Bounds for the Regularity Radius of Delone Sets

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ICERM — July 2026

Basic Problem

- Characterize global properties of a geometric object $\mathcal{O}$ in a d-dimensional Euclidean space $\mathbb{E}^d$ in terms of its local configurations $C(\mathcal{O})$!

If the local configurations of $\mathcal{O}$ have properties $a, b, c, ...$ etc., then the entire object $\mathcal{O}$ has properties $x, y, z, ...$ etc.

- <u>Specifically:</u> Detect transitivity properties of the symmetry group $G(\mathcal{O})$ locally!

- Objects in $\mathbb{E}^d$ could be
  - Tilings
  - Delone sets (uniformly distributed discrete point sets)

- Local configurations could be coronas, clusters, neighborhoods, vertex-links...

Motivation comes from Crystallography

The standard mathematical model for a periodic crystal involves two concepts:

- a uniformly distributed discrete point set X, a Delone set (representing the atomic positions), and
- a crystallographic group of symmetries of X that acts on X with finitely many orbits.

Then X is the union of these orbits!

- Main question: how does the crystallographic group of symmetries appear?

- The Local Theorem for Delone Sets clarifies the connection between local and global structure of a crystal and explains the emergence of the crystallographic group through the congruence of local arrangements.

Tilings

How can a space be tiled by copies of one or more shapes?

– Long History! Hilbert's 18th Problem!

– Great relevance in geometry, geometry of numbers, crystallography, arts ...

- **copies:** translates, congruent copies, isomorphic polytopes ...

- **shapes:** convex polytopes, topological polytopes ...

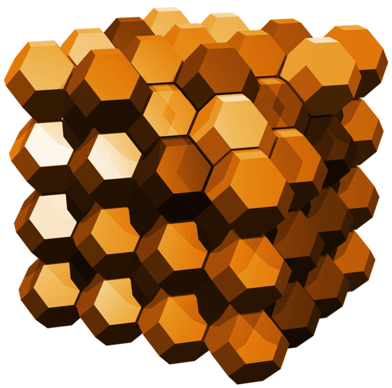
Tilings of Euclidean d-Space $\mathbb{E}^d$

Tiling $\mathcal{T}$ — family of *convex* polytopes, called the tiles of $\mathcal{T}$, which cover $\mathbb{E}^d$ without gaps and overlaps.

(Minkowski: If the tiles in a tiling are convex and compact, then each tile is a convex polytope.)

- **$\mathcal{T}$ is locally finite if each point in $\mathbb{E}^d$ has a neighborhood meeting only finitely many tiles.**

- **$\mathcal{T}$ is face-to-face if the intersection of any two tiles is either empty or a face of each (of any dimension).**

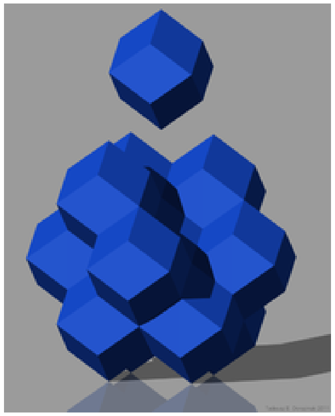


truncated octahedra

Tilings (cont.)

- $\mathcal{T}$ is **normal** if the tiles are uniformly bounded in size.

- $\mathcal{T}$ is **monohedral** if any two tiles are congruent.



rhombic dodecahedra

Fundamental Problem: Space Fillers in $\mathbb{E}^d$

Classify all convex d-polytopes that admit a monohedral tiling of $\mathbb{E}^d$.

Variants require face-to-face or isohedral (tile-transitive).

- **Planar case has been solved recently!** *Only 15 types of pentagonal tiles (Rao 2017)!*
  - All triangles, quadrangles, and certain hexagons, tile $\mathbb{E}^2$.
  - If $\mathcal{T}$ is a normal tiling of the plane by n-gons, then $n \leq 6$.

