An isometry classification of periodic point sets

Vitaliy Kurlin & Olga Anosova
(University of Liverpool)

Crystals and lattices

Crystal structure is an ordered arrangement of particles in a lattice that extends in all directions. A *lattice* is defined as $\Lambda = \{\sum_{i=1}^{n} c_i v_i \,:\, c_i \in \mathbb{Z}\}$ for some linear basis $v_1, \ldots, v_n$ in $\mathbb{R}^n$.

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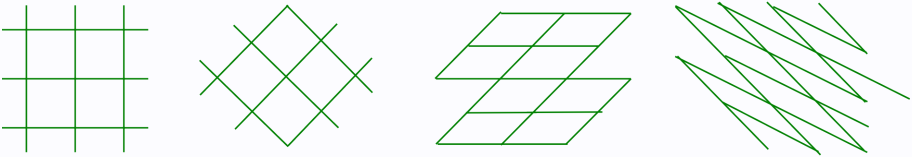

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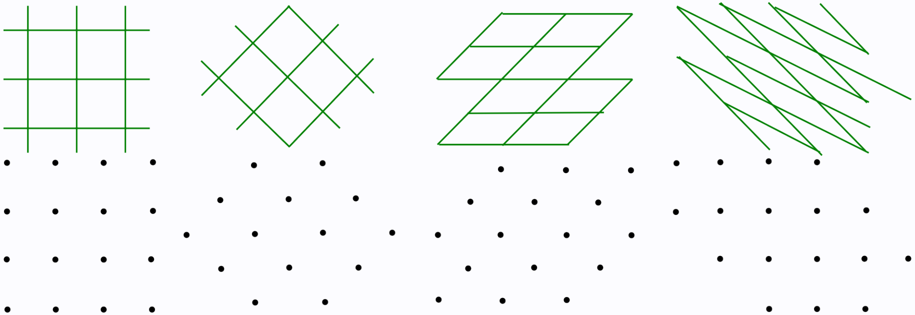
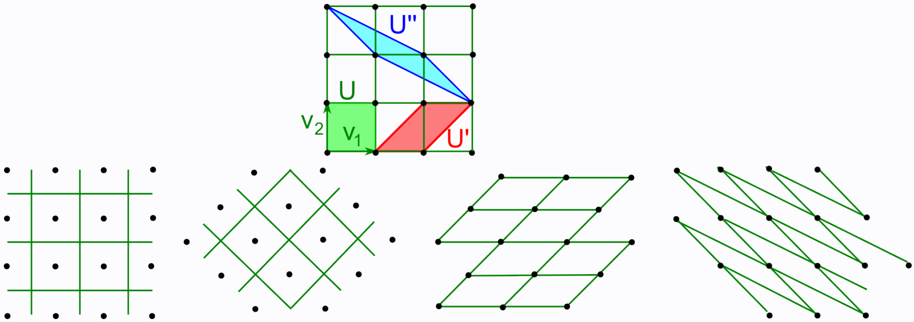


Lattices and Unit cells



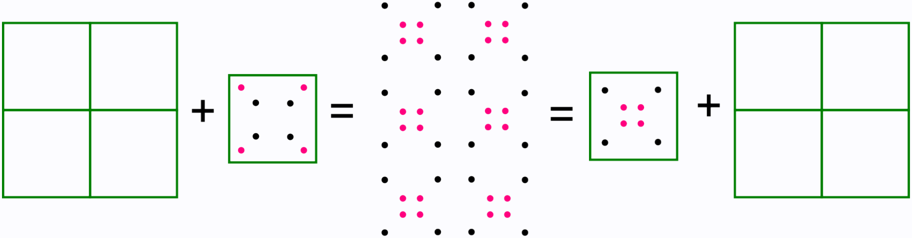
There are infinitely many different linear bases that generate the same square lattice.

A *unit cell* is the the parallelepiped $U = \{\sum_{i=1}^{n} c_i v_i \ : \ c_i \in [0,1)\}$ spanned on the linear basis $v_1, \ldots, v_n$.

Crystals as periodic point sets

Crystal structure is often presented in terms of the geometry of arrangement of particles (motif) in the unit cell.

A *motif* is a finite set of points $M \subset U$. Then a crystal is described by a *periodic point set* $S = M + \Lambda = \{u + v \ : \ u \in M, v \in \Lambda\}$.



Isometry invariants

Crystal structures can be studied up to *rigid motions*, which preserve distances and orientation.

An **isometry** is a map f that preserves all interpoint distances: $|p - q| = |f(p) - f(q)|$.

