Multiregular Point Systems

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Abstract

This paper gives several conditions in geometric crystallography which force a structure X in $\mathbb{R}^n$ to be an ideal crystal. An ideal crystal in $\mathbb{R}^n$ is a finite union of translates of a full-dimensional lattice. An (r, R)-set is a discrete set X in $\mathbb{R}^n$ such that each open ball of radius r contains at most one point of X and each closed ball of radius R contains at least one point of X. A multiregular point system X is an (r, R)-set whose points are partitioned into finitely many orbits under the symmetry group $Sym(X)$ of isometries of $\mathbb{R}^n$ that leave X invariant. Every multiregular point system is an ideal crystal and vice versa. We present two different types of geometric conditions on a set X that each imply that it is a multiregular point system. The first is that if X "looks the same" when viewed from $n + 2$ points $\{\mathbf{y}_i : 1 \leq i \leq n + 2\}$, such that one of these points is in the interior of the convex hull of all the others, then X is a multiregular point system. The second is a "local rules" condition, which asserts that if X is an (r, R)-set and all neighborhoods of X within distance ρ of each $\mathbf{x} \in X$ are isometric to one of k given point configurations, and ρ exceeds CRk for $C = 2(n^2 + 1) \log_2(\frac{2R}{r} + 2)$, then X is a multiregular point system that has at most k orbits under the action of $Sym(X)$ on $\mathbb{R}^n$. In particular, ideal crystals have perfect local rules under isometries.

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1. Introduction

One of the central problems in long-range order is to characterize the various types of ordered discrete structures in $\mathbb{R}^n$ that are possible. The symmetry group $Sym(X)$ of a discrete set X is the set of all Euclidean isometries of $\mathbb{R}^n$ that map X to itself. Crystalline materials have the highest possible symmetry. An *ideal crystal* or *periodic crystal* is a discrete set X in $\mathbb{R}^n$ which is a finite union of translates of a full-dimensional lattice L in $\mathbb{R}^n$. An ideal crystal is just a discrete set X that contains a full-dimensional lattice L in its symmetry group; however, $Sym(X)$ need not act transitively on X. This definition of ideal crystal extends a definition of a three-dimensional crystal composed of several species of atoms that was proposed in 1888 by Sohncke [25, p. 433].

The recent discovery and study of quasicrystals (see [25]) raises the question: what geometric and physical conditions force a structure to be crystalline rather than quasicrystalline? In this paper we prove several results giving minimal geometric conditions on a discrete set X in $\mathbb{R}^n$ that are sufficient to imply that X is an ideal crystal. These conditions involve concepts in geometric crystallography, and particularly the notion of multiregular point system which we define below.

Geometric crystallography was initiated by Bravais [1] and Sohncke ([27]–[29]), see also [9], [14, Chapter 2] and [24]. The basic structures that it studies are *Delone sets*, also called *Delaunay sets* or *(r, R)-sets*, which are those sets X in $\mathbb{R}^n$ that satisfy the two conditions:

(i) *Uniform discreteness.* There is an $r > 0$ such that any open ball of radius r in $\mathbb{R}^n$ contains at most one point of X.

(ii) *Relative denseness.* There is an $R > 0$ such that any closed ball of radius R in $\mathbb{R}^n$ contains at least one point of X.

These sets are named after B. N. Delone who introduced them in 1937, see [6], [12].

Geometric crystallography is concerned with how a Delone set X looks when viewed from each of its points. A *regular point system* X is a Delone set such that X "looks the same" from every point $\mathbf{x} \in X$. Regular point systems X are exactly those Delone sets whose symmetry group $Sym(X)$ acts transitively on X, so that X is a single orbit $Sym(X).\mathbf{x}$ of $Sym(X)$. Alternatively, we define the (global) *star $ST_{\mathbf{y}}(X)$ of a set X* centered at a point $\mathbf{y} \in \mathbb{R}^n$ to be the collection of line segments from $\mathbf{y}$ to every $\mathbf{x} \in X$, namely

$$ST_{\mathbf{y}}(X) := \{[\mathbf{y}, \mathbf{x}] : \mathbf{x} \in X\} \ .$$

Then X is a regular point system if for each pair $\mathbf{x}_1, \mathbf{x}_2 \in X$ there exists an isometry $g = g(\mathbf{x}_1, \mathbf{x}_2)$ such that

$$g(ST_{\mathbf{x}_1}(X)) = ST_{\mathbf{x}_2}(X) \ .$$

We set

$$ST(X) := \{ST_{\mathbf{x}}(X) : \mathbf{x} \in X\} \ ,$$

and let $|ST(X)|$ denote the number of distinct isometry classes among all $ST_{\mathbf{x}}(X)$ for $\mathbf{x} \in X$. A regular point system is just a Delone set X with the property that $|ST(X)| = 1$.

One of the major results of geometric crystallography is that a regular point system is an ideal crystal. However not all ideal crystals are regular point systems.

Definition 1.1. *A multiregular point system* is any Delone set X such that the action of its symmetry group $Sym(X)$ partitions the points of X into a finite number of orbits. That is, a multiregular point system is any Delone set X such that $|ST(X)|$ is finite.

Every ideal crystal is a multiregular point system. In fact multiregular point systems coincide with ideal crystals, as was shown by Galiulin [11]. The following theorem includes this result, and also gives another characterization of multiregular point systems, in terms of the concept of crystallographic group, for which we give several equivalent definitions in §2.

Theorem 1.1. *The following conditions on a set X in $\mathbb{R}^n$ are equivalent.*

(i). *X is a multiregular point system. That is, X is a Delone set and the set of isometry classes among $\{ST_{\mathbf{x}}(X) : \mathbf{x} \in X\}$ is finite.*

(ii). X is an ideal crystal. That is, X is a finite union of translates of an n-dimensional lattice L, with $X = \cup_{i=1}^{k}(\mathbf{x}_i + L)$.

(iii). X is a discrete set whose symmetry group $Sym(X)$ is a crystallographic group.

The equivalence (ii) ⇔ (iii) is a well known corollary of Bieberbach's first theorem (see [27, Theorem 2]). We give a proof of Theorem 1.1 at the end of §2.

The first type of geometric condition on a set X that we consider requires that suitable finite sets of global stars $ST_{\mathbf{y}_i}(X)$ of X are isometric. These conditions are global in the sense that a star involves lines to every point of X; however only finitely many stars are used. One such result is:

Theorem 1.2. *Let X be a discrete set in $\mathbb{R}^n$ and let Y be a finite set in $\mathbb{R}^n$ with $|Y| = n+2$, such that the convex hull of Y is a full-dimensional simplex containing one point of Y in its interior. If the $n+2$ stars $\{ST_{\mathbf{y}}(X) : \mathbf{y} \in Y\}$ are all isometric, then $Sym(X)$ is a crystallographic group, and X is an ideal crystal.*

It is easy to show that every ideal crystal contains a set $Y \subseteq X$ having the properties above. We derive this result in §3 as a special case of a more general criterion (Theorem 3.1).

The condition on Y in Theorem 1.2 cannot be relaxed to merely requiring that the convex hull of Y be full-dimensional. For example, let X in $\mathbb{R}^3$ be the 12 vertices of a regular icosahedron, and take $Y = X$. Here $Sym(X)$ is the alternating group A_5, which is transitive on X, and all $\{ST_{\mathbf{x}}(X) : \mathbf{x} \in X\}$ are isometric, but X is not an ideal crystal.

The second type of geometric condition that we consider consists of "local rules" that require that the elements in X in a fixed finite neighborhood of each $\mathbf{x} \in X$ to be isometric to one of a finite set of point configurations.

Definition 1.2. A set of *local rules* of radius ρ_0 is a finite collection $\mathcal{L} = \{L_i\}$ of discrete sets L_i with $\mathbf{0} \in L_i$ and with each L_i contained in the closed ball $B(\mathbf{0}; \rho_0)$ of radius ρ_0 around $\mathbf{0}$. A set X satisfies the *local rules $\mathcal{L}$ under isometries* if for each $\mathbf{x} \in X$ the set $(X - \mathbf{x}) \cap B(\mathbf{0}; \rho_0)$ is a rotation of some set L_i in $\mathcal{L}$.

In 1976 Delone et al. [6] showed that if X is an (r, R)-set in $\mathbb{R}^n$ such that all neighborhoods of X within a distance $\rho_0 = \rho_0(r, R, n)$ of each point $\mathbf{x} \in X$ are isometric, then X is a regular point system. In 1988 Dolbilin and Shtogrin [8] announced an analogous result for multiregular point systems. We prove here such a result for multiregular point systems and give an explicit

distance bound $\rho_0(r, R, n, k)$, where $k = |ST(X)|$, stated below.