- Space filler problem rephrased: What are the analogues of the triangles, quadrangles, pentagons and hexagons in d-space?

Regular Tessellations (Honeycombs) in $\mathbb{E}^d$

$d = 2$: with triangles, hexagons, squares
$\{3,6\}, \{6,3\}, \{4,4\}$

$d \geq 1$: with d-cubes, $\{4,3,...,3,4\}$

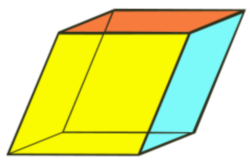
$d = 4$:
- with 24-cells, $\{3,4,3,3\}$
- with 4-crosspolytopes (generalized octahedra), $\{3,3,4,3\}$

Regular: geometric symmetry group is transitive on the flags

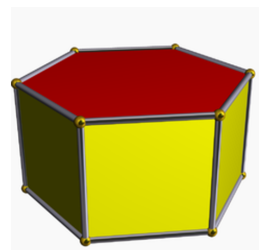
(flag: maximal chain of mutually incident faces in the tiling).

Tiling by translation

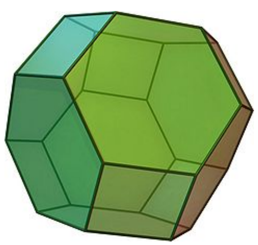
- **Parallelohedra:** Convex polytopes that tile $\mathbb{E}^d$ by translation. Will admit a unique face-to-face lattice tiling!
- **The five parallelohedra in $\mathbb{E}^3$ (Fedorov).**



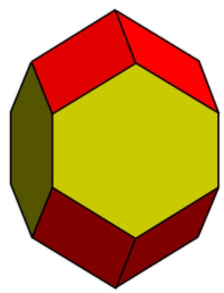
Rhombohedron



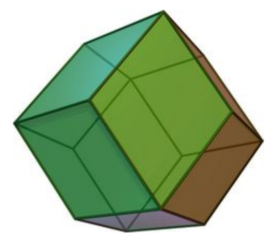
Hexagonal Prism



Truncated Octahedron

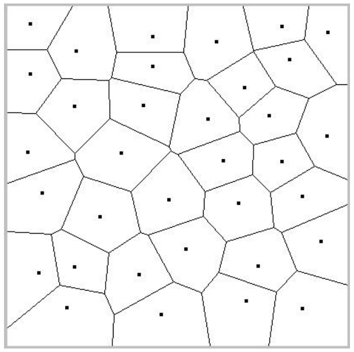


Elongated Dodecahedron



Rhombic Dodecahedron

• **Famous Voronoi Conjecture:** Every parallelohedron is an affine image of a Voronoi region of some lattice.

Voronoi regions 

• Proved for $d \leq 4$ and for primitive parallelohedra. There are just $2, 5, 52$ parallelohedra if $d = 2$, 3 or 4, resp.

• Voronoi Conjecture recently confirmed for $d = 5$ (Garber 2025)! In $\mathbb{E}^5$, 100,000+ examples!

Problem: Finitely many combinatorial types of space filler?

- Delone-Tarasov Bound: For space fillers admitting isohedral face-to-face tilings $\mathcal{T}$,

$$\#\ \text{facets} \ \leq\ 2^d(h - \tfrac{1}{2}) - 2,$$

where h is the index of the translation subgroup in $S(\mathcal{T})$.

  - Bieberbach theorems: h is bounded.
  - In $\mathbb{E}^3$: # facets $\leq$ 378 (here, $h \leq 48$)

- How realistic is this bound in $\mathbb{E}^3$?

- World record by Engel, 1980: several isohedral space fillers in $\mathbb{E}^3$ with 38 facets!

