Modelling Aperiodic Solids: Concepts and Properties of Tilings and their Physical Interpretation

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Quasicrystals
Quasiperiodicity
Translation module, Repetitivity
Local Isomorphism
Mutual Local Derivability
Matching Rules
Covering Rules
Maximal Coverings

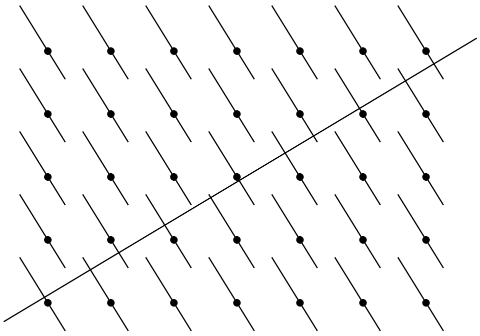
Quasicrystals

- intermetallic alloys
- well ordered, but aperiodic
- non-crystallographic symmetries: 5-, 8-, 10- or 12-fold rotation axis, icosahedral symmetry
- *quasiperiodic*: density formally given by Fourier series

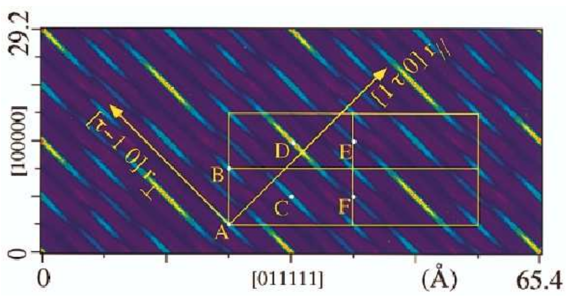
$$\rho(\mathbf{x}, x^{\perp}) = \sum_{\mathbf{h}\in\mathbb{Z}^n} a_{\mathbf{h}}\, e^{i\sum_j h_j (\mathbf{k}_j + \mathbf{k}_j^{\perp})\cdot(\mathbf{x}+\mathbf{x}^{\perp})}$$

with $n > d$ rationally independent basis vectors $\mathbf{k}_j$

In real space: cut through n-dimensional crystal



Electron density in 5-fold plane of i-ZnMgHo:

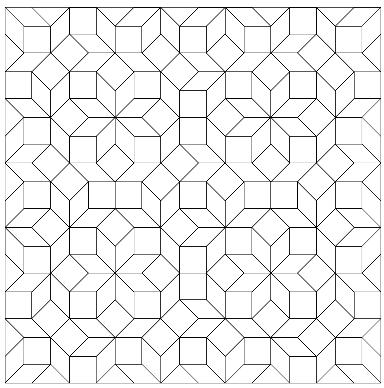


(H. Takakura et al., Phys. Rev. Lett. **86**, 236 (2001))

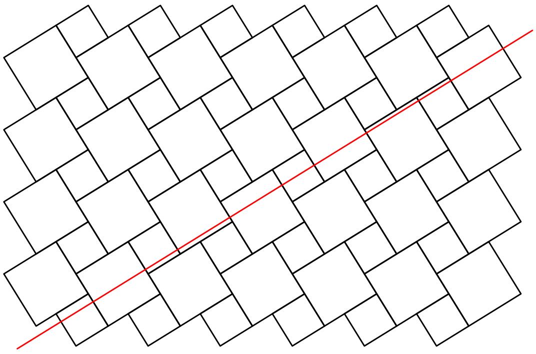
Atom positions form Delone set:
uniformly discrete and relatively dense
(minimal distance of atoms, no big voids).

For any R: only finitely many patches of radius R up to translation (*finite local complexity)*.

Can describe quasicrystal as decoration of a tiling, with finitely many tiles up to translation:



Quasiperiodic tilings: section through higher-dimensional periodic tiling:



Translation module, repetitivity

Translation module $T(P)$ of a patch P:
$\mathbb{Z}$-module generated by distance vectors between all translates of P.

Finite local complexity: $T(P)$ has finite rank!

Limit translation module T: intersection of all $T(P)$.