Definition 1.3. Given $\rho \in \mathbb{R}_{>0}$, the ρ-*star* of X centered at $\mathbf{y} \in \mathbb{R}^n$ is the set of line segments

$$ST_{\mathbf{y}}(X; \rho) := \{[\mathbf{x}, \mathbf{y}] : \mathbf{x} \in X \quad \text{and} \quad ||\mathbf{x} - \mathbf{y}|| \leq \rho\} \ .$$

The set of all ρ-stars of X is denoted

$$ST(X; \rho) := \{ST_{\mathbf{x}}(X; \rho) : \mathbf{x} \in X\} \ .$$

We let $|ST(X; \rho)|$ denote the number of isometry classes among the $ST_{\mathbf{x}}(X; \rho)$ for $\mathbf{x} \in X$, and define the function

$$N_X(\rho) := |ST(X; \rho)| \ , \quad 0 < \rho < \infty \ .$$

In §4 we prove:

Theorem 1.3. *Let X be a Delone set in $\mathbb{R}^n$ with constants (r, R). If for some radius ρ_0 the number $k = N_X(\rho_0)$ of isometry classes of its ρ_0-stars satisfies*

$$N_X(\rho_0) < \frac{\rho_0}{CR} \ , \tag{1.1}$$

with

$$C = 2(n^2 + 1) \log_2 \left(\frac{2R}{r} + 2\right) \ , \tag{1.2}$$

then X is a multiregular point system, and the global stars $\{ST_{\mathbf{x}}(X) : \mathbf{x} \in X\}$ of X are partitioned into exactly k orbits under the action of $Sym(X)$. Furthermore the only Delone sets Y all of whose ρ-stars are isometric to ρ-stars of X are sets globally isometric to X, i.e.

$$Y = Q(X + \mathbf{t}) \quad for \quad some \quad \mathbf{t} \in \mathbb{R}^n \ , \quad Q \in O(n, \mathbb{R}) \ . \tag{1.3}$$

The bound (1.1) in Theorem 1.3 is best possible as a function of ρ_0 up to the value of C, for in §4 we give examples of (r, R)-sets X in $\mathbb{R}^n$ which are not multiregular point systems, but have the property that $N_X(\rho)$ is approximately $(\frac{\sqrt{n}}{2})\frac{\rho}{R}$ for large ρ.

The interest of Theorem 1.3 to crystallography is that it asserts that the atomic structure of any ideal crystal is completely determined by "local conditions" of a fixed radius around each atom separately.

Definition 1.4. Two sets X and X' are *locally isomorphic* if for each finite neighborhood in X an isometric copy of it can be found in X', and vice-versa.

Definition 1.5. A set of local rules $\mathcal{L}$ are *perfect local rules under isometries* if whenever two sets X and X' satisfy $\mathcal{L}$ then X and X' are locally isomorphic. That is, $\mathcal{L}$ determines a unique *local isomorphism class* of sets.

Theorem 1.3 shows that if X is a multiregular point system with parameters (r, R) and with k orbits under the action of $Sym(X)$, then the set $\mathcal{L}$ of ρ_0-stars of X for any

$$\rho_0 > CRk \tag{1.4}$$

is a set of perfect local rules under isometries for X, for by (1.3) the local isomorphism class of X consists only of sets isometric to X. Thus every ideal crystal satisfies perfect local rules under isometries.

There are also various "quasicrystalline" structures that have perfect local rules under isometries. For further discussions and references concerning "perfect local rules" for ideal crystals and quasicrystals, see [15], [17], [19] and [25].

One question remaining about Theorem 1.3 is the extent to which the bound for C in (1.3) can be improved. The value of C in (1.3) depends on n, R and r. It is possible that there exists a smaller bound for C which is a function of the dimension alone. Shtogrin [26] showed for $n = 2$ and $k = 1$ that $\rho > 4R$ suffices for X to be a multiregular point system, and gave an example showing that $4R$ is the best possible value. Dolbilin and Shtogrin [7] showed that for $n = 3$ and $k = 1$ the condition $\rho > 10R$ suffices. Their proof methods do not apply in dimensions $n \geq 4$. Engel [5, Theorem 9.9] announced a general result of this type for $k = 1$, namely that (1.4) can then be weakened to the condition $\rho > 6R$, independent of the dimension. However his proof is incomplete, since it depends on his unproved Conjecture 9.7.

In this paper $\log x$ and $\log_2 x$ represent logarithms to base e and 2, respectively.

2. Crystallographic Groups

In this section we give several characterizations of crystallographic groups, most of which are well known. First, we set some notation. The Euclidean norm on $\mathbb{R}^n$ is denoted $\|\mathbf{x}\| = (\sum_{i=1}^{n} x_i^2)^{1/2}$. For $\rho > 0$, let $B(\mathbf{x}; \rho)$ denote the closed ball of radius ρ around $\mathbf{x}$, given by

$$B(\mathbf{x}; \rho) := \{\mathbf{y} : \|\mathbf{y} - \mathbf{x}\| \leq \rho\} .$$

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Let $B°(\mathbf{x}; \rho)$ denote the corresponding open ball and $\partial B(\mathbf{x}; \rho)$ its boundary,

$$\partial B(\mathbf{x}; \rho) := \{\mathbf{y} : ||\mathbf{y} - \mathbf{x}|| = \rho\} .$$

A subset X of $\mathbb{R}^n$ is *discrete* if it is closed and for each $\mathbf{x} \in X$ there is a radius $\rho_{\mathbf{x}} > 0$ such that

$$X \cap B(\mathbf{x}; \rho_{\mathbf{x}}) = \{\mathbf{x}\} .$$

Let $\mathbb{E}^n$ denote the space $\mathbb{R}^n$ endowed with the Euclidean metric. The Euclidean group $\mathcal{E}_n = Sym(\mathbb{E}^n)$ denotes the group of isometries of $\mathbb{R}^n$. It is a real Lie group of dimension $\frac{n(n+1)}{2}$ and is a semidirect product of the orthogonal group $O(n, \mathbb{R}) = \{Q : QQ^T = I\}$ and the translation group $\mathbb{R}^n$. We denote its elements $g = (Q, \mathbf{t})$ where Q is the *rotational part* of g and $\mathbf{t}$ is the *translational part* of g, with multiplication

$$g'g = (Q', \mathbf{t}')(Q, \mathbf{t}) = (Q'Q, \mathbf{t}' + Q'\mathbf{t}) .$$

A general element $g \in \mathcal{E}_n$ acts on $\mathbb{R}^n$ by

$$g.\mathbf{x} = Q\mathbf{x} + \mathbf{t} . \tag{2.1}$$

The following definitions concern subgroups G of the Euclidean group $\mathcal{E}^n$.

Definition 2.1. A group G is a *discrete subgroup* of $\mathcal{E}_n$ if it is a closed subgroup of $\mathcal{E}_n$ and the topology induced on G from the standard (Euclidean) topology on $\mathcal{E}_n$ is discrete. That is, for each $g \in G$ there is an open set U of $\mathcal{E}_n$ such that $G \cap U = \{g\}$.

Definition 2.2. A group G *acts discontinuously*[1] on $\mathbb{R}^n$ if for every $\mathbf{x} \in \mathbb{R}^n$ the orbit

$$G.\mathbf{x} := \{g.\mathbf{x} : g \in G\}$$

is a discrete set in $\mathbb{R}^n$.

In this definition we allow the possibility that there are distinct $g_1, g_2 \in G$ with $g_1.\mathbf{x} = g_2.\mathbf{x}$.

Definition 2.3. A group G *acts uniformly* on $\mathbb{R}^n$ if the orbit space $\mathbb{R}^n/G$ is compact in the quotient topology.

This definition implies that the translational parts $\mathbf{t}$ of elements of G span $\mathbb{R}^n$ as a vector space. Indeed, call a group G of isometries *irreducible* if for each invertible affine map $\alpha : \mathbb{R}^n \rightarrow \mathbb{R}^n$

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[1] Schwartzenberger [23] terms this "*acts discretely* on $\mathbb{R}^n$."

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the group $G' = \alpha G \alpha^{-1}$ has the property that the translational parts of all elements of G' span $\mathbb{R}^n$. A group G of isometries is irreducible if and only if it acts uniformly on $\mathbb{R}^n$, see Charlap [2, p. 3].

Definition 2.4. A group G is *crystallographic* if it acts uniformly and discontinuously on $\mathbb{R}^n$. (This is the definition of Charlap [2, p. 4].)

Definition 2.5. A group G is a *space group* if the subgroup T of all pure translations in G is an n-dimensional lattice. (See Schwarzenberger [16, p. 26].)

The following theorem gives several necessary and sufficient conditions for a group G to be crystallographic. All of these criteria are quite well known, except for (v), which will be the criterion we mainly use in this paper.

Theorem 2.1. *The following properties of a group G contained in the Euclidean group $\mathcal{E}_n = Sym(\mathbb{E}^n)$ are equivalent.*

(i). *G is a crystallographic group. That is, G acts uniformly and discontinuously on $\mathbb{R}^n$.*

(ii). *G is a space group. That is, the subgroup of pure translations T in G is an n-dimensional lattice, which is necessarily the maximal abelian subgroup of G.*

(iii). *G is a discrete subgroup of $\mathcal{E}_n$ and $\mathcal{E}_n/G$ is compact.*

(iv). *Every orbit $G.\mathbf{x} = \{g.\mathbf{x} : g \in G\}$ is a Delone set in $\mathbb{R}^n$.*

(v). *There exists one orbit $G.\mathbf{x}$ which is a discrete, relatively dense set in $\mathbb{R}^n$.*

Remark. We later obtain an even weaker version of (v) in Corollary 3.1.

