Locally Isometric Delone Sets

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The atomic structure of crystalline materials exhibits a very high symmetry. One of the central problems of the local theory for regular systems is to explain the genesis of the symmetry of crystalline structures through geometric features of their fragments of relatively small size.

An ideal crystal is a discrete set X in $\mathbb{R}^d$ which is a finite union of translates of a full-rank lattice Λ. However, generally saying, $\mathrm{Sym}(X)$ contains not only pure translations. Therefore, the crystalline structure X can be described in another way: X is a finite union of several $\mathrm{Sym}(X)$-orbits. An each orbit $\mathrm{Sym}(X) \cdot x$ is a regular system, i.e., a Delone set whose symmetry group acts point-transitively. The concept of the regular system generalizes the concept of the lattice. Though regular systems are arranged more complicate than lattices, by the Schoenflis-Bieberbach theorem, any regular system is a union of several translates of a lattice.

The regularity properties and conditions can be described in terms of ρ-clusters. Given $x \in X$ and $\rho > 0$, a subset of all points $x' \in X$ with distance $|xx'| \leq \rho$ is a *ρ-cluster* $C_x(\rho)$ of the point x. Given x and y from X, two ρ-clusters $C_x(\rho)$ and $C_y(\rho)$ are said to be *equivalent* if for some Euclidean isometry g $g(x) = y$ and $g(C_x(\rho)) = C_y(\rho)$. For given ρ the number of all classes of ρ-clusters in X is denoted by $N(\rho)$. The *cluster counting function* $N(\rho)$ is a positive, integer-valued,

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non-decreasing function. For any regular system $N(\rho) = 1$ for all $\rho > 0$.

The *regularity radius* is defined by the two conditions. First, equivalence of all $\hat{\rho}_d$-clusters in a Delone set $X \subset \mathbb{R}^d$, i.e., condition $N(\hat{\rho}_d) = 1$, implies the regularity of the X. Second, $\hat{\rho}_d$ is the minimal value in the sense that for $\forall \varepsilon > 0$ there is a Delone set X with $N(\hat{\rho}_d - \varepsilon) = 1$, which is not a regular system. As proved recently, $\hat{\rho}_d \geq d2R$.

From now on we denote by X a Delone set in which all $2R$-clusters are assumed to be equivalent, i.e. $N(2R) = 1$. We call a set X with $N(2R) = 1$ *locally isometric*. From $\hat{\rho}_d \geq d2R$ it follows that a locally isometric Delone set, generally saying, is not a regular systems. However, for some classes of Delone sets, e.g., for locally antipodal sets, as we showed recently for any d, condition $N(2R) = 1$ implies X to be a regular system.

Now we will focus on locally isometric Delone sets in $\mathbb{R}^3$. Due to long ago proven Stogrin's lemma, for such sets the groups $S_x(2R)$ of the $2R$-clusters are unable to contain a rotation axis of the order to exceed 6. The list of finite groups with this restriction is finite. Assuming each group from this list as a group $S_x(2R)$ for a Delone set, by means of numerous non-trivial geometric arguments one can prove that $\hat{\rho}_3 \leq 10R$.

On the background of the estimates $6R \leq \hat{\rho}_3 \leq 10R$ it is particularly interesting that for most groups, that are possible as $S_x(2R)$, the condition $N(2R) = 1$ is sufficient for regularity of a Delone set. Moreover, on this way we get another proof of the estimate $\hat{\rho}_3 \leq 10R$. This result represents also notable progress towards improving the upper bound for $\hat{\rho}_3$.