Resurrecting the space group of an aperiodic pattern

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Quasicrystals: pattern formation and aperiodic order,
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Some clarifications, added after talk:

- In this talk I explained how one may arrive at a notion of an aperiodic space group, through topology, in particular through the study of homotopical invariants of associated moduli spaces of patterns. This was a later observation—with our original and main goal being on the calculation of cohomological invariants—but one that I thought would be of most interest at this conference.
- This meant that, unfortunately, I had overlooked the notion of space group currently used in the theory of quasicrystals. This is an important concept that has been in regular usage for some decades, with several important mathematical developments (such as classification theorems) as well as being of practical importance to experimentalists.
- The title of course was not any sort of statement on this standard usage of 'space group' for quasicrystals, but rather simply the idea that the basic, classical definition of the space group of a periodic pattern breaks down when applied to an aperiodic pattern (slide 6), and that this talk discussed *one approach* (via topology) of how to recover an interesting extension of this classical idea which applies to aperiodic patterns too.
- Given all of this, clearly the definition of the 'space group' of an aperiodic pattern as used in this talk (and our paper) should be renamed. It would also be interesting to connect the space pro-group here and the usual space group of a quasicrystal when considering classes of patterns to which they both apply. After making some progress on this, it appears that whilst the space pro-group here is more complicated and captures extra information (which may or may not be a good thing, depending on the intended application), there is a mechanism with which to compare these invariants.

Joint work with John Hunton, Durham University.

Paper on the arXiv (as of last Tuesday):

J. Hunton and J. Walton, Aperiodic space groups and the topology of rotational tiling spaces.

arXiv:1806.00670

Periodic Patterns

Throughout, $T \subset \mathbb{R}^d$ is a 'pattern' (tiling/Delone set) with FLC.

If T is periodic then it is 'essentially interchangeable' (up to MLD) with its **space group**:

$$\Gamma := \{\text{isometries of } \mathbb{R}^d \text{ preserving } T\},$$

with group operation given by composition of symmetries.

For example, in $\mathbb{R}^2$ there are 17 such *wallpaper groups* up to isomorphism. In $\mathbb{R}^3$ there are 219 space groups up to isomorphism.

Point group extension

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The (positive) space group is an extension

$$\mathbb{Z}^d \to \Gamma \to G$$

where $G \leqslant \mathrm{SO}(d)$ is the (positive) **point group**.

It is the group of 'rotational parts' of symmetries of T. E.g., for the periodic tesselation of squares it's $\mathbb{Z}/4$.

Hulls of aperiodic patterns

If T is aperiodic then Γ, as defined earlier, is woefully insufficient (T doesn't have many, if any, *global* symmetries!).

The structure of 'almost symmetries' of T can be captured, though, via topology.

The **translational hull**:

$$\Omega_t := \{\text{tilings with same finite patches as } T \text{ up to translation}\}$$

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Example

If T is periodic then the hull consists only of translates of T and $\Omega_t \cong \mathbb{R}^d/\mathbb{Z}^d$ is a d-torus.

Rotational hulls

The **rotational hull**:

$$\Omega_r := \{\text{tilings with same finite patches as } T \textbf{ up to rigid motion}\}$$

(again, with 'obvious' topology).