Proof. (i) $\Leftrightarrow$ (ii). The direction (i) $\Rightarrow$ (ii) is Bieberbach's first theorem, see Buser [2], Charlap [2, p. 17], Milnor [18] or Vince [31]. Besides being of finite index in G, T is the unique maximal, normal, abelian subgroup of G, see [2, p. 18]. For (ii) $\Rightarrow$ (i) we use [2, p. 4 bottom] to obtain that G acts uniformly. Next T is of finite index in G [16, p. 26] and acts discontinuously on $\mathbb{R}^n$. We complete this step by using the observation that if G contains a subgroup of finite index that acts discontinuously on $\mathbb{R}^n$, then G also acts discontinuously on $\mathbb{R}^n$.

(ii) $\Rightarrow$ (iii). This is a theorem in Schwarzenberger [16, p. 27].

(iii) $\Rightarrow$ (i). This is also a theorem of Bieberbach, see Schwarzenberger [16, p. 29].

(ii) $\Rightarrow$ (iv). Any orbit $T.\mathbf{x}$ is a translate of the n-dimensional lattice $T.\mathbf{0}$. Since $[G:T]$ is finite and T is a normal subgroup of G, the set $G.\mathbf{x}$ consists of $[G:T]$ translates of $T.\mathbf{0}$, hence it is a Delone set.

(iv) $\Rightarrow$ (v). Trivial.

(v) $\Rightarrow$ (iii). Since $G.\mathbf{x}$ is relatively dense, the vectors in $G.\mathbf{x}$ span $\mathbb{R}^n$, because they clearly cannot all lie in an $(n-1)$-dimensional affine subspace. This, together with $G.\mathbf{x}$ being a discrete set, implies that any element g of G sufficiently close to the identity e must be the identity, hence G is a discrete subgroup of $\mathcal{E}_n$.

To show that $\mathcal{E}_n/G$ is compact, it suffices to show that for any $g' \in \mathcal{E}_n$ with $g'.\mathbf{z} = Q'\mathbf{z} + \mathbf{t}'$ we can find some element $g \in G$, say $g.\mathbf{z} = Q\mathbf{z} + \mathbf{t}$, such that the element $g'g$ with

$$g'g.\mathbf{z} = Q'Q\mathbf{z} + Q'\mathbf{t} + \mathbf{t}'$$

has $||Q'\mathbf{t} + \mathbf{t}'||$ bounded, because any region $O(n, \mathbb{R}) \times \{\mathbf{t} : ||\mathbf{t}|| \le R'\}$, for any R', is a compact subset of $\mathcal{E}_n$. Let $||Q||_2$ denote the Frobenius norm on matrices, which is

$$||Q||_2 = \big(\sum_{i,j=1}^{n} Q_{ij}^2 \big)^{1/2} = (Tr(QQ^T))^{1/2} \ ,$$

and note that orthogonal matrices Q satisfy $||Q||_2 = \sqrt{n}$. We now view the orbit $G.\mathbf{x}$ as generated by that element $\mathbf{x}$ in the orbit which minimizes $||\mathbf{x}||$. Then $||\mathbf{x}|| \le R$ since $G.\mathbf{x}$ is relatively dense with constant R. By relative denseness we can also find $\mathbf{y} \in G.\mathbf{x}$ such that

$$||\mathbf{y} - (Q')^{-1}\mathbf{t}'|| \le R \ .$$

Next choose a $g \in G$ with $\mathbf{y} = g.\mathbf{x} = Q\mathbf{x} + \mathbf{t}$. Then $g'g$ has translation part satisfying

$$
\begin{aligned}
||Q'\mathbf{t} + \mathbf{t}'|| &= ||Q'(\mathbf{y} - Q\mathbf{x}) + \mathbf{t}'|| \ , \\
&\le ||Q'||_2 \, ||\mathbf{y} - (Q')^{-1}\mathbf{t}'|| + ||Q'||_2 \, ||Q||_2 \, ||\mathbf{x}|| \ , \\
&\le (\sqrt{n} + n)R \ ,
\end{aligned}
$$

which is the desired bound. $\square$

¿From Theorem 2.1 we easily deduce Theorem 1.1.

Proof of Theorem 1.1. (i). $\Rightarrow$ (iii). Choose a radius ρ sufficiently large that the ball $B(\mathbf{0}; \rho)$ contains representatives $\{\mathbf{x}_i : 1 \le i \le |ST(X)|\}$ of each type of global star $ST_{\mathbf{x}_i}(X)$. For

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any $\mathbf{x} \in X$ there exists some $\mathbf{x}_j$ such that $ST_{\mathbf{x}}(X)$ is isometric to $ST_{\mathbf{x}_j}(X)$ via an isometry $g = g(\mathbf{x}, \mathbf{x}_j) \in Sym(X)$. Then for each i,

$$||g^{-1}.\mathbf{x}_i - \mathbf{x}|| = ||g^{-1}.(\mathbf{x}_i - \mathbf{x}_j)|| \leq 2\rho \ ,$$

and $ST_{g^{-1}.\mathbf{x}_i}(X)$ is isometric to $ST_{\mathbf{x}_i}(X)$. Thus each of the sets

$$X_i := \{\mathbf{x} \in X : ST_{\mathbf{x}}(X) \text{ is isometric to } ST_{\mathbf{x}_i}(X)\}$$

is relatively dense with constant $2\rho + R$. Since

$$X_i \subseteq Sym(X).\mathbf{x}_i \subseteq X \ ,$$

it follows that the $Sym(X)$-orbit of $\mathbf{x}_i$ is discrete and relatively dense, hence $Sym(X)$ is a crystallographic group by property (v) of Theorem 2.1.

(iii). $\Rightarrow$ (ii). X is invariant under the maximal abelian subgroup T contained in $Sym(X)$, which is an n-dimensional lattice since $Sym(X)$ is a crystallographic group. Now X is a union of orbits $T.\mathbf{x}$, each of which is a translate of the lattice $L = T.\mathbf{0}$. Since X is a discrete set, there can only be finitely many such orbits.

(ii) $\Rightarrow$ (i). Immediate. $\quad\square$

For each crystallographic group G there exists some multiregular point system such that $G = Sym(X)$. This contrasts with the situation for regular point systems. For example, there is no regular point system X with $Sym(X)$ equal to a group G of pure translations $\mathbb{Z}^n$. Indeed the orbit $G.\mathbf{x}$, which is a translate of a full-rank lattice, has a strictly larger symmetry group than G, for $Sym(G.\mathbf{x})$ contains a reflection $g.\mathbf{y} := \mathbf{x}_0 - \mathbf{y}$ around any given point $\mathbf{x}_0 \in G.\mathbf{x}$. For this reason the classification of regular point systems differs from that of crystallographic groups.

We conclude this section with the following consequence of Theorem 1.1. Call a set X in $\mathbb{R}^n$ *fully periodic* if it is invariant under some full rank lattice L of translations. We have: *If X is a Delone set, then X is not fully periodic if and only if $|ST(X)|$ is infinite.*

3. Global Star Criterion

We show that a discrete set X is an ideal crystal provided that certain sets of global stars $\{St_{\mathbf{y}}(X) : \mathbf{y} \in Y\}$ are all isometric.

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Definition 3.1. An arbitrary set Y in $\mathbb{R}^n$ is an *enclosing set* if there is a point $\mathbf{y} \in Y$ which is contained in the interior of the convex hull of the remaining points $Y \backslash \{\mathbf{y}\}$. We call any such $\mathbf{y} \in Y$ an *enclosed point*.

This definition requires that the convex hull of Y in $\mathbb{R}^n$ be full dimensional, i.e., the points of Y do not all lie in some hyperplane. An enclosing set Y necessarily has cardinality $|Y| \geq n + 2$, and $|Y| = n + 2$ occurs when Y consists of the vertices of a n-simplex plus one point in the interior of the simplex. We prove:

Theorem 3.1. *Let X be a discrete set in $\mathbb{R}^n$ and suppose that Y is a (finite or infinite) set such that all the stars $\{ST_{\mathbf{y}}(X) : \mathbf{y} \in Y\}$ are isometric. If Y is an enclosing set, then $Sym(X)$ is a crystallographic group, and X is an ideal crystal.*

In this result the set X and the star centers Y are not necessarily related, and we may have $X \cap Y = \emptyset$. Theorem 1.2 directly follows as a special case of Theorem 3.1.

Theorem 3.1 also gives the following relaxation of property (v) in Theorem 2.2.

Corollary 3.1. *If G is a group of isometries of $\mathbb{R}^n$ that contains an orbit $G.\mathbf{x}$ which is discrete and is also an enclosing set, then G is a crystallographic group.*

Proof. Apply Theorem 3.1 with $Y = X = G.\mathbf{x}$. $\qquad \square$

Before proving Theorem 3.1, we derive some equivalent conditions for a set Y to be an enclosing set.

Definition 3.2. Given $\rho > 0$, a point $\mathbf{y}$ of a set Y in $\mathbb{R}^n$ is a *ρ-point* of Y if every ball $B(\mathbf{x}; \rho)$ that contains $\mathbf{y}$ on its boundary $\partial B(\mathbf{x}; \rho)$ also contains a point of $Y \backslash \{\mathbf{y}\}$.

