d)$.

By the Schoenflies–Bieberbach theorem, every crystal $G \cdot X_0$ decomposes into a finite number ($\le mh$) of congruent parallel lattices of rank d:

$$G \cdot X_0 = \bigcup_{i=1}^{m} \bigl(T \cdot x_i \cup T \cdot g_2(x_i) \cup \ldots \cup T \cdot g_h(x_i)\bigr), \qquad x_i \in X_0.$$

Consider the *group* of a ρ-cluster $C_x(\rho)$ as a subgroup $S_x(\rho)$ of $\mathrm{Iso}(d)$ that consists of isometries s such that

$$s\colon\ x \mapsto x, \qquad s\colon\ C_x(\rho) \mapsto C_x(\rho),$$

and denote by $M_x(\rho)$ the order of the group $S_x(\rho)$. Since X is a Delaunay set (with parameters r and R), the dimension of the affine hull of the ρ-cluster is finite for every $\rho \ge 2R$; hence, the function $M_x(\rho) \ge 1$ is defined on $[2R, \infty)$ and is integer-valued, left-continuous, piecewise constant, and nonincreasing. That the order $M_x(\rho)$ does not increase is because each symmetry of a larger ρ'-cluster $C_x(\rho')$ must also leave invariant a smaller ρ-cluster $C_x(\rho)$, $\rho < \rho'$. Therefore, the group $S_x(\rho')$ of the larger cluster $C_x(\rho')$ either coincides with the group $S_x(\rho)$ or is a proper subgroup of the latter.

A Delaunay set X is said to be *locally antipodal* if for every point $x \in X$ the $2R$-cluster $C_x(2R)$ is centrally symmetric with respect to the point x, i.e., if for every $x \in X$ the group $S_x(2R)$ contains the central symmetry with respect to x.

Theorem 1 [8]**.** *A locally antipodal Delaunay set X is globally antipodal with respect to each of its points x.*

Theorem 2 [9]**.** *Any locally antipodal Delaunay set $X \subset \mathbb{R}^d$ can be represented as*

$$X = \bigcup_{i=1}^{N} (x + v_i + \Lambda), \tag{1.1}$$

where $x \in \mathbb{R}^d$ is a point, Λ is a d-dimensional lattice, and the vectors $v_1, v_2, \ldots, v_N$, where $1 \le N \le 2^d - 1$, are representatives of some cosets of the quotient lattice $\frac{\Lambda}{2}/\Lambda$.

Theorem 3. *Let X be a locally antipodal Delaunay set with a parameter R, and let $Y \subset \mathbb{R}^d$ be an arbitrary* (*not necessarily Delaunay*) *set in which the $2R$-cluster $C'_y(2R)$ of every point $y \in Y$ is antipodal with respect to y. Suppose that $x \in X \cap Y$ and $C_x(2R) = C'_x(2R) \subset X \cap Y$. Then $X = Y$.*

The hypothesis of the theorem does not require that Y should be a Delaunay set; i.e., we do not even rule out the possibility that the $2R$-cluster $C_y(2R)$ is an infinite set. And only for one point $x \in X \cap Y$ we assume that the $2R$-cluster $C'_x(2R)$ in the set Y coincides with the $2R$-cluster $C_x(2R)$ of the Delaunay set X. Theorem 3 strengthens a theorem announced in [9] in which both sets X and Y are assumed to be Delaunay sets.

The following theorem is an easy corollary of Theorem 3.

Theorem 4 [8, 9]**.** *Let $N(2R) = 1$ for a locally antipodal Delaunay set X. Then X is a regular system, i.e., $N(\rho) \equiv 1$ for all $\rho > 0$.*

Proof. Let us prove that for an arbitrary pair $x, x' \in X$ there exists an isometry g such that $g(x) = x'$ and $g(X) = X$. Indeed, since $N(2R) = 1$, there exists a g such that $g(x) = x'$ and $g(C_x(2R)) = C_{x'}(2R)$.

Set $Y := g^{-1}(X)$. It is clear that the sets X and Y satisfy the hypothesis of Theorem 3. Therefore, $X = Y$. Hence, $g(X) = g(Y) = g(g^{-1}(X)) = X$. Thus, the symmetry group of X acts on X transitively. Since X is a Delaunay set, it follows that X is a regular system. Theorem 4 is proved. $\square$

2. PROOFS OF THEOREMS 1–3

Proof of Theorem 1. Suppose the contrary, i.e., that some locally antipodal Delaunay set X is not centrally symmetric with respect to some of its points x_0. Then there exists a point $x_1 \in X$ such that the point x'_1 symmetric to it with respect to x_0 does not belong to X. Since X is a Delaunay set, we can assume without loss of generality that the point x_1 minimizes the distance $|x_1 - x_0|$ over all points x_1 with the indicated property.