Hence mathematically a crystal is an **isometry class of periodic point sets**.

Problem: How to split periodic point sets into isometry classes?

Mathematical approach: via an **isometry invariant** I, that is a function I such that if periodic sets S, Q are isometric, then $I(S) = I(Q)$. This invariant is called **complete** if $I(S) = I(Q)$ implies that S, Q are isometric.

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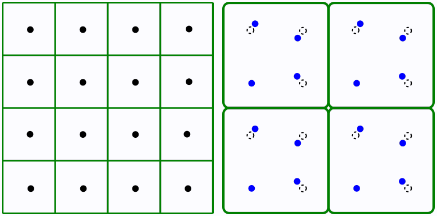

All discrete invariants (including symmetry groups) are discontinuous. Pseudo-symmetries have a manually chosen threshold.

Crystal Structure Prediction would benefit from continuously quantifying similarities between simulated crystals with different symmetry groups.

Measuring perturbations of points

The most natural way to measure thermal vibrations of atoms is by max displacement $d_f(S,Q) = \sup_{p \in S} |p - f(p)|$ for a fixed bijection $f : S \to Q$ between given periodic sets S, Q.

Bottleneck distance $d_B(S,Q) = \inf_{f:S \to Q} d_f(S,Q)$ is minimized over all bijections $f : S \to Q$.

Though d_B is impractical to compute, we can look for a distance d between invariants such that $d(I(S), I(Q)) \leq C d_B(S,Q)$ for a Lipschitz constant C, which is independent of S, Q.

Isometry classification problem

Find a function $I : \{\text{crystals}\} \to \{\text{numbers}\}$

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3) *(Lipschitz) Continuity* : the invariant I slightly changes under perturbations to quantify a similarity,
that is there exists a factor (constant) C such that $d(I(S), I(Q)) \leq C d_B(S, Q)$ for the bottleneck distance d_B and a suitable distance d between invariant values.

More classification requirements

4) *Computability* : a polynomial time in a motif size (that is in the number *m* of atoms in a unit cell).

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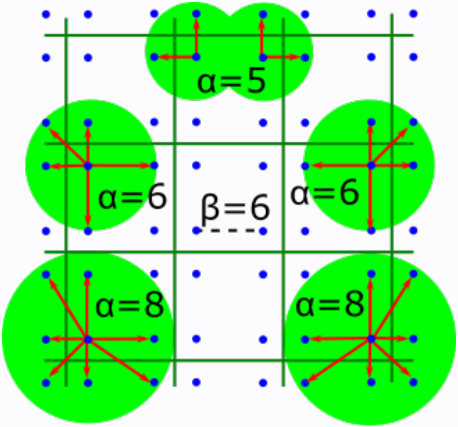
We'll define **isosets** : complete and continuous.

Local clusters of a point $p \in S$

In a periodic set, the *local α-cluster* of a point $p \in S$ at a radius α is $C(S, p; \alpha) = \{q - p : q \in S, \ |q - p| \le \alpha\}$.

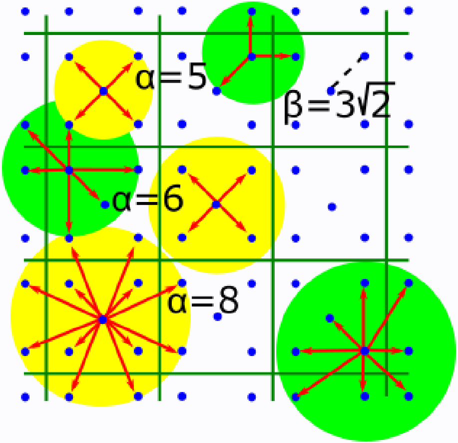


This set S has all α-clusters $C(S, p; \alpha)$ isometric to each other for any radius α.

In any S, points p, q are α-*equivalent* if $C(S, p; \alpha)$ and $C(S, q; \alpha)$ are isometric.

A set with two types of α-clusters

If α is small, for any point $p \in S$, its α-cluster $C(S, p; \alpha)$ consists of the single center p.