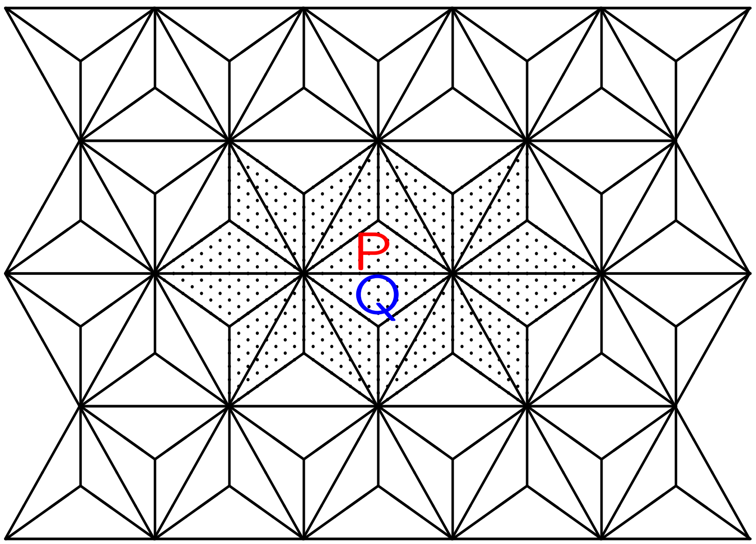
- Bochis, Sabariego, Santos, 2011: In $\mathbb{E}^3$, Voronoi regions for single crystallographic point orbits have # facets $\leq$ 92.

Local Theorem for Monohedral Tilings

(Delone, Dolbilin, Shtogrin, Galiulin, 1970's)!

- How can we detect tile-transitivity (isohedrality) locally, that is, in the local (central) coronas of the tiling.

Centered Coronas



The 1^{st} corona of tile P.

Tiles P and Q have the same 1^{st} coronas.

- Centered k^{th} corona $(P, C^k(P))$ of tile P in a tiling

$$C^0(P) := \{P\}$$
$$C^1(P) := \{S \mid S \cap P \neq \emptyset\}$$
$$C^k(P) := \{S \mid S \cap R \neq \emptyset \text{ for some } R \in C^{k-1}(P)\}$$

Note: Coronas are sets of tiles, *not* unions of tiles!

- Pairwise congruence of coronas $(P, C^k(P))$ and $(Q, C^k(Q))$:

there exists an isometry γ of $\mathbb{E}^d$ such that

$$\gamma(P) = Q, \;\; \gamma(C^k(P)) = C^k(Q).$$

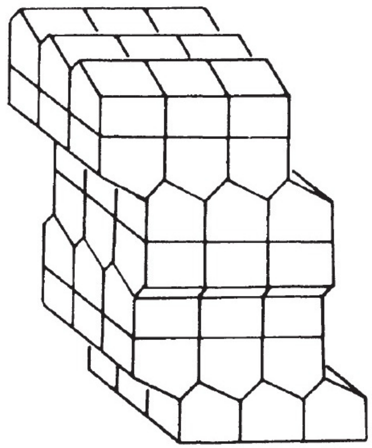
- k-th corona group: symmetry group of $(P, C^k(P))$

$$S^k(P) := \{\gamma \in S(P) \mid \gamma(C^k(P)) = C^k(P)\}.$$

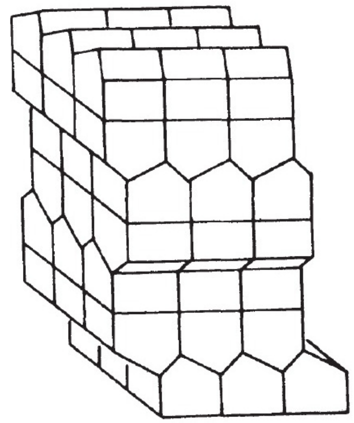
Note: $S(P) = S^0(P) \supseteq S^1(P) \supseteq S^2(P) \supseteq S^3(P) \supseteq \dots$

Finite groups! Only finitely many proper descents!

Pairwise congruence of 1^{st} coronas is not enough to imply pairwise congruence of 2^{nd} corona!! (Engel)



C2/c



$P4_122$

Two isohedral tilings with pairwise congruent 1^{st} coronas, but their 2^{nd} coronas are not pairwise congruent. (There are similar examples where one tiling is isohedral but the other is not.)

