LOCAL SOURCES OF GLOBAL ORDER IN CRYSTALS

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One of the most fundamental problems of crystallography is the problem of crystal formation. Since the crystallization is a process which results from mutual interaction of just nearby atoms, it was believed (L. Pauling, R. Feynmann et al) that the long-range order of the atomic structure of the resulting crystal comes out certain local rules restricting the arrangement of nearby atoms. However, before 1970's there were no whatever rigorously proved statements about the link between local arrangements of nearby atoms and global ordering in a crystallographic structure. In the early 1970's B. Delone (Delaunay) and R.Galiulin initiated a problem to find such a link. Delone's students N.Dolbilin and M. Stogrin developed the beginnings of the so-called local theory of crystals.

The motivation of the local theory are as follows. An appropriate concept for describing positions of atoms of whatever solid structure (at the zero temperature) is a Delone set (or an (r,R)-system). However structures with long-range order such that as crystals involve a concept of the space group as well. A mathematical model of an ideal crystalline matter is defined now as a Delone set which is invariant with respect to some space (crystallographic) group. Thus, a mathematical model of an ideal crystal uses two concepts: a Delone set (which is of local character) and a space group (which is of global character). Meanwhile, as already said, the structure of a crystal is a result of the interaction of the nearby atoms. In this context the main aim of the local theory of a crystal was and is a rigorous derivation of global order of a crystalline structure from the pairwise geometric identity of local arrangements of the structure around each its atom. Mathematically, a crystal is defined as a Delone set X which is an orbit of some finite set under some crystallographic group. In the talk it is supposed to expose several basic theorems on how the local identity of a Delone set in the neighborhoods of all its points within certain radius R implies that the set is a crystal. There will be introduced all necessary definitions and stated some open questions.

Given Delone point set $X \subset \mathbb{R}^d$ with parameters $r > 0$ and $R > 0$, X is called a *crystal* if there is a certain crystallographic group G and a finite subset $X_0 \subset \mathbb{R}^d$ such that X is an G-orbit of X_0: $X = G \cdot X_0$. A particular case of a crystal is a *regular point set*: X_0 consists of a single point: $X_0 = \{x\}$.

Given Delone set X, $x \in X$, and $\rho > 0$, a ρ-*cluster* is a subset $C_x(\rho) := \{y \in X \mid |xy| \leq \rho\}$. Two ρ-clusters $C_x(\rho)$ and $C_{x'}(\rho)$ are *equivalent* if there is an isometry g such that $g(x) = x'$ and $g(C_x(\rho)) = C_{x'}(\rho)$. Denote by $N(\rho)$ the number of equivalence classes of ρ-clusters in X. Here we assume that a Delone set is of *finite type*, i.e. $N(\rho) < \infty$ for any $\rho > 0$.

The function $N(\rho)$ is an integer valued, continuous from the left, monotonically increasing, piece-wise constant function. X is a crystal if and only if $N(\rho) \leq m_0 < \infty$ for any $\rho > 0$. If $m_0 = 1$ then X is a regular point set.

Let $S_x(\rho)$ be a group of all isometries s which leave the center x fixed and the cluster $C_x(\rho)$ invariant. If ρ grows the group $S_x(\rho)$ can jump down: $S_x(\rho) \supseteq S_x(\rho')$ if $\rho < \rho'$.

In the talk we are going to tell about the following theorems.

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Theorem [Local Theorem, Delone, N.D.,M.Stogrin, R.Galiulin]. *A Delone set (=(r, R)-set) is a regular set if and only if for some radius ρ two conditions hold:*
$N(\rho + 2R) = 1$ *and*
$S_{\mathbf{x}}(\rho) = S_{\mathbf{x}}(\rho + 2R)$.

Theorem [Stogrin, N.D.]. $d = 2$. $N(4R) = 1$.

$N(4R - \varepsilon) = 1$ is not enough

Theorem [N.D.]. $d = 3$: $N(10R) = 1 \Rightarrow X$ *is a regular point set*

Theorem [N.D.]. *Let $X \subset \mathbb{R}^d$ be such that*
(1) $N(2R) = 1$,
(2) $2R$*-cluster* $C_x(2R)$ *is centrally symmetrical.*
Then X is RPS.

Theorem [N.D., A.Magazinov]. *Let $X \subset \mathbb{R}^d$ be such that $2R$-cluster $C_x(2R)$ for $\forall x \in X$ is centrally symmetrical.*
Then X is a crystal.

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