Set $\rho := |x_1 - x_0|$. Since the cluster $C_{x_0}(2R)$ is centrally symmetric, we have $\rho > 2R$.

Let z and z' be the points lying on the line segment $[x_0 x_1]$ at a distance of R and $2R$ from the point x_1, respectively. It is easy to see that the balls $B_z(R)$ and $B_{z'}(2R)$ are tangent to the sphere $\partial B_{x_0}(\rho)$ from the inside at the point x_1. In addition, the ball $B_{z'}(2R)$ is homothetic to the ball $B_z(R)$ with homothety center at the point x_1 and with ratio 2.

In view of conditions (r) and (R) from the definition of a Delaunay set, the intersection $X \cap B_z(R)$ cannot consist of a single point x_1. Therefore, we can choose a point $x_2 \neq x_1$ such that $x_2 \in X \cap B_z(R)$. It is clear that

$$|x_2 - x_1| \leq 2R.$$

By the hypothesis of the theorem, the cluster $C_{x_2}(2R)$ is antipodal. Moreover, $x_1 \in C_{x_2}(2R)$. Therefore, if x_3 is a point symmetric to x_1 with respect to x_2, then $x_3 \in X$. On the other hand, it is easy to see that $x_3 \in B_{z'}(2R)$ and $x_3 \neq x_1$. Consequently,

$$|x_3 - x_0| < \rho.$$

Finally, the conditions $x_2 \in B_z(R)$ and $x_2 \neq x_1$ imply

$$|x_2 - x_0| < \rho.$$

Let x'_1, x'_2, and x'_3 be the points symmetric to x_1, x_2, and x_3 with respect to x_0. In view of the choice of the point x_1 (as a closest point to x whose antipode with respect to x does not belong to X), we have $x'_2 \in X$ and $x'_3 \in X$. However, since $|x'_3 - x'_2| = |x_3 - x_2| \leq 2R$, the point x'_3 belongs to the cluster $C_{x_2}(2R)$. Since the cluster $C_{x_2}(2R)$ is antipodal with respect to x_2, it follows that the point x'_1, which is symmetric to x'_3 with respect to x'_2, also belongs to $C_{x_2}(2R) \subset X$. Thus, $x'_1 \in X$. But this contradicts the assumption that the point symmetric to x_1 with respect to x does not belong to X. $\square$

Similar arguments will be used in the proof of Theorem 3.

Proof of Theorem 2. Denote by $t(v)$ the parallel translation by a vector v, and let $T(X)$ be the group of all translational isometries of the set X. Set

$$\Lambda := \{v\colon\ t(v) \in T(X)\}.$$

It is clear that the set Λ is discrete; therefore, it is a lattice. Let us show that the rank of the lattice Λ is d.

It is easy to see that for any pair of points $x, x' \in X$ we have $2(x' - x) \in \Lambda$. Indeed, by Theorem 1, the central symmetries with respect to each of the points x and x' are symmetries of the set X. Hence, the parallel translation by the vector $2(x' - x)$, which is the composition of these symmetries, is also a symmetry of the set X. Since X is a Delaunay set, it follows that the rank of the lattice Λ is d.

The Delaunay set X is a union of a finite number of lattices that are congruent and parallel to the lattice Λ, i.e.,

$$X = \bigcup_{i=1}^{N} (x_i + \Lambda).$$

However, by what has been proved above, for $i = 2, 3, \dots, N$ we have $x_i - x_1 \in \Lambda/2$. Setting $x := x_1$ and $v_i = x_i - x_1$ $(i = 1, 2, \dots, N)$, we obtain (1.1). The inequality $N \le 2^d$ follows from the fact that the number of classes in $\Lambda/2\Lambda$ is at most 2^d. The case $N = 2^d$ is also impossible, because then

$$T(X) = \{v\colon\ v \in \Lambda/2\}.$$

In this case the set T is a lattice for which Λ is a proper sublattice. However, this contradicts the definition of the lattice Λ as a maximal group of translations of the set X. $\square$

Proof of Theorem 3. We will prove the inclusions $X \subseteq Y$ and $Y \subseteq X$.

1. Let us prove that $X \subseteq Y$.

Suppose the contrary: $X \setminus Y \neq \varnothing$. Since X is a Delaunay set, one can choose a point $x_1 \in X \setminus Y$ that is closest to the point x among the points of the set $X \setminus Y$.

Set $\rho := |x_1 - x|$, and let $C'_y(\rho)$ be a cluster in the set Y. Notice that $x \in X \cap Y$ and that the equality $C_x(2R) = C'_x(2R)$ rules out the case of $\rho \le 2R$. Therefore, we can assume that $\rho > 2R$.