Local Theorem for Monohedral Tilings

(Delone, Dolbilin, Shtogrin, Galiulin, 1974)

$\mathcal{T}$ is isohedral iff there exists $k > 0$ such that

- any two centered k^{th} coronas are pairwise congruent, and
- $S^k(P) = S^{k-1}(P)$ for some tile (hence all tiles) P.

Notes

- Universal bound: $k \leq k_d$ ($k_2 = 1$, $k_3 = 5$, bound related to Delone-Tarasov bound for space-fillers)
- P asymmetric: $\mathcal{T}$ is isohedral iff $k = 1$.
- $k = 1$ is not enough for $d = 3$ (Engel), but it is for $d = 2$ and polygonal tiles (Dolbilin, Schattschneider).

DELONE SETS (mathematical models for crystals)

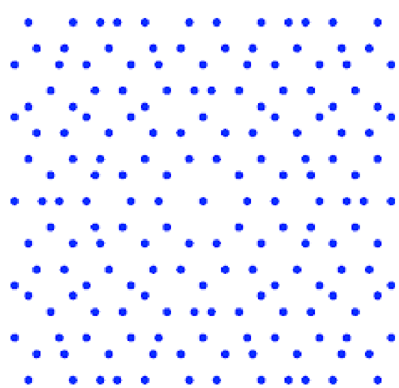
Delone set $X \subset \mathbb{E}^d$ of type (r, R), with $r, R > 0$

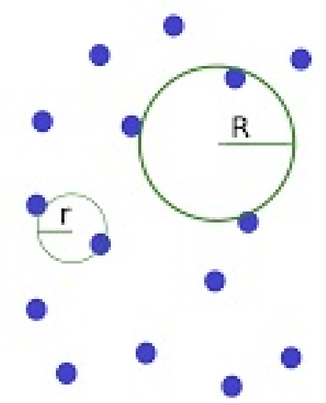
– Any two points of X are at distance $\geq 2r$.

Every *open* ball in $\mathbb{E}^d$ of radius r contains at most one point of X.

– R is the radius of the largest *empty* <u>open</u> ball.

Every *closed* ball in $\mathbb{E}^d$ of radius R contains at least one point of X.





Delone sets used in modeling of crystals (location of atoms).

Fedorov: Delone set X called an *ideal crystal* if its symmetry group $S(X)$ has finitely many orbits on X.

Regular systems (regular point sets)

Delone set X is called a *regular system* if its symmetry group $S(X)$ acts transitively on X.

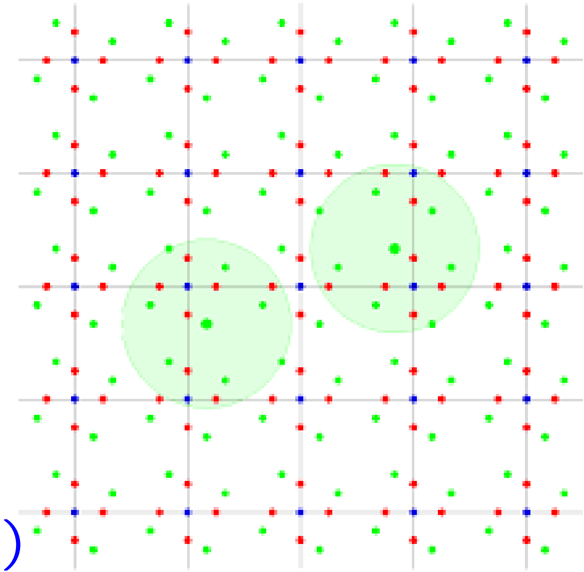
– Point orbits of crystallographic groups!

– "Ideal crystals" are unions of finitely many regular systems (Fedorov's definition)!

Basic question: How can we tell from local data that X is a regular system?

Some more terminology ....

