Local Groups in Delone Sets: Results and Conjectures

N.P. Dolbilin

[1]

We will discuss new results on local symmetry that occurs in arbitrary (not just periodic) Delone sets. It seems unexpected that these results, formulated and proved for completely arbitrary Delone sets in plane and in 3D space, imply a number of rather meaningful statements on Delone sets with additional conditions, in particular, statements on regular systems (i.e., Delone sets with transitive groups) including point lattices. Before formulating the theorems and conjectures that will be presented in the talk, we remind some necessary notions.

A set $X \subset \mathbb{R}^d$ is called a *Delone set* if there are some positive r, R such that
(1) r is the largest radius of equal balls centered at points from X that pack space $\mathbb{R}^d$, or in other words, $\inf_{x,x' \in X} |xx'| = 2r$;
(2) R is the smallest radius of equal balls centered at points of X that cover space $\mathbb{R}^d$, or in other words, $\sup_{y \in \mathbb{R}^d} \inf_{x \in X} |yx| = R$.

Given $x \in X$ and $\rho > 0$, a set of all points $x' \in X$ for which $|xx'| \leq \rho$, we call *ρ-cluster* of point x and denote it by $C_x(\rho)$. Clusters $C_{x_1}(\rho)$ and $C_{x_2}(\rho)$ of two points of X are said to be *equivalent* if there is a isometry $g \in Iso(d)$ such that $g(x_1) = x_2$ and $g(C_{x_1}(\rho)) = C_{x_2}(\rho)$. The *$\rho$-cluster group* $C_x(\rho)$ is a set of all isometries $s \in Iso(d)$ such that $s(x) = x$ and $s(C_x(\rho)) = C_x(\rho)$. A *regular system* is defined as a Delone set X with a transitive symmetry group. In particular, an integer lattice built on some basis is a particular case of a regular system since the group of translations of the lattice acts on it transitively.

Groups of bounded clusters in a set X, despite the fact that they may not enter the symmetry group of the entire set X, play important role in the study of a condensed matter. We focus on groups $S_x(2R)$ of clusters of radius $2R$, where R is the covering radius for a Delone set. The clusters of this radius are of especial interest. We call $S_x(2R)$ the *local group* at x and denote it $G_x := S_x(2R)$. Since $2R$-cluster is always of full dimension d, the local group G_x at any point x of a Delone set is finite.

Let X be a Delone set in $\mathbb{R}^2$ or $\mathbb{R}^3$, we call its *crystal kernel* a subset $X_{cr} \subseteq X$ of all points $x \in X$ with local groups G_x containing rotations of only crystallographic orders 2,3,4 or 6.

Conjecture 1 (crystal kernel conjecture, [1]). *The crystal kernel X_{cr} of a Delone set $X \subset R^3$ with covering radius R is a Delone set with some covering radius $R_{cr} \geq R$.*

The validity of this hypothesis immediately implies the following statement

[1]Steklov Mathematical Institute of the Russian Academy of Sciences
This work is supported by the Russian Science Foundation under grant 20-11-19998

Conjecture 2 (no 5-th fold local symmetry conjecture)**.** *In $\mathbb{R}^2$ and $\mathbb{R}^3$, there is no Delone set in which all the local groups G_x contain rotations of the 5-th order.*

This statement implies immediately the theorem on the absence of the 5-fold axes in 2D and 3D lattices. Moreover, the statement generalizes this classical theorem of geometric crystallography in two directions at once. The statement approves the impossibility of 5th-order rotations at all points, firstly, not only of the whole set but even of local rotations within $2R$-clusters. Secondly, this fact is true not only for lattices but also for arbitrary Delone sets.

In [2, 3], the crystal kernel conjecture is proved for $d = 2$. Thus for $d = 2$, Conjecture 2 is established also.

Theorem 1 (crystal kernel theorem for plane)**.** *For a Delone set $X \subset \mathbb{R}^2$ with covering radius R, its crystal kernel X_{cr} is a Delone set with covering radius $R_{cr} < 2R$. Moreover, this estimate is exact.*

Now let X be a Delone set in space $\mathbb{R}^3$ and $\widetilde{X} \subset X$ of all points $x \in X$ at which local groups G_x do not contain rotations of order higher than 6. The following inclusion is obviously true:

$$X_{cr} \subseteq \widetilde{X} \subseteq X$$

The following theorem is proved (see [1, 4]).

Theorem 2. *In an arbitrary Delone set $X \subset R^3$, the subset $\widetilde{X}$ of all points, at which local groups do not contain rotations of order higher than 6, is a Delone set. Moreover, $\widetilde{R} < 3R$, where R and R' are the covering radiuses for X and $\widetilde{X}$, respectively.*

‘

References

[1] Nikolay Dolbilin, Local groups in Delone sets, *Lecture Notes in Computational Sciences and Engineering* by Springer International Publishing, vol. **143**, https://www.springer.com/book/9783030767976 (2021), 10 pp. (Published online).

[2] N. P. Dolbilin, M. I. Shtogrin, "On crystalinity of local groups in a Delone set in Euclidean plane", Comp.Math.and Math.Phys., 2021, 12pp, (accepted, to appear).

[3] N. P. Dolbilin, M. I. Shtogrin, "Local groups in Delone sets: the hypothesis and results". Russian Survey, 2022, (accepted, to appear).

[4] N. P, Dolbilin, M. I.Shtogrin, "Local groups in Delone sets in space" (in print).