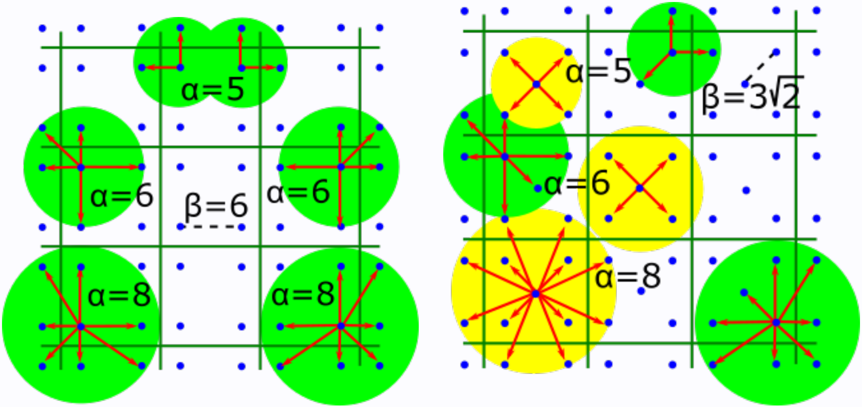


For any small radius α, all p are α-equivalent.

The 2-regular periodic point set S on the left has two non-isometric types of α-clusters $C(S, p; \alpha)$ for $\alpha \geq 4$.

The α-partition $P(S; \alpha)$

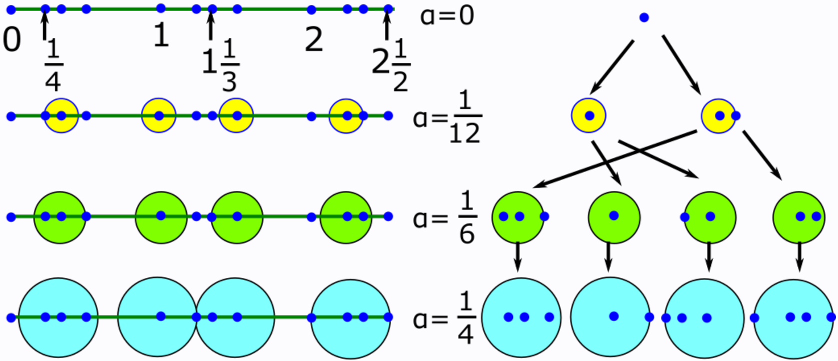
For a fixed radius α, any periodic point set S splits into classes of α-equivalent points $p \in S$, which form the α-partition $P(S; \alpha)$.



Left: 1-class partition, right: 2-class partition for any α.

The isotree $\mathrm{IT}(S)$ of a periodic set

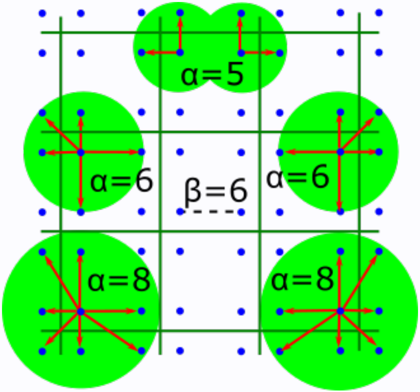
is formed by α-equivalence classes of points represented by their α-clusters over all $\alpha \geq 0$.

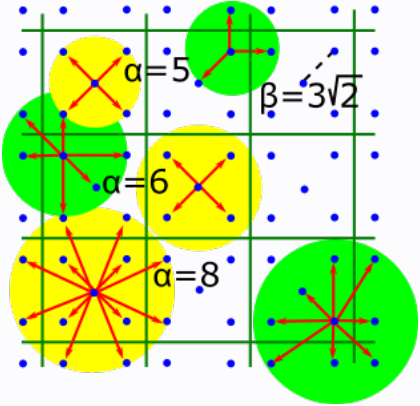


4 classes $0+\mathbb{Z}$, $\frac{1}{4}+\mathbb{Z}$, $\frac{1}{3}+\mathbb{Z}$, $\frac{1}{2}+\mathbb{Z}$ for $\alpha = \frac{1}{4}$.

The bridge length $\beta(S)$

Consider all paths: finite sequences of points $p_0, \ldots, p_m \in S$.
$\beta(S) = \min_{\text{all paths}} \max_{i=1,\ldots,m} |p_i - p_{i-1}|$ is the minimum 'jump' needed to reach any point.





The key concept: a stable radius α

For a periodic set S, a radius α is *stable* if

1) α-partitions stabilize: $P(S;\alpha) = P(S;\alpha-\beta)$;

2) the symmetry groups (of self-isometries of local clusters with fixed centers) stabilize for any point p in a motif of S, so $\mathrm{Sym}(S,p;\alpha) = \mathrm{Sym}(S,p;\alpha-\beta)$.