X a Delone set in $\mathbb{E}^d$



- ρ-cluster at $x \in X$: $\quad C_x(\rho) := X \cap B_x(\rho)$

(all points of X at distance at most ρ from x)

Centered clusters! Clusters are full-dimensional if $\rho \geq 2R$.

- Cluster group $S_x(\rho)$ (local symmetry group)

$S_x(\rho)$ is the stabilizer of point $x \in X$ in the symmetry group of $C_x(\rho)$.

Cannot get larger as the radius ρ increases.

- Equivalence of clusters

ρ-clusters $C_x(\rho)$, $C_{x'}(\rho)$ said to be *equivalent* iff there exists an isometry σ of $\mathbb{E}^d$ such that

$$\sigma(C_x(\rho)) = C_{x'}(\rho), \quad \sigma(x) = x'.$$

Note: equivalence = congruence plus "center to center"

- Cluster counting function

$N(\rho) :=$ #(equivalence classes of ρ-clusters)

$N(\rho)$ is a non-decreasing function.

- For regular systems X, any two ρ-clusters of X are equivalent $\forall \rho \geq 0$ (that is, $N(\rho) = 1 \; \forall \rho \geq 0$).

Local Theorem for Delone Sets

(Delone, Dolbilin, Stogrin, Galiulin, 1976)

Explains the emergence of a crystallographic group of symmetries for a regular Delone set X!

X a Delone set of type (r, R) in $\mathbb{E}^d$

Thm: X is a regular system iff there exists a radius $\rho_0 > 0$ such that

- Any two $(\rho_0 + 2R)$-clusters of X are equivalent (that is, $N(\rho_0 + 2R) = 1$).
- The cluster groups of X stabilize at radius ρ_0, that is,
$$S_x(\rho_0) = S_x(\rho_0 + 2R)$$
for some point (and hence all points) x in X.

Conditions: $\exists \rho_0 > 0 : N(\rho_0+2R) = 1$ & $S_x(\rho_0) = S_x(\rho_0+2R)$

Consequences: If these two conditions hold, then actually

- $N(\rho) = 1 \, \forall \rho > 0$,
- $S_x(\rho)$ is the stabilizer of x in the full symmetry group of $X \ \forall \rho \geq \rho_0$.

Example: A "locally asymmetric" Delone set X of type (r, R) with mutually equivalent $4R$-clusters is regular!

Proof: $S_x(2R)$ is trivial by assumption, so pick $\rho_0 = 2R$.

Regularity Radius – important problem

Goal: Find small numbers ρ such that each Delone set X of type (r, R) with equivalent ρ-clusters is a regular point set.

Regularity radius

$$\widehat{\rho_d} \;=\; \text{smallest such } \rho \qquad (\text{depends on } d, r, R)$$

Does exist! By definition of $\widehat{\rho_d}$,

- Each Delone set X with equivalent $\widehat{\rho_d}$-clusters is a regular system.
- For all $\rho < \widehat{\rho_d}$ there exists a Delone set X with equivalent ρ-clusters which is not a regular system.

Estimates for $\widehat{\rho_d}$

Upper bound (Dolbilin, Lagarias & Senechal, 1998)

$$\hat{\rho}_d \leq 2R(d^2 + 1)\log_2(2R/r + 2)$$

Known prior to 2017

$\hat{\rho}_1 = 2R$, $\hat{\rho}_2 = 4R$ (Dolbilin, Stogrin)

$\hat{\rho}_d \geq 4R$, for $d \geq 2$ (Dolbilin)

Important question: nature of dependency on d?

Lower Bounds

Thm (Baburin, Bouniaev, Dolbilin, Erokhovets, Garber, Krivovichev & S., 2017) *

$$\widehat{\rho}_d \geq 2dR, \text{ for } d \geq 1.$$

– Lower bound grows linearly in d!

– Case $d = 3$ gives $\widehat{\rho}_3 \geq 6R$.