Definition 3.3. An *oriented hyperplane* H is a hyperplane

$$H := H_{\mathbf{c},d} = \{\mathbf{x} : \langle \mathbf{c}, \mathbf{x} \rangle = d\} \,,$$

together with a particular labelling H^+, H^- of the two open half-spaces it determines. The data $(\mathbf{c}, d)$ with $\mathbf{x} \neq \mathbf{0}$ determine these open half-spaces by

$$H^+ = \{\mathbf{x} : \langle \mathbf{c}, \mathbf{x} \rangle > d\} \quad \text{and} \quad H^- = \{\mathbf{x} : \langle \mathbf{c}, \mathbf{x} \rangle < d\} \,.$$

We prove:

Lemma 3.1. *The following conditions on a point $\mathbf{y}$ in a set Y in $\mathbb{R}^n$ are equivalent.*

(i). *$\mathbf{y}$ is an enclosed point of Y, i.e. $\mathbf{y}$ is in the interior of the convex hull of $Y \backslash \{\mathbf{y}\}$.*

(ii). **y** *is a ρ-point of* Y, *for some finite* $\rho > 0$.

(iii). *Every oriented hyperplane* H *containing* **y** *satisfies*

$$H^+ \cap Y \neq \emptyset \quad and \quad H^- \cap Y \neq \emptyset .$$

Proof. (i) $\Rightarrow$ (iii). We prove the contrapositive. Suppose (iii) fails. If some hyperplane H has $Int(H^+ \cap Y) = \emptyset$ then the convex hull of Y is contained in the closed half-space $\overline{H}^- = H \cup H^-$, and **y** $\in H$ is on its boundary, hence **y** can't be an (n-dimensional) interior point of the convex hull of Y, and (i) fails.

(iii) $\Rightarrow$ (ii). We prove the contrapositive. Suppose (ii) fails. Then there are arbitrarily large closed balls $B(\mathbf{x}_j; \rho_j)$ which have **y** on their boundary and contain other no point of Y. Let H_j be the tangent hyperplane to $\partial B(\mathbf{x}_j; \rho_j)$ at **y**, oriented so that $B(\mathbf{x}_j; \rho_j) \backslash \{\mathbf{y}\} \subseteq H^+$. Extract a subsequence of H_j that tend to a limit hyperplane H containing **y**. Along this subsequence the sets $B(\mathbf{x}_j; \rho_j) \backslash \{\mathbf{y}\}$ exhaust all of H^+, hence H^+ contains no point of Y, contradicting (iii).

(ii) $\Rightarrow$ (i). Let $\tilde{Y}(\mathbf{y}) := Y \cap B(\mathbf{y}; 2\rho)$, which consists of all points of Y contained in some closed ball $B(\mathbf{x}; \rho)$ that contains **y** on its boundary. We show that $\tilde{Y}$ contains **y** as an enclosed point. Suppose not. Then there is an oriented hyperplane H through **y** which contains no point of $Y \backslash \{\mathbf{y}\}$ on one side H^+ of it. Consider the closed ball $B(\mathbf{x}; \rho)$ contained in H^+ which is tangent to H at **y**. It contains no point of $Y \backslash \{\mathbf{y}\}$, which contradicts (ii). $\quad \square$

We also need the following simple criterion for a set Y to be relatively dense.

Lemma 3.2. *An arbitrary set* Y *in* $\mathbb{R}^n$ *is relatively dense if and only if there is some* $\rho > 0$ *such that each point* **y** $\in Y$ *is a ρ-point of* Y.

Proof. If Y is relatively dense with parameter R, then every point **y** $\in Y$ is an R-point. Indeed relative density implies that every ball $B(\mathbf{x}, R)$ with **y** $\in \partial B(\mathbf{x}, R)$ contains some other point of Y.

Conversely, if every point of Y is a ρ-point, for fixed $\rho > 0$, then Y is relatively dense with parameter ρ. Suppose not, so that there is some empty ball $B(\mathbf{z}; \rho')$ with $\rho' > \rho$. Choose a point **y** $\in Y$ that is a closest point to **z**, and translate the ball in the direction **y** $-$ **z** until **y** $\in Y$ is on its boundary. The resulting ball $B(\mathbf{z}'; \rho)$ contains no point of $Y \backslash \{\mathbf{y}\}$ by the triangle inequality, for any other point in it would be closer to **z** than **y**. This contradicts **y** being a ρ-point of Y.

$\quad \square$

Proof of Theorem 3.1. By hypothesis, for each point $\mathbf{y}_i, \mathbf{y}_j$ of Y there is an isometry g_{ij} of $\mathbb{R}^n$ that maps $\mathbf{y}_i$ to $\mathbf{y}_j$ and $ST_{\mathbf{y}_i}(X)$ to $ST_{\mathbf{y}_j}(X)$. We do not require that any of the $\mathbf{y}_i$ be in X. Let G be the group of isometries generated by all the possible g_{ij}'s. Then $Y \subseteq G.\mathbf{y}$ for any fixed $\mathbf{y} \in Y$. Since each $g_{ij} \in Sym(X)$, we have $G \subseteq Sym(X)$. The main part of the proof will be to show that G is a crystallographic group.

Consider an orbit $G.\mathbf{x}$ for some $\mathbf{x} \in X$ and let $Aff(G.\mathbf{x})$ denote the smallest affine subspace spanned by the elements of $G.\mathbf{x}$. We show that $dim(Aff(X)) = n$. Assume the contrary, that $G.\mathbf{x}$ spans some affine subspace $P^k = Aff(G.\mathbf{x})$ of dimension $k < n$. Now G must leave P^k invariant, i.e. $g(P^k) = P^k$ for all $g \in G$. Since $g(P^k) = P^k$ for all $g \in G$, we have

$$dist(\mathbf{y}, P^k) = dist(g.\mathbf{y}, P^k) \ ,$$

where $dist(\mathbf{y}, F) := \inf\{||\mathbf{y} - \mathbf{z}|| : \mathbf{z} \in F\}$. Thus the orbit $G.\mathbf{y}$ lies on a cylinder

$$C_\alpha := \{\mathbf{z} \in \mathbb{R}^n : dist(\mathbf{z}, P^k) = \alpha\} \ .$$

The constant $\alpha > 0$, for if $\alpha = 0$, then $Y \subseteq G.\mathbf{y} \subseteq P^k$, which contradicts the property that the points of an enclosing set Y span $\mathbb{R}^n$. If $k < n$, then the cylinder $C_\alpha \cong P^k \times S^{n-k}$ is a convex set, hence a supporting hyperplane H to a point $\mathbf{y} \in Y$ on the surface of the cylinder leaves the entire cylinder C_α in one closed half-space $\overline{H^-} = H \cup H^-$, say. Then $H^+ \cap Y = \emptyset$, which by Lemma 3.1 (iii) shows that Y is not an enclosing set, a contradiction. Thus $k = n$.

We next show that $Sym(X)$ acts discontinuously on $\mathbb{R}^n$. We must show that every orbit $Sym(X).\mathbf{z}$ is a discrete set. We know that $Sym(X).\mathbf{x} \subseteq X$ is a discrete set, and $Aff(Sym(X).\mathbf{x}) = \mathbb{R}^n$ because $\mathbb{R}^n = Aff(G.\mathbf{x}) \subseteq Aff(Sym(X).\mathbf{x})$. Now $Aff(Sym(X).\mathbf{x}) = \mathbb{R}^n$ implies that there exist $n + 1$ points $\{\mathbf{x}_i : 1 \le i \le n + 1\}$ which form a full-dimensional simplex in $\mathbb{R}^n$, so we can write

$$\mathbf{z} = \sum_{i=1}^{n+1} a_i \mathbf{x}_i \ , \quad \text{with} \ \sum_{i=1}^{n+1} a_i = 1 \ .$$

Here $(a_1, a_2, \ldots, a_{n+1})$ are barycentric coordinates of $\mathbf{z}$ and

$$||\mathbf{z} - \mathbf{x}_i|| \le c_0 := \sum_{i=1}^{n+1} (|a_i| + 1) \ ||\mathbf{x}_i|| \ , \quad 1 \le i \le n + 1 \ .$$

We now argue by contradiction. Suppose that $Sym(X).\mathbf{z}$ is not discrete. Then there exists a sequence of distinct points $\{\mathbf{z}_j = g_j.\mathbf{z} : j \ge 1\}$ tending to a limit point $\mathbf{z}_\infty$. However

$$g_j.\mathbf{z} = \sum_{i=1}^{n+1} a_i(g_j.\mathbf{x}_i) \ , \tag{3.1}$$

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and all $g_j.\mathbf{x}_i \in Sym(X).\mathbf{x}$. Now we have

$$||\mathbf{z}_\infty - g_j.\mathbf{x}_i|| \leq ||\mathbf{z}_\infty - \mathbf{z}_j|| + ||g_j.\mathbf{z} - g_j.\mathbf{x}_i|| \leq ||\mathbf{z}_\infty - \mathbf{z}_j|| + c_0 \ .$$

Whenever $||\mathbf{z}_\infty - \mathbf{z}_j|| \leq 1$, the point $g_j.\mathbf{x}_i$ lies in the fixed ball $B(\mathbf{z}_\infty; c_0 + 1)$. Since X is discrete, there are only finitely points of $Sym(X).\mathbf{x}$ in this ball, hence by (3.1) there are only finitely many possible choices for $g_j.\mathbf{z}$ having $||\mathbf{z}_\infty - g_j.\mathbf{z}|| \leq 1$, which contradicts the distinctness of all $\mathbf{z}_j$. Thus $Sym(X)$ acts discontinuously on $\mathbb{R}^n$. In particular $Sym(X).\mathbf{y}$ is a discrete set, hence $G.\mathbf{y}$ is a discrete set.