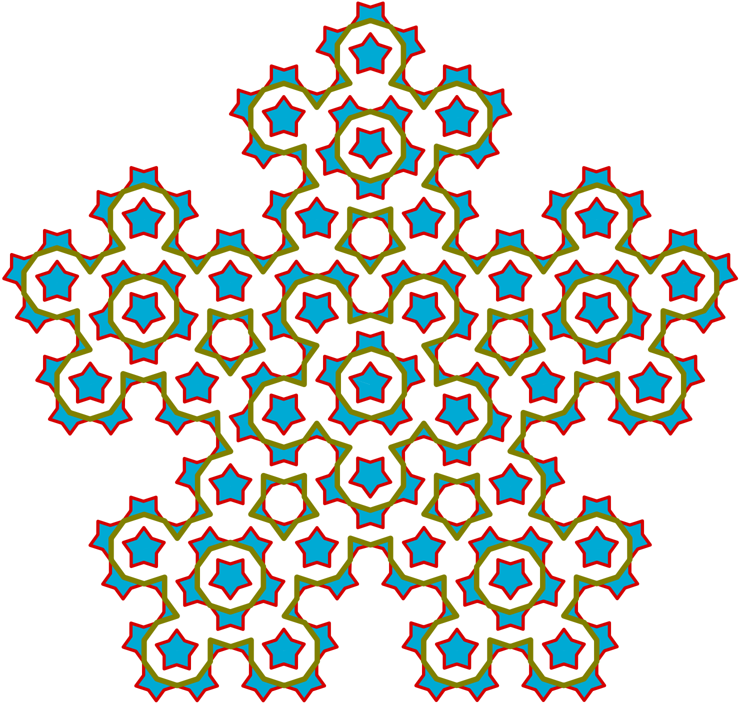
Example

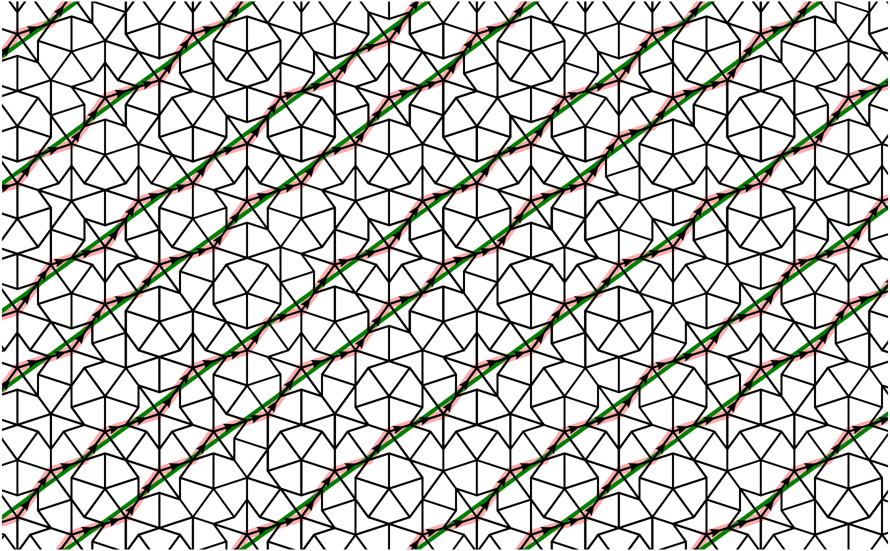
If T is periodic then Ω_r is a manifold of dimension $d + d(d+1)/2$...
whose topology depends on the rotational symmetries of T!

Example

If T is a Penrose tiling then Ω_r is the space of 'all Penrose tilings', constructed from rigid motions of Penrose rhombs fitting together according to their matching rules.

Question: what do the topologies of the hulls tell us about the tilings? What can we say about the topologies of the hulls?





Aperiodic point group

There is still a simple notion of the point group G:

Let $g \in \mathrm{SO}(d)$ be in the point group G if: whenever P is a finite patch of T then $g(P)$ also belongs to T, up to a translation.

Example

If T is periodic then G coincides with the standard (positive) point group.

Example

If T is a Penrose tiling then $G \cong \mathbb{Z}/10$ (but note: there is no Penrose tiling with tenfold rotational symmetry).

One last hull

The rotation group G naturally acts on Ω_t (by rotating tilings). The quotient space Ω_t/G has been considered before. We consider instead the *homotopy quotient*:

$$\Omega_G := (\Omega_t \times EG)/G.$$

Here, EG = contractible space equipped with free G-action.

Also known as the *Borel construction*. 'Morally correct' quotient for the purposes of homotopy theory.

Spin point groups

We have the *spin group* $\mathrm{Sp}(d)$ given as the universal cover of $\mathrm{SO}(d)$. For $d = 2$ it is the $\mathbb{Z}$ cover $\mathbb{R} \xrightarrow{q} S^1$.

For $d > 2$ the quotient $\mathrm{Sp}(d) \xrightarrow{q} \mathrm{SO}(d)$ is a $\mathbb{Z}/2$ cover.