**On the origin of crystallinity: a lower bound for the regularity radius of Delone sets, Acta Cryst. A74 (2018), 61–629*

Thm: $\widehat{\rho}_d \geq 2dR$

Proof: Construction of layered Delone sets in $\mathbb{E}^d$ ("Engel sets"). The layers are very fine $(d-1)$-dimensional grids shifted relative to each other in a rather sophisticated way.

For all $0 < \varepsilon < 2dR$, there is an Engel set X_ε with mutually equivalent $(2dR-\varepsilon)$-clusters which is not regular. This implies $\widehat{\rho}_d \geq 2dR$.
(In fact, for all $\rho < 2dR$ there is a Delone set with equivalent ρ-clusters which is not a regular system. To see this, take $\varepsilon = 2dR - \rho$ and look at the Engel set X_ε. This has equivalent ρ-clusters but is not regular.)

Upper Bounds

X a Delone set with mutually equivalent $2R$-cluster,

Ω:= # prime factors of $|S_{\mathrm{x}}(2R)|$ (counted with multiplicities).

(For any group, $\Omega(G) + 1 \leq \log(2|G|)$.)

Tower Bound Theorem

If the $2(\Omega+2)R$-clusters of X are mutually equivalent, then X is a regular system.

Proof: Recall LocalThm: $\exists \rho_0 > 0 : N(\rho_0{+}2R) = 1 \,\&\, S_x(\rho_0) = S_x(\rho_0{+}2R)$.

In the chain of cluster groups,

$$S_{\mathrm{x}}(2R) \supseteq S_{\mathrm{x}}(4R) \supseteq \ldots \supseteq S_{\mathrm{x}}(2(\Omega+1)R) \supseteq S_{\mathrm{x}}(2(\Omega+2)R),$$

the descents cannot all be proper (otherwise $|S_X(2R)|$ has at least $\Omega+1$ prime factors). If $S_{\mathrm{x}}(2j_0R) = S_{\mathrm{x}}(2(j_0+1)R)$ for some j_0 (say), then the Local Theorem applies with $\rho_0 = 2j_0R$ and shows that X is regular.

Upper Bound for $\widehat{\rho_3}$

Thm (Dolbilin, Garber, Leopold & S., 2021)

$$\hat{\rho}_3 \leq 10R.$$

Thus,

$$6R \leq \hat{\rho}_3 \leq 10R.$$

Proof strategy

- $S_{\mathbf{x}}(2R)$ is a finite subgroup of $O(3)$! Finite subgroups of $O(3)$ are known! Essentially a finite list.
- Establish regularity of X for specific groups $S_{\mathbf{x}}(2R)$.
  - For example, "locally antipodal" Delone sets are regular systems (Dolbilin, Magazinov).
  - If $S_{\mathbf{x}}(2R)$ contains the rotation group of the cube or the tetrahedron, then X is regular.

- Eliminate specific groups as $2R$-cluster groups.
  - For any X with mutually equivalent $2R$-clusters, the rotations in $S_{\mathrm{x}}(2R)$ must have order ≤ 6. If order 6 occurs, then X is regular. (Shtogrin)
  - $S_{\mathrm{x}}(2R)$ cannot contain the icosahedral rotation group.

- Builds on a Dolbilin paper from 2021 which almost proves the 10R-upper bound. Missing piece: the symmetry group of the regular antiprism over a square cannot occur as the cluster group $S_{\mathrm{x}}(2R)$ for a Delone set with equivalent $2R$-clusters.

Conjectures on asymptotic growth of $\widehat{\rho_d}$

(Dolbilin, Garber, S. & Senechal, 2025)

Conjecture 1 (Weak Conjecture):

$$\hat{\rho}_d = O(d^2 \log d)R$$

Conjecture 2 (Strong Conjecture):

$$\hat{\rho}_d = O(d \log d)R$$

Conjectures imply

$$2dR \leq \hat{\rho}_d \leq O(d^2 \log d)R$$

and

$$2dR \leq \hat{\rho}_d \leq O(d \log d)R,$$

respectively. Bounds depend only on R and d, not on r.