Now choose $\mathbf{y}$ to be an enclosed point of Y, so it is a ρ-point for some $\rho > 0$ by Lemma 3.1. Now for any isometry $g \in G$, the point $g.\mathbf{y}$ is a ρ-point of $g(Y)$, because property (iii) of Lemma 3.1 is invariant under isometries. Since $Y \subseteq G.\mathbf{y}$ we have $g(Y) \subseteq G.\mathbf{y}$, hence $g.\mathbf{y}$ is a ρ-point of Y. Thus every point of $G.\mathbf{y}$ is a ρ-point, so $G.\mathbf{y}$ is a relatively dense set by Lemma 3.2.

It follows that G is a crystallographic group by property (v) of Theorem 2.1. Thus $\mathbb{R}^n/G$ is compact, hence $\mathbb{R}^n/Sym(X)$ is also compact, so $Sym(X)$ acts uniformly on $\mathbb{R}^n$. We conclude that $Sym(X)$ is a crystallographic group. Finally, Theorem 2.2 shows that X is an ideal crystal.
$\square$

For later use we show that for any finite partition $X = \cup_{i=1}^k X_i$ of a relatively dense set, at least one set X_i is an enclosing set. The following lemma shows that this conclusion holds more generally for finite sets X that are relatively dense on any sufficiently large finite region. We say that a set X is R-relatively dense in the ball $B(\mathbf{y}; \rho)$ if every closed ball $B(\mathbf{z}; R)$ contained in $B(\mathbf{y}; \rho)$ contains a point of X.

Lemma 3.3. *Let X be a set in $\mathbb{R}^n$ which is partitioned into k subsets,*

$$X = \bigcup_{i=1}^k X_i \ , \quad with \ \ X_i \cap X_j = \emptyset \ \ if \ \ i \neq j \ .$$

If X is R-relatively dense in some ball $B(\mathbf{y}; \rho)$ with $\rho \geq 3^k R$, then at least one subset X_i is an enclosing set.

Proof. We proceed by induction on k. For the base case $k = 1$, if $X = X_1$ is R-relatively dense in $B(\mathbf{y}; 3R)$, then there exists some $\mathbf{x} \in X$ with $||\mathbf{x} - \mathbf{y}|| \leq R$. The set $\tilde{X}(\mathbf{x}) = X \cap B(\mathbf{x}; 2R)$ of all points of X within distance $2R$ of $\mathbf{x}$ contains $\mathbf{x}$ as an enclosed point, as in the proof of

Lemma 3.1 (ii) $\Rightarrow$ (i), because it includes each point of X in any $B(\mathbf{z}; R)$ that contains $\mathbf{x}$ on its boundary, and all such $B(\mathbf{z}; R) \subseteq B(\mathbf{y}; 3R)$.

Now suppose that the lemma is true for all partitions of X into $k-1$ subsets. Consider a partition of X into k subsets, and suppose that there is a ball $B(\mathbf{y}; 3^k R)$ on which X is R-relatively dense. If the set X_k is $3^{k-1}R$-relatively dense on $B = B(\mathbf{y}; 3^k R)$, then the set X_k is an enclosing set, by applying the base case $k=1$. If it is not, then there is some ball $B' = B(\mathbf{y}'; 3^{k-1}R)$ inside $B(\mathbf{y}; 3^k R)$ that contains no point of X_k. Now set $X' = X \cap B'$ and $X_i' = X_i \cap B'$, $1 \le i \le k-1$. Then since $X_k' = X_k \cap B' = \emptyset$, we have a partition

$$X' = \bigcup_{i=1}^{k-1} X_i' \,,$$

and X' inherits the R-relatively dense property on $B(\mathbf{y}'; 3^{k-1}R)$ from that of X on B. By the induction hypothesis one of the X_i' is an enclosing set, and since $X_i' \subseteq X_i$ the enclosing set property holds for the corresponding X_i. This completes the induction step. $\quad\square$

4. Local Star Criterion

We deduce results on the multiregularity of a point set X from conditions on a set of its local stars (ρ-stars) centered at a Delone subset of points Y of X. In Corollary 4.1 below we recover the main result stated in Dolbilin and Shtogrin [8], which generalizes that of Delone et al. [6].

Recall the definition

$$ST_\mathbf{y}(X; \rho) := \{[\mathbf{y}, \mathbf{x}] : \mathbf{x} \in X \;\; \text{and} \;\; ||\mathbf{x} - \mathbf{y}|| \le \rho\} \,.$$

This implies that

$$ST_\mathbf{y}(X; \rho) \subseteq ST_\mathbf{y}(X; \rho') \quad \text{if} \;\; \rho \le \rho' \,. \tag{4.1}$$

Definition 4.1. The *local stabilizer* of the ρ-star centered at $\mathbf{y}$, denoted $Lsym_\mathbf{y}(X; \rho)$, is the group of isometries g that fix $\mathbf{y}$ and leave $ST_\mathbf{y}(X; \rho)$ invariant. That is, it consists of all $g \in Sym(\mathbb{E}^n)$ such that $g.\mathbf{y} = \mathbf{y}$ and

$$g(ST_\mathbf{y}(X; \rho)) = ST_\mathbf{y}(X; \rho) \,.$$

$Lsym_{\mathbf{y}}(X;\rho)$ is a subgroup of the group of rotations centered at $\mathbf{y}$. The relation (4.1) implies that

$$Lsym_{\mathbf{y}}(X;\rho) \supseteq Lsym_{\mathbf{y}}(X;\rho') \quad \text{if} \ \ \rho \le \rho' \ . \tag{4.2}$$

Definition 4.2. The (global) *stabilizer $Lsym_{\mathbf{y}}(X)$* centered at $\mathbf{y}$ is the subgroup of elements of $Sym(X)$ that fix $\mathbf{y}$.

We clearly have

$$Lsym_{\mathbf{y}}(X) \subseteq Lsym_{\mathbf{y}}(X;\rho) \ , \quad \text{for any } \rho \ .$$

Any group $Lsym_{\mathbf{y}}(X;\rho)$ or $Lsym_{\mathbf{y}}(X)$ is conjugate in $Sym(\mathbb{E}^n)$ to a subgroup of the orthogonal group $O(n,\mathbb{R})$ by applying the conjugacy that translates $\mathbf{y}$ to the origin, i.e. $t_{-\mathbf{y}} g t_{\mathbf{y}} \in O(n,\mathbb{R})$, where $t_{\mathbf{y}}.\mathbf{x} = \mathbf{x} + \mathbf{y}$.

We generalize these definitions to apply to a partition $X = Y \cup Z$ of a set X. We define the *partitioned ρ-star*

$$ST_{\mathbf{w}}(Y,Z;\rho) := ST_{\mathbf{w}}(Y;\rho) \cup ST_{\mathbf{w}}(Z;\rho) = ST_{\mathbf{w}}(X;\rho) \ ,$$

and we consider two such partitioned ρ-stars *isometric* if there is an isometry $g \in Sym(\mathbb{E}^n)$ with $g.\mathbf{w} = \mathbf{w}'$ which satisfies

$$g(ST_{\mathbf{w}}(Y;\rho)) = ST_{\mathbf{w}'}(Y;\rho) \ , \quad \text{and} \ \ g(ST_{\mathbf{w}}(Z;\rho)) = ST_{\mathbf{w}'}(Z;\rho) \ .$$

We call any such isometry g a *$(Y,Z;\rho)$-isometry.* We set

$$ST_W(Y,Z;\rho) := \{ST_{\mathbf{w}}(Y,Z;\rho) : \mathbf{w} \in W\} \ ,$$

and let $|ST_W(Y,Z;\rho)|$ denote the number of $(Y,Z;\rho)$-isometry classes among the members of $ST_W(Y,Z;\rho)$.

Finally, we define the *local stabilizer $Lsym_{\mathbf{w}}(Y,Z;\rho)$* of the partitioned ρ-star by

$$Lsym_{\mathbf{w}}(Y,Z;\rho) = Lsym_{\mathbf{w}}(Y;\rho) \cap Lsym_{\mathbf{w}}(Z;\rho) \ ,$$

and the *stabilizer $Lsym_{\mathbf{w}}(Y,Z)$* by

$$Lsym_{\mathbf{w}}(Y,Z) = Lsym_{\mathbf{w}}(Y) \cap Lsym_{\mathbf{w}}(Z) \ .$$

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We obtain the following criterion:

Theorem 4.1. *Let X be a discrete set which has a partition $X = Y \cup Z$ in which Y is a Delone set. Suppose that $\rho \geq 4R$ is such that*

(a). $|ST_Y(Y, Z; \rho)| = |ST_Y(Y, Z; \rho - 2R)| = k$.

(b). $Lsym_{\mathbf{y}}(Y, Z; \rho) = Lsym_{\mathbf{y}}(Y, Z; \rho - 2R)$ *for all* $\mathbf{y} \in Y$.