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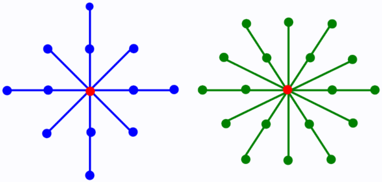
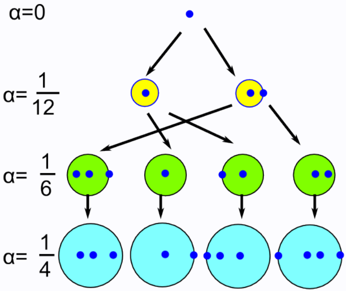


The isosets of the square and hexagonal lattices at the stable radius 2 consist of one cluster.

Minimal stable radius $\alpha(S)$

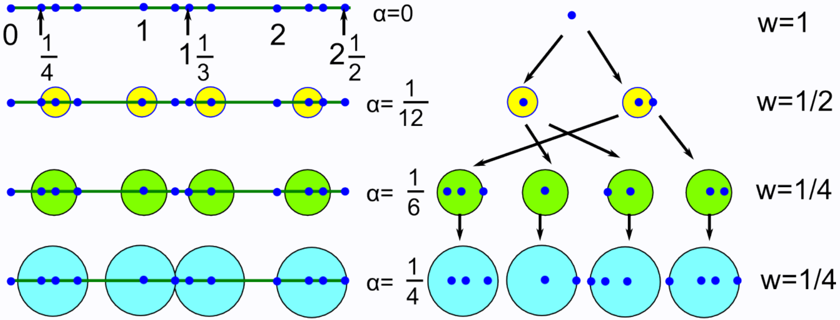
With increasing α, classes of $P(S;\alpha)$ can only be subdivided, not merged: if $\alpha' > \alpha$, the partition $P(S;\alpha')$ refines $P(S;\alpha)$.



Any periodic set with m points in a motif has at most m classes in any α-partition, hence a stable radius exists. All stable radii form an interval $[\alpha(S), +\infty)$ with the minimal stable radius $\alpha(S)$. For our goal upper bounds of $\alpha(S), \beta(S)$ will suffice.

The isoset invariant $I(S; \alpha)$

consists of *isometry classes* $[C(S, p; \alpha)]$ for all points p in a motif of S. If a class is repeated for k of m points in the motif, it has the weight k/m.



A complete classification

Theorem. Periodic point sets $S, Q \subset \mathbb{R}^n$ with a common stable radius α are isometric *if and only if* there is a bijection between their isosets $I(S; \alpha) \to I(Q; \alpha)$ respecting all weights.

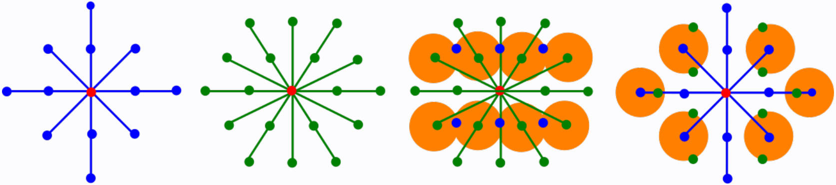
Any periodic crystal is uniquely identified (can be explicitly reconstructed in $\mathbb{R}^n$) by a finite list of isometry classes of its local α-clusters.

A stable radius α should now replace arbitrary cut-offs since isosets are complete invariants.

Continuity of complete isosets

A continuous **metric on isosets** is defined below.

Step 1: the distance between isometry classes of α-clusters is a Hausdorff distance minimized over rotations around the common center, also tolerant to points close to the boundary.



Step 2: use Earth Mover's Distance between isosets as weighted distributions of isometry classes.

Step 3: $\mathrm{EMD}(I(S;\alpha), I(Q;\alpha)) \leq 2d_B(S, Q)$.

Isosets of crystals summary

Periodic point sets model all crystalline solids.

A periodic point set S is uniquely determined up to isometry in $\mathbb{R}^n$ by its isoset $I(S;\alpha)$, which is
a weighted distribution of isometry classes of α-clusters $[C(S,p;\alpha)]$ at a stable radius α.

The isosets define continuous coordinates on the space of isometry classes of all crystals.

Further developments are in arXiv:2103.02749, Introduction to Periodic Geometry and Topology, V.Kurlin & O.Anosova

Summary of crystallographic invariants

	Invariant	Complete	Continuous	Run time	Reconstruct
Niggli's cell (for lattices)	Yes	Yes	No	Fast in practice	Yes
Symmetry groups	Yes	No	No	Fast in practice	
Density function ψ_k	Yes	in generic cases	Yes, with a distance	$O(mk^3)$	unclear
AMD_k, PDD_k	Yes	unclear	Yes, with with a distance	near linear in m, k	unclear
Isosets	Yes	Yes	Yes, with a distance	$O(m^3)$	Yes