Support for the Weak Conjecture $\hat{\rho}_d = O(d^2 \log d)R$

Conjectures proved for specific families $\mathcal{X}$ of Delone sets (with parameters r, R)!

$\mathcal{X}$-regularity radius

$$\hat{\rho}_d(\mathcal{X}) := \begin{cases} \text{smallest } \rho \text{ such that each } \rho\text{-isometric Delone} \\ \text{set } X \text{ from } \mathcal{X} \text{ is a regular system.} \end{cases}$$

Thm: For the family $\mathcal{X}$ of $2R$-isometric Delone sets with *full-dimensional* sets of points at minimal distance from all $x \in X$, we even have

$$\hat{\rho}_d(\mathcal{X}) = O(d^2)R$$

(The $O(d^2)$ term is roughly $2d \log \tau_d \sim 0.8022 d^2$, with τ_d the kissing number. Here, no log-term!)

Thm: For the family $\mathcal{X}$ of $2R$-isometric Delone sets with *full-dimensional* sets of $2r$-reachable points from any $x \in X$,

$$\widehat{\rho}_d(\mathcal{X}) = O(d^2 \log d)R.$$

(Point $y \in X$ is said to be *t-reachable* from $x \in X$ if y can be reached from x in finitely many steps of size at most t within X.)

An analogous theorem also holds for the sets of $2ar$-reachable points, with $a \geq 1$.

Support for the Strong Conjecture $\widehat{\rho}_d = O(d \log d) R$

Plausibility comes from the lower bound and yet another conjecture.

Group Order Problem: Bound the size of the $2R$-cluster groups $S_{\mathbf{x}}(2R)$ in a $2R$-isometric Delone set in $\mathbb{E}^d$.

Group Order Conjecture: $|S_{\mathbf{x}}(2R)|$ is bounded by $2^d \cdot d!$.

(True for $d = 2, 3$. For $d \geq 4$, there is a bound depending on d, r, R.)

Implication for $\widehat{\rho}_d$:

Group Order Conjecture says: $|S_{\mathbf{x}}(2R)| \le 2^d \cdot d!$

Apply the Tower Bound Theorem. Using $\Omega(G) + 1 \le \log(2|G|)$ with $G = S_{\mathrm{x}}(2R)$ shows

$$\Omega(S_{\mathrm{x}}(2R)) + 1 \le \log(2^{d+1} d!) =: C(d) = O(d \log d),$$

so

$$2(\Omega(S_{\mathrm{x}}(2R)) + 2) \le 2(C(d) + 1)$$

The Tower Bound Theorem says that a Delone set X with equivalent $2(\Omega(S_{\mathrm{x}}(2R))+2)R$-clusters is regular. So, in particular, if even the larger $2(C(d) + 1)R$-clusters are equivalent, then X is regular. Thus,

$$\widehat{\rho}_d \ \le \ 2(C(d) + 1)R = O(d \log d)R.$$

..... Thank You! .....

Abstract Bounds for the Regularity Radius of Delone Sets

Delone sets are uniformly discrete point sets X in Euclidean d-space used in the modeling of crystals. They are characterized by two parameters r and R, where (usually) $2r$ is the smallest inter-point distance of X and R is the radius of a largest "empty ball" that can be placed into the interstices of X. The local theory for Delone sets searches for local conditions on X that guarantee the emergence of a crystallographic group of symmetries producing X as an orbit set consisting of a single point orbit or finitely many point orbits, respectively. The regularity radius $t(d)$ is defined as the smallest positive number s such that each Delone set X with congruent clusters of radius t in Euclidean d-space is a

regular system, that is, a point orbit under a crystallographic group. We discuss bounds for the regularity radius in terms of R, and present conjectures that have been verified for some particularly interesting classes of Delone sets. This is joint work with Nikolai Dolbilin, Alexey Garber and Marjorie Senechal.