Then $Sym(Y) \cap Sym(Z) \subseteq Sym(X)$ is a crystallographic group. Furthermore each of X and Y is a multiregular point system, and the points of X fall into at most k orbits under the action of $Sym(X)$.

In hypothesis (b) the groups $Lsym_{\mathbf{y}}(Y, Z; \rho)$ for $\mathbf{y} \in Y$ are not all necessarily isomorphic. The proof implies that they fall in at most k isomorphism classes. Lemma 4.2 below shows that, for any value of ρ that satisfies (a), (b), we have

$$Lsym_{\mathbf{y}}(Y, Z) = Lsym_{\mathbf{y}}(Y, Z; \rho) , \quad \text{all } \mathbf{y} \in Y . \tag{4.3}$$

Theorem 4.1 says nothing about the group $Sym(Z)$, but the proof implies that $Sym(Z)$ acts uniformly on $\mathbb{R}^n$. The theorem includes the special case $Z = \emptyset$, in which case we make the convention that $Sym(Z) = Sym(\mathbb{E}^n) = \mathcal{E}_n$. This special case is:

Corollary 4.1. *Let X be an (r, R) set for which there exists some $\rho \geq 4R$ such that:*

(a). $|ST_X(X; \rho)| = |ST_X(X; \rho - 2R)| = k$.

(b). $Lsym_{\mathbf{x}}(X; \rho) = Lsym_{\mathbf{x}}(X; \rho - 2R)$ *for all* $\mathbf{x} \in X$.

Then X is a multiregular point system whose points fall in exactly k orbits under the action of $Sym(X)$. Furthermore

$$Lsym_{\mathbf{x}}(X) = Lsym_{\mathbf{x}}(X; \rho) \quad \text{for all } \mathbf{x} \in X . \tag{4.4}$$

We have exactly k orbits because condition (a) shows that there are at least k distinct orbits under the action of $Sym(X)$.

An important part of the proof of Theorem 4.1 is to show that the set X possesses global symmetries. We establish this in two preliminary lemmas, in which we assume all hypotheses of Theorem 4.1 are in force.

Lemma 4.1. *Let $\mathbf{y}, \mathbf{y}' \in Y$ and suppose $\rho \geq 4R$ and that there exists $g \in Sym(\mathbb{E}^n)$ which is a $(Y, Z; \rho - 2R)$-isometry that maps $ST_{\mathbf{y}}(X; \rho - 2R)$ to $ST_{\mathbf{y}'}(X; \rho - 2R)$. Then g is also a*

$(Y, Z; \rho)$-*isometry that maps* $ST_\mathbf{y}(X; \rho)$ *to* $ST_{\mathbf{y}'}(X; \rho)$.

Proof. The hypothesis (a) in Theorem 4.1 implies that the isometry class of a star $ST_\mathbf{y}(Y, Z; \rho - 2R)$ uniquely determines the isometry class of the star $ST_\mathbf{y}(Y, Z; \rho)$. Thus the $(Y, Z; \rho - 2R)$-isometry hypothesis implies that $ST_\mathbf{y}(X; \rho)$ is $(Y, Z; \rho)$-isometric to $ST_{\mathbf{y}'}(X; \rho)$, and we let $g' \in Sym(\mathbb{E}^n)$ be such an isometry between them. Now

$$g^{-1} \circ g'(ST_\mathbf{y}(X; \rho - 2R)) = g^{-1}(ST_{\mathbf{y}'}(X; \rho - 2R)) = ST_\mathbf{y}(X; \rho - 2R) \ .$$

Thus $g^{-1} \circ g' \in Lsym_\mathbf{y}(X; \rho - 2R)$. Now hypothesis (b) of Theorem 4.1 gives

$$g'' = g^{-1} \circ g' \in Lsym_\mathbf{y}(X; \rho) \ .$$

Thus $g = g' \circ (g'')^{-1}$ is a $(Y, Z; \rho)$-isometry. □

Next we show that any such local symmetry is a global symmetry of both Y and Z.

Lemma 4.2. *Let* $\mathbf{y}, \mathbf{y}' \in Y$ *and suppose* $\rho \geq 4R$ *and that there is a* $(Y, Z, \rho - 2R)$-*isometry* $g \in Sym(\mathbb{E}^n)$ *from* $\mathbf{y}$ *to* $\mathbf{y}'$, *so that*

$$g(ST_\mathbf{y}(X; \rho - 2R)) = ST_{\mathbf{y}'}(X; \rho - 2R) \ .$$

Then $g \in Sym(Y) \cap Sym(Z)$. *In particular,*

$$Lsym_\mathbf{y}(Y, Z) = Lsym_\mathbf{y}(Y, Z; \rho) \ .$$

Proof. Since Y is an (r, R)-set, we can connect $\mathbf{y}$ to any $\bar{\mathbf{y}} \in Y$ by a finite chain $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_m$ with $\mathbf{y}_0 = \mathbf{y}$ and $\mathbf{y}_m = \bar{\mathbf{y}}$, such that

$$||\mathbf{y}_i - \mathbf{y}_{i-1}|| \leq 2R \quad \text{for} \ \ 1 \leq i \leq m \ . \tag{4.5}$$

This is proved in [6, Section 2], as follows. If $||\bar{\mathbf{y}} - \mathbf{y}|| = R'$ then the closed ball $\overline{B} = B(\bar{\mathbf{y}}; R')$ contains only finitely many points of Y, and $\mathbf{y}$ lies its boundary. The closed ball

$$\overline{B}_0 := B(\mathbf{y} + \frac{R}{R'}(\bar{\mathbf{y}} - \mathbf{y}); R) \subseteq \overline{B}$$

contains $\mathbf{y}_0 = \mathbf{y}$ on its boundary, and by relative denseness it must contain another point $\mathbf{y}_1 \in Y$. Then $||\mathbf{y}_1 - \mathbf{y}_0|| \leq 2R$ and

$$||\mathbf{y}_1 - \bar{\mathbf{y}}|| < ||\mathbf{y}_0 - \bar{\mathbf{y}}|| \ ,$$

since $\mathbf{y}$ is the furthest point in $\overline{B}_0$ from $\bar{\mathbf{y}}$. Now $\mathbf{y}_1 \in \overline{B}$, so we can repeat the same argument to find $\mathbf{y}_2 \in Y \cap \overline{B}$ with $||\mathbf{y}_2 - \mathbf{y}_1|| \leq 2R$ and

$$||\mathbf{y}_2 - \bar{\mathbf{y}}|| < ||\mathbf{y}_1 - \bar{\mathbf{y}}|| .$$

Continue this process to produce $\mathbf{y}_3, \mathbf{y}_4, \ldots$, and since there are only finitely many points of Y in $\overline{B}$, this process terminates with some $\mathbf{y}_m = \bar{\mathbf{y}}$, which gives (4.5).

By hypothesis $\rho \geq 4R$, hence

$$\mathbf{y}_1 \in B(\mathbf{y}_0; 2R) \subseteq B(\mathbf{y}_0; \rho - 2R) .$$

Thus

$$\mathbf{y}_1 \in X \cap B(\mathbf{y}_0; \rho - 2R) \subseteq X \cap B(\mathbf{y}_0; \rho) ,$$

so Lemma 4.1 applies to give

$$g.\mathbf{y}_1 \in ST_{\mathbf{y}'}(X; \rho) .$$

Now g is a $(Y, Z; \rho)$-isometry that takes $ST_{\mathbf{y}}(X; \rho)$ to $ST_{\mathbf{y}'}(X; \rho)$, hence it is a $(Y, Z; \rho - 2R)$-isometry of $ST_{\mathbf{y}_1}(X; \rho - 2R)$ to some $ST_{\mathbf{y}_1'}(X; \rho - 2R)$ with $\mathbf{y}_1' \in Y$. Lemma 4.1 then implies that g is a $(Y, Z; \rho)$-isometry of $ST_{\mathbf{y}_1}(X; \rho)$ to $ST_{\mathbf{y}_1'}(X; \rho)$. Since $ST_{\mathbf{y}_2}(X; \rho - 2R) \subseteq ST_{\mathbf{y}_1}(X; \rho)$ by Lemma 4.1 we get that g is a $(Y, Z; \rho - 2R)$ isometry of $ST_{\mathbf{y}_2}(X; \rho - 2R)$ to some $ST_{\mathbf{y}_2'}(X; \rho - 2R)$. Continuing in this fashion, we eventually obtain that g is a $(Y, Z; \rho)$ isometry of $ST_{\bar{\mathbf{y}}}(X; \rho)$ to some $ST_{\bar{\mathbf{y}}'}(X; \rho)$. In particular

$$g.\bar{\mathbf{y}} = \bar{\mathbf{y}}' \in Y .$$

By a similar argument $g^{-1}.\bar{\mathbf{y}} \in Y$, for all $\bar{\mathbf{y}} \in Y$, hence $g \in Sym(Y)$.