T can be non-trivial.
In quasiperiodic case: projection of higher-dimensional lattice.

Dual T^* of T: union of all $T^*(P)$, with $T^*(P)$ the linear functionals on $T(P)$ with values in $\mathbb{Z}$.

Primitive substitution tilings, canonical projection tilings: pure point part of diffraction pattern has support contained in T^*.

T trivial $\longrightarrow$ T^* not finitely generated.

Tiling is called *repetitive*, if the set of translates of any patch is relatively dense.

Homogeneity condition with physical motivation!

Equivalence concepts I: Local Isomorphism

Two tilings are called *locally isomorphic*, if any patch in one occurs also in the other (up to translation), and vice versa.

Such tilings are indistinguishable by any local means.

Finite range interactions cannot distinguish them
$\longrightarrow$ physically equivalent.

Tilings form local isomorphism (LI) classes.

Repetitive tilings: LI class invariant under translation.

LI class can be given natural a topology: two tilings are close if they agree in a large ball around the origin, up to a small translation.

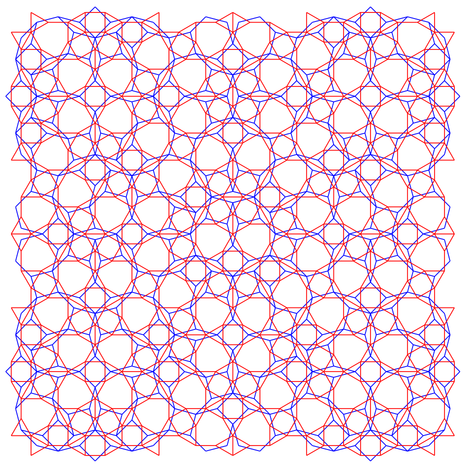
Translations then act by homeomorphisms on LI class
$\longrightarrow$ tiling dynamical system.

Repetitive tilings: tiling dynamical system is *minimal*.

The *symmetry* of a tiling should be defined as the symmetry of its LI class.

Equivalence concepts II: Local Derivability

Given the set of atoms, there is some arbitraryness in the choice of a tiling:



Two tilings are *mutually locally derivable* (MLD),
if one can be constructed in a local way from the other, and vice versa.

Translation module is an invariant of a MLD class, can only increase under local derivation.

MLD induces a bijection between LI classes.

Matching Rules

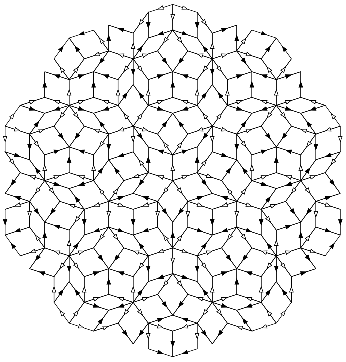
R-*atlas* of a tiling: collection of all patches of radius up to R; It is an invariant of the LI class.

Some LI classes are completely characterized by the R-atlas $\mathcal{A}_R$ for some fixed, finite R: any tiling with R-patches from $\mathcal{A}_R$ is also in this LI class.

Such an LI class of tilings is said to have *perfect matching rules* of radius R.

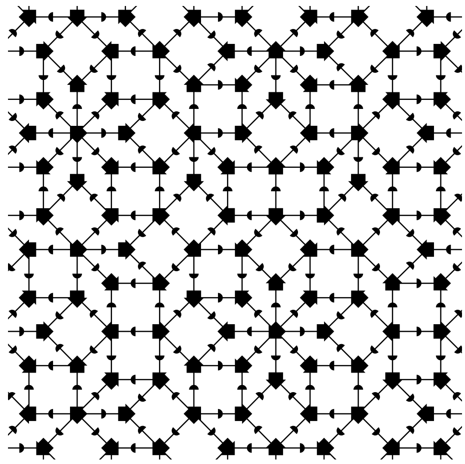
Finite range matching rules can never distinguish different tilings from the same LI class.

Having finite range matching rules is an invariant of an MLD class, but the matching rules radius may change under local derivation.



Some LI classes of tilings admit finite range perfect matching rules only after a *non-local* decoration.