Let z and z' be the points lying on the line segment $[xx_1]$ at a distance of R and $2R$ from the point x_1, respectively. Notice that z and z' may not lie in X or in Y. It is easy to see that the balls $B_z(R)$ and $B_{z'}(2R)$ are tangent to the sphere $\partial B_x(\rho)$ from the inside at the point x_1. Moreover, the ball $B_{z'}(2R)$ is homothetic to the ball $B_z(R)$ with homothety center at x_1 and with ratio 2. Therefore, the following strict inclusions are valid:

$$B_x(\rho) \supset B_{z'}(2R) \setminus \{x_1\} \supset B_z(R) \setminus \{x_1\}.$$

By conditions (r) and (R), the intersection $X \cap B_z(R)$ cannot consist of a single point x_1, because the point x_1 is located on the boundary of the ball $B_z(R)$. Therefore, we can choose a point $x_2 \neq x_1$ in X such that $x_2 \in X \cap B_z(R)$. It is clear that $|x_2 - x_1| \le 2R$. Moreover, $|x_2 - x| < \rho$. The assumption that x_1 is the closest point to x in $X \setminus Y$ implies that the point $x_2 \in X$ also belongs to Y: $x_2 \in Y$.

By the hypothesis of the theorem, the cluster $C_{x_2}(2R)$ is antipodal. Moreover, $x_1 \in C_{x_2}(2R)$. Therefore, if x_3 is the point symmetric to x_1 with respect to x_2, then $x_3 \in X$.

On the other hand, it is easy to see that $x_3 \in B_{z'}(2R)$ and $x_3 \neq x_1$. Therefore, $|x_3 - x| < \rho$. By the choice of the value of ρ, we have $x_3 \in Y$.

Thus, we have $x_2 \in Y$, $x_3 \in Y$, and $|x_3 - x_2| \le 2R$. Finally, consider the cluster $C'_{x_2}(2R)$, which, according to the hypothesis of the theorem, is symmetric with respect to the point x_2 and contains the point x_3. Hence, it also contains the point x_1, i.e., $x_1 \in Y$. We have obtained a contradiction to the assumption that $x_1 \in X \setminus Y$. Thus, the inclusion $X \subseteq Y$ is proved.

2. Let us prove that $Y \subseteq X$. Suppose the contrary: $Y \setminus X \neq \varnothing$.

Take an arbitrary point $y_1 \in Y \setminus X$, and let $|y_1 - x| = \rho$, where $\rho > 2R$. Let us show that there exists an infinite sequence of points

$$y_1, y_2, \dots, y_n, \dots$$

such that

(1) $y_i \in Y \setminus X$,

(2) $|y_{i+1} - x| < |y_i - x|$, and

(3) $(y_i + y_{i+1})/2 \in X$.

Let us show that there exists a point y_2 that does not violate conditions (1)–(3); the subsequent terms of the sequence can be constructed in a similar way.

Let z and z' be the points lying on the line segment $[xy_1]$ at a distance of R and $2R$ from the point y_1, respectively. It is easy to see that the balls $B_z(R)$ and $B_{z'}(2R)$ are tangent to the sphere $\partial B_x(\rho)$ from the inside at the point y_1. Moreover, the ball $B_{z'}(2R)$ is homothetic to the ball $B_z(R)$ with homothety center at y_1 and with ratio 2.

By condition (R), the intersection $X \cap B_z(R)$ is nonempty. Therefore, one can choose a point $x_1 \in X \cap B_z(R)$. Since $x_1 \in X$, we have (as shown above) $x_1 \in Y$.

The cluster $C'_{x_1}(2R)$ is antipodal. Hence, it contains a point y_2 symmetric to the point y_1 with respect to x_1. Thus, condition (3) for $i = 1$ is satisfied. If it turned that $y_2 \in X$, then the cluster $C_{x_1}(2R)$ would also contain y_1 (together with y_2). But this is impossible, because $y_1 \notin X$. Hence, condition (1) for $i = 2$ is satisfied. Finally, condition (2) for $i = 1$ takes the form $|y_2 - x| < \rho$. This inequality is valid because $y_2 \in B_{z'}(2R)$.

Thus, we have found a sequence $\{y_i\}$ satisfying conditions (1)–(3). Next, we apply Theorem 2. Notice that by condition (3), the subsequence $\{y_{2k+1}\}$ consists of points of the form $y_1 + v$, where the vector v belongs to the lattice Λ from formula (1.1).

It follows from condition (2) that all terms of the sequence $\{y_i\}$ are different and lie in the ball $B_x(\rho)$, with $\rho := |x - y_1|$. However, the ball $B_x(\rho)$ can contain only a finite number of different points of the form

$$y_1 + v, \qquad \text{where} \quad v \in \Lambda.$$

The contradiction obtained proves the inclusion $Y \subseteq X$.

The theorem is proved. □

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