Next consider an arbitrary $\bar{\mathbf{z}} \in Z$. Since Y is an (r, R)-set, the closed ball $B(\bar{\mathbf{z}}; R)$ contains some point $\bar{\mathbf{y}} \in Y$. By the argument above g is a $(Y, Z; \rho)$-isometry of $ST_{\bar{\mathbf{y}}}(X; \rho)$ to some $ST_{\bar{\mathbf{y}}'}(X; \rho)$. Thus the point $\bar{\mathbf{z}}$ is mapped to a point $\bar{\mathbf{z}}' \in Z$ in $ST_{\bar{\mathbf{y}}'}(X; \rho)$, i.e. $g.\bar{\mathbf{z}} = \bar{\mathbf{z}}' \in Z$. Similarly $g^{-1}.\bar{\mathbf{z}} \in Z$, so $g \in Sym(Z)$. $\square$

Proof of Theorem 4.1. Partition the Delone set

$$Y := \bigcup_{j=1}^{k} Y_j ,$$

in which the Y_j comprise the $(Y, Z; \rho)$-isometry classes of $ST_{\mathbf{y}}(Y, Z; \rho)$ and $k = |ST_Y(Y, Z; \rho)|$. For each $\mathbf{y}, \mathbf{y}' \in Y_j$ there is some $g = g_{\mathbf{y}, \mathbf{y}'} \in Sym(\mathbb{E}^n)$ which is a $(Y, Z; \rho)$-isometry from

$ST_{\mathbf{y}}(Y, Z; \rho)$ to $ST_{\mathbf{y}'}(Y, Z; \rho)$. By Lemma 4.2 each $g_{\mathbf{y}, \mathbf{y}'} \in Sym(Y) \cap Sym(Z)$. Let G denote the subgroup of $Sym(\mathbb{E}^n)$ generated by all such $g_{\mathbf{y}, \mathbf{y}'}$ for $1 \leq j \leq k$. Then

$$G \subseteq Sym(Y) \cap Sym(Z) \subseteq Sym(X) .$$

Since Y is a Delone set and $G \subseteq Sym(Y)$, it follows that G acts discontinuously on $\mathbb{R}^n$.

Next, Lemma 3.3 implies that some Y_j is an enclosing set. Choose any $\mathbf{y} \in Y_j$, and since all $g_{\mathbf{y}, \mathbf{y}'} \in G$ for $\mathbf{y}' \in Y_j$, we have

$$Y_j \subseteq G.\mathbf{y} \subseteq (Sym(Y) \cap Sym(Z)).\mathbf{y} \subseteq Sym(Y).\mathbf{y} \subseteq Y .$$

Then $Sym(Y) \cap Sym(Z)$ and $Sym(Y)$ are both crystallographic groups by Corollary 3.1, and Y is a multiregular point system by Theorem 1.1.

Finally, since

$$Y_j \subseteq G.\mathbf{y} \subseteq Sym(X).\mathbf{y} \subseteq X ,$$

it follows that $Sym(X)$ is a crystallographic group by Corollary 3.1, and X is a multiregular point system by Theorem 1.1. The number of isomorphism classes of $\{ST_{\mathbf{x}}(X) : \mathbf{x} \in X\}$ is at most k, because the action of $Sym(Y) \cap Sym(Z)$ on X gives k isomorphism classes by Lemma 4.2, and $Sym(Y) \cap Sym(Z) \subseteq Sym(X)$. □

In the remainder of this section we consider the special case $Y = X$ and $Z = \emptyset$, and prove Theorem 1.3 using Corollary 4.1. We begin with the following bound.

Lemma 4.3. *If X is an (r, R)-set in $\mathbb{R}^n$ and $\mathbf{x} \in X$ then*

$$|Lsym_{\mathbf{x}}(X; 2R)| \leq \left(\frac{2R}{r} + 1\right)^{n^2} . \tag{4.6}$$

Proof. The point $\mathbf{x} \in X$ is an R-point by the proof of Lemma 3.2. In particular the finite set $\tilde{X} := X \cap \overline{B}(\mathbf{x}; 2R)$ contains $\mathbf{x}$ as an enclosed point, by the proof of Lemma 3.1. We can find $n + 1$ points $\mathbf{x}_0 = \mathbf{x}, \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in \tilde{X}$ which form a full-dimensional simplex. (See the proof of Caratheodory's theorem in [28, (2.2.12)].) Each element g of $Lsym_{\mathbf{x}}(X; 2R)$ fixes $\mathbf{x}$, and is completely determined by specifying the images $g.\mathbf{x}_i$ of $\mathbf{x}_i$ for $1 \leq i \leq n$. Now

$$||g.\mathbf{x}_i - \mathbf{x}_0|| = ||g.\mathbf{x}_i - g.\mathbf{x}_0|| = ||\mathbf{x}_i - \mathbf{x}_0|| \leq 2R ,$$

hence each image $g.\mathbf{x}_i$ lies in $\tilde{X}$. To prove (4.6) it therefore suffices to show that

$$|\tilde{X}| \leq \left(\frac{2R}{r} + 1\right)^n , \tag{4.7}$$

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for there are then at most $(\frac{2R}{r} + 1)^{n^2}$ choices for $\{g.\mathbf{x}_i : 1 \leq i \leq n\}$. To prove (4.6), note that since X is an (r, R)-set, the open balls $B^{\circ}(\mathbf{x}'; r)$ are pairwise disjoint. For if two balls had a common point $\mathbf{w}$, the open ball $B^{\circ}(\mathbf{w}; r)$ would contain two points of X, contradicting the r-uniformly discrete property. All these balls lie inside the ball $B(\mathbf{x}; 2R + r)$. Comparing the volumes that these balls cover gives

$$Vol\left(\bigcup_{\mathbf{x}' \in \tilde{X}} B^{\circ}(\mathbf{x}'; r) \right) \leq \kappa_n r^n |\tilde{X}| \leq \kappa_n (2R + r)^n = Vol(B(\mathbf{x}; 2R + r)) \ ,$$

in which κ_n denotes the volume of an n-dimensional unit ball, and this yields (4.7). $\quad\square$

Proof of Theorem 1.3. We suppose that X is an (r, R)-set having the property that all ρ_0-stars $\{ST_{\mathbf{x}}(X; \rho_0) : \mathbf{x} \in X\}$ fall in $k = N_X(\rho_0)$ isometry classes, and that

$$\rho_0 > 2f(n, r, R)Rk \ ,$$

with

$$f(n, r, R) := (n^2 + 1) \frac{\log(\frac{2R}{r} + 2)}{\log 2} \ .$$

We deduce Theorem 1.3 from Corollary 4.1, by showing that the two hypotheses

    (a). $N_X(\rho_j) = N_X(\rho_j - 2R) = k' \leq k$,

    (b). $Lsym_{\mathbf{x}}(X; \rho_j) = Lsym_{\mathbf{x}}(X; \rho_j - 2R)$ for all $\mathbf{x} \in X$,

must simultaneously hold for some

$$\rho_j := 2jR \ \ \text{with} \ \ 2 \leq j \leq kf(n, r, R) \ .$$

Note that all $\rho_j \geq 4R$.

    First, we observe that $N_X(\rho)$ is a nondecreasing function of ρ, hence

$$N_X(\rho_j) \leq N_X(\rho_0) = k \ .$$

Thus $N_X(\rho_j)$ can assume at most k different values. Second, the function $|Lsym_{\mathbf{x}}(X; \rho)|$ is a nonincreasing function of ρ by (4.2). If

$$|Lsym_{\mathbf{x}}(X; \rho_j)| \neq |Lsym_{\mathbf{x}}(X; \rho_{j-1})| \ ,$$

then

$$\log |Lsym_{\mathbf{x}}(X; \rho_j)| \leq \log |Lsym_{\mathbf{x}}(X; \rho_{j-1})| - \log 2 \ , \tag{4.8}$$

since a strict subgroup of a finite group G has index at least 2 in G.

We now argue by contradiction. So suppose that for each j with $2 \leq j \leq f(n, r, R)$, at least one of (a) or (b) does not hold for ρ_j. If condition (a) does not hold for ρ_j, and $j \geq 3$, then

$$N_X(\rho_j) > N_X(\rho_{j-1}) \ ,$$

so this can happen for at most $k - 1$ different values of j. To deal with condition (b), we select representatives $\{\mathbf{x}_i : 1 \leq i \leq k\}$ of each of the k isometry classes of $\{ST_{\mathbf{x}}(X; \rho_0) : \mathbf{x} \in X\}$ and define the quantity

$$I_j := \sum_{i=1}^{k} \log |Lsym_{\mathbf{x}_i}(X; \rho_j - 2R)| \ , \quad \text{for} \ \ 2 \leq j \leq k f(n, r, R) \ .$$

Lemma 3.3 gives

$$\log |Lsym_{\mathbf{x}}(X; 2R)| \leq n^2 \log \left(\frac{2R}{r} + 1 \right) \ ,$$

hence

$$I_2 \leq k n^2 \log \left(\frac{2R}{r} + 1 \right) \ .$$

If (b) does not hold for a given ρ_j with $j \geq 3$, then (4.8) applies to at least one of the representative classes $\mathbf{x}_i$, hence

$$I_j \leq I_{j-1} - \log 2 \ .$$

Since all $I_j \geq 0$, this can occur for at most $k n^2 \log_2(\frac{2R}{r} + 1)$ values of j. Thus

$$\#\{j\} \leq k + k n^2 \log_2 (\frac{2R}{r} + 1) \ .$$

We obtain a contradiction since

$$\#\{j\} \geq k f(n, r, R) - 1 > k + k n^2 \log_2 (\frac{2R}{r} + 1) \ ,$$

in which we used

$$k \log_2 (\frac{2R}{r} + 2) > k \log_2 (4) \geq k + 1 \ ,$$

since $R/r > 1$ for $n \geq 2$.