Example: Ammann-Beenker tiling



The vertex decoration is non-local.

Finite range perfect matching rules make it possible that the LI class forms the set of ground state structures of some *finite range* interaction.

Covering Rules

The atlas of allowed R-patches is often rather big, and thus the matching rules complicated.

A simpler solution is often obtained with covering rules: the structure is required to be covered by copies of some patch or cluster.

Overlaps are allowed, but are subject to some constraints.

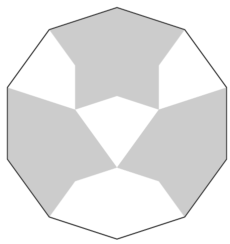
Ideally, the overlap constraints are imposed by the internal structure of the patch.

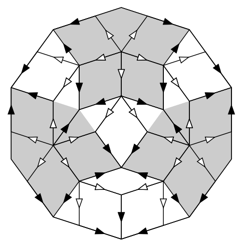
Physical motivation: the covering patch represents an energetically favourable local configuration.

If the whole structure is covered, all local configurations are favourable.

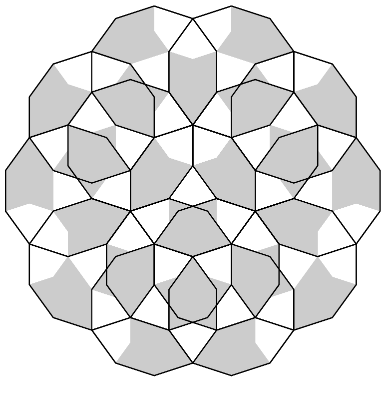
Gummelt's Aperiodic Decagon

Petra Gummelt (1995, 1996) defined overlap rules for a decagon, such that the set of admissible coverings of the plane is MLD to the LI class of Penrose tilings:



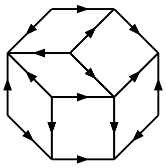


In the overlap region the coloring must match:

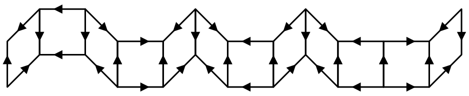


Covering Cluster for Octagonal Tiling

The following cluster completely covers the arrowed octagonal tiling:



The arrowing enforces the alternation condition:



This is not a *perfect* matching rule: it enforces ordered, quasiperiodic tilings, which are in general only 4-fold symmetric (A. Katz, 1995).

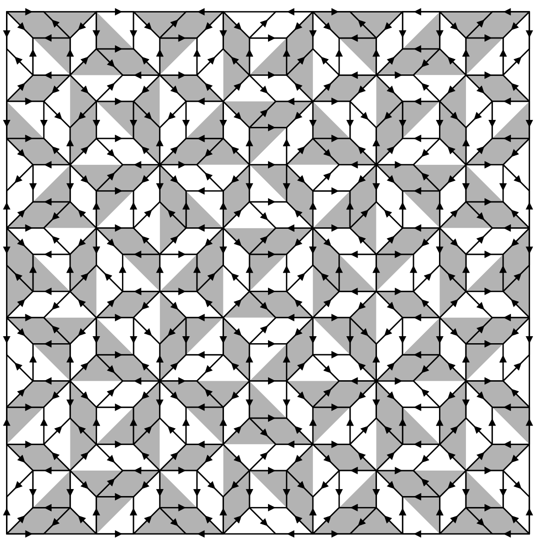
The covered tilings form a 1-parameter family of LI classes; however, among these the octagonal one has the *highest octagon density*.

The octagonal LI class consists of those structures that are *maximally covered*.

Each octagon corresponds to an octagonal prism. Prisms of different coloring are shifted against each other in the vertical direction.

The overlap rules due to the atomic decoration enforce the alternation condition, and thus an ordered tiling.

Among these structures the octagonal ones have the highest cluster density.



For physical applications, the arrowing can be encoded by the atomic decoration.

Structure of octagonal AlMnSi can be interpreted as maximal cluster covering (S.I. Ben-Abraham, F.G.).

This structure is a stacking of layers $\ldots ABAB' \ldots$