Now suppose that Y is a Delone set all of whose ρ_0-stars are isometric to one of $\{ST_{\mathbf{x}}(X; \rho_0) : \mathbf{x} \in X\}$. We reduce to the case that $\mathbf{0} \in Y$ by translating Y to $Y - \mathbf{y}$, if necessary. The proof

above produced ρ_j with $4R \leq \rho_j \leq \rho$ such that (a) and (b) above hold, and these conditions imply that any $(\rho_j - 2R)$-star of Y extends in a unique way to a ρ_j-star of Y.

By hypothesis

$$ST_{\mathbf{0}}(Y; \rho_j) = Q(ST_{\mathbf{x_0}}(X; \rho_j) - \mathbf{x_0}) , \tag{4.9}$$

for some $Q \in O(n, \mathbb{R})$ and $\mathbf{x_0} \in X$. Now each $\mathbf{y} \in Y \cap B(\mathbf{0}; \rho_j - 2R)$ has $ST_{\mathbf{y}}(Y; \rho_j - 2R) \subseteq ST_{\mathbf{0}}(Y, \rho_j)$, and this $(\rho_j - 2R)$-star extends uniquely to $ST_{\mathbf{y}}(Y; \rho_j)$. The extensions cover all points of Y in the ball $B(\mathbf{0}; \rho_j + R)$ because $ST_{\mathbf{0}}(Y; \rho_j)$ inherits the (r, R)-property of X to within distance R of its boundary. Since the uniqueness of these extensions holds for both X and Y, we obtain

$$ST_{\mathbf{0}}(Y; \rho_j) = Q(ST_{\mathbf{x_0}}(X; \rho_j + R) - \mathbf{x_0}) .$$

Repeating the same argument, by induction on $k \geq 1$, we obtain

$$ST_{\mathbf{0}}(Y; \rho_j + kR) = Q(ST_{\mathbf{x_0}}(X; \rho_j + kR) - \mathbf{x_0}) , \quad \text{all } k \geq 1 .$$

Thus $Y - \mathbf{y} = Q(\mathbf{x} - \mathbf{x_0})$, which gives (1.3). $\square$

The following examples show that some hypothesis like (1.1) is needed in Theorem 1.3 to conclude that X is a multiregular point system.

Definition 4.3. A Delone set X is has the *locally finite atlas property under isometries*, or is a *Delone set of finite type under isometries*, if $|ST(X; \rho)|$ is finite for each finite $\rho > 0$.

In this case the function

$$N_X(\rho) := |ST(X; \rho)| , \quad 0 < \rho < \infty ,$$

is a non-decreasing integer-valued function. Theorem 1.3 states that if

$$N_X(\rho) < \frac{\rho}{CR} ,$$

for $C = 2(n^2 + 1) \log_2(\frac{2R}{r} + 2)$, then $N_X(\rho)$ is necessarily a bounded function. The examples below exhibit Delone sets X with $N_X(\rho) \to \infty$ as $\rho \to \infty$, in one case with $N_X(\rho)$ growing linearly in ρ.

Many studies of quasicrystalline structures have considered equivalence of neighborhoods under translations rather than under isometries. Let $N_X^*(\rho)$ denote the number of translation-equivalence classes of ρ-stars of X. We clearly have

$$N_X(\rho) \leq N_X^*(\rho) , \quad \text{for } \rho > 0 . \tag{4.10}$$

Definition 4.4. A Delone set X has the *locally finite atlas property under translations*, or is a *Delone set of finite type under translations*, if $N_X^*(\rho)$, is finite for all $\rho > 0$.

This property obviously implies the locally finite atlas property under isometries. It is studied in [16].

Example 4.1. (*Crystal with "defects"*) Consider the set X in $\mathbb{R}^2$ given by

$$X = \{(m, n) \in \mathbb{Z}^2 : n \neq 0\} \cup \{(m + \theta, 0) : m \in \mathbb{Z}\}$$

where θ is a constant with $0 < \theta < \frac{1}{2}$. It is a Delone set with $r = \frac{1}{2}$ and $R = \frac{\sqrt{2}}{2}$. It is not a multiregular set, since the row of "defects" along the x-axis makes $|ST(X)| = \infty$. However X has the locally finite atlas property under translations, with

$$\lfloor \rho \rfloor \leq N_X(\rho) = N_X^*(\rho) \leq \lfloor \rho \rfloor + 2 \ ,$$

with a complete set of isometry classes of ρ-stars having centers contained in the set $\mathbf{x}_0 = (\theta, 0)$ and $\{\mathbf{x}_i = (0, i) : 1 \leq i \leq \lfloor \rho \rfloor + 1\}$. Its local stabilizers are

$$Lsym_{\mathbf{x}}(X; \rho) = \begin{cases} \mathbb{Z}/2\mathbb{Z} & \text{if } \mathbf{x} = (m + \theta, 0) \ , \\ \{1\} & \text{if } \mathbf{x} = (m, n) \ , \text{ with } 1 \leq |n| < \rho \ , \\ D_8 & \text{if } \mathbf{x} = (m, n) \ , \text{ with } |n| \geq \rho \ , \end{cases}$$

in which D_8 is the symmetry group of the square. For any $k \geq 3$, if $\rho = k - 3/2$ then $|ST(X; k - 3/2)| = k$. The scaled set $X' = \sqrt{2}RX$ is thus an (r, R)-set in $\mathbb{R}^2$ with $\rho = \sqrt{2}R(k - 3/2)$ which has $|ST(X'; \rho)| = k$.

There are similar examples in $\mathbb{R}^n$. Consider the set X in $\mathbb{R}^n$ given by

$$X = \{(m_1, \ldots, m_n) \in \mathbb{Z}^n : |m_n| > 1\} \cup \{(m_1 + \theta, \ldots, m_{n-1} + \theta, 0) : (m_1, \ldots, m_{n-1}) \in \mathbb{Z}^{n-1}\} \ ,$$

with $0 < \theta < \frac{1}{2}$, which is an (r, R)-set with $r = \frac{1}{2}$, $R = \frac{1}{2}\sqrt{n}$. It is not a multiregular point system, but its group of symmetries $Sym(X)$ includes an $(n-1)$-dimensional lattice of translations. The set $X' = \frac{2}{\sqrt{n}}RX$ is an (r, R)-set that has $|ST(X'; \rho)| = k$ for $\rho = \frac{2}{\sqrt{n}}R(k - \frac{3}{2})$.

Example 4.2. (*Penrose tilings*) Many constructions proposed in connection with quasicrystals give aperiodic Delone sets X which have the locally finite atlas property under translations. Penrose tilings provide examples. Penrose tilings are tilings of $\mathbb{R}^2$ by two types of polygonal tiles called "kites" and "darts," respectively, see [4], [5], [11, p. 539], and [25]. We associate to any Penrose tiling $\mathcal{T}$ a Delone set $X = X(\mathcal{T})$ by choosing a fixed point in each "kite" and "dart."

Such tilings have a *repetitivity property* (under translations), which is that there is a function $L_X(\rho)$ such that a translate of each finite configuration ("patch") of tiles of diameter ρ occurs inside any ball of diameter $L_X(\rho)$. For Penrose tilings one can take $L_X(\rho) = (\tau^5 + 2)\rho \doteq 13.09\rho$, where $\tau = \frac{1+\sqrt{5}}{2}$, see Grünbaum and Shephard [11, p. 563]. We show that

$$N_X^*(\rho) \le 270\rho^2 \ \text{ for } \ \rho \ge 3 \ . \tag{4.11}$$

This holds since all "kites" and "darts" that touch a ball of radius 6.55ρ are completely contained in a ball of radius $6.55\rho + (\tau + 1) \le 8\rho$, for $\rho \ge 3$, and each "kite" and "dart" has area at least $\frac{3}{4}$. Thus $270\rho^2$ is an upper bound for the number of points of X that lie in any ball of radius 6.55ρ, and these points include among them representatives of all translation-equivalence classes of ρ-stars.

We can choose the Penrose tiling $\mathcal{T}$ to have no global symmetry, in which case $X = X(\mathcal{T})$ has $Sym(X) = \{1\}$. If we choose ρ so that $N_X(\rho) = k$, then (4.11) implies that ρ grows at least proportionally to $\sqrt{k}$ as $k \to \infty$.

For other properties of Penrose tilings, see [4], [5], [13], [21], [22] and [25].

Example 4.3. *(Pinwheel Tilings)* The pinwheel tilings of the plane studied in Radin [20] have the locally finite atlas property under isometries, but do not have the locally finite atlas property under translations. We obtain a Delone set X from the Conway tesselation of the plane described in §2 of [20] and [23, Sect. 7.4] by choosing a fixed point in each prototile. It can be proved that $N_X(\rho)$ is finite, with $N_X(\rho) = O(\rho^2)$. Radin's results imply that $N_X^*(\rho) = +\infty$ for $\rho > 4R$.

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