For $d = 3$, $\mathrm{Sp}(3) \cong S^3$.

We can lift our finite point group $G \leqslant \mathrm{SO}(d)$ to $\widetilde{G} \leqslant \mathrm{Sp}(d)$. For example, for $d = 2$: $G \cong \mathbb{Z}/n$ and $\widetilde{G} \cong \mathbb{Z}$.

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Remark

$\mathrm{Sp}(d)$ is convenient from the perspective of homotopy theory: it has trivial π_1 and π_2.
For $d = 3$ the groups $\widetilde{G}$ can be better behaved than G. The group cohomology of $\widetilde{G}$ is 4-periodic (but this need not be the case for G, such as the icosahedral group).

Homotopical invariants of periodic patterns

Theorem

Let $T \subset \mathbb{R}^d$ be periodic. Then there exists a natural isomorphism of extensions (*):

$$\begin{array}{ccccc} \pi_1(\Omega_t) & \longrightarrow & \pi_1(\Omega_G) & \longrightarrow & G \\ \downarrow \cong & & \downarrow \cong & & \| \\ \mathbb{Z}^d & \longrightarrow & \Gamma & \longrightarrow & G \end{array}$$

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\mathbb{Z}^d \arrow[r] & \Gamma \arrow[r] & G
\end{tikzcd}$$

Theorem

Let $T \subset \mathbb{R}^d$ be periodic. Then there exists a pullback of extensions:

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So:

1. The space group can be recovered as the fundamental group of the homotopy quotient Ω_G.
2. The fundamental group of Ω_r is the 'spin version' of Γ (a $\mathbb{Z}$ cover for $d = 2$, $\mathbb{Z}/2$ cover for $d > 2$).

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Unfortunately the fundamental group is not an appropriate invariant to apply to an aperiodic tiling space; these are 'pathological spaces' (c.f., the Warsaw circle).

But shape theory gives us the correct replacement: the **pro-fundamental group** $\pi_1^{\text{pro}}(X)$.

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Definition

We call $\pi_1^{\mathrm{pro}}(\Omega_G)$ the **space pro-group**, and denote it by Γ^{pro}.

Aperiodic space groups

To get an honest group (rather than pro-group), we can pass to the inverse limit:

Definition

We call the inverse limit $\Gamma := \varprojlim \Gamma^{\mathrm{pro}}$ the **space group** of T.

If T is fixed by the full point group (c.f., 'symmorphic space groups') then Γ is an extension (in fact, a split one):

$$\varprojlim \pi_1^{\mathrm{pro}}(\Omega_t) \to \Gamma \to G.$$

We can calculate Γ precisely in some cases:

Example

Let $T = \text{Fibonacci}^3 \subset \mathbb{R}^3$. Then Γ is the semi-direct product of $F_2 \oplus F_2 \oplus F_2$ and $G =$ the rotational symmetries of a cube (we can describe the action of G on $(F_2)^3$ precisely).

Example

If $T \subset \mathbb{R}^2$ is a canonical $3 \to 2$ cut and project tiling (a 'stepped surface') then Γ is the semi-direct project of $\mathbb{Z}^3$ and $\mathbb{Z}/2$ (with non-trivial element acting by $x \mapsto -x$).

Natural fibrations

These results come from some natural (and computationally useful!) fibre-bundle descriptions of Ω_G and Ω_r, along with a useful network of maps connecting them all.

For example: Ω_r can be expressed as a fibre bundle:

$$\Omega_t \to \Omega_r \to \mathrm{SO}(d)/G.$$

These can be useful for cohomology calculations.

We can use the Serre spectral sequence, amongst some other technical tricks, to compute the cohomology of the 6-manifold of placements of the cube tessellation in $\mathbb{R}^3$:

Theorem

For $T \subset \mathbb{R}^3$ the periodic tessellation by unit cubes:

$$H^n(\Omega_r;\mathbb{Z}) \;=\; \begin{cases} \mathbb{Z} & n=0 \\ 0 & n=1 \\ \mathbb{Z}/2\oplus\mathbb{Z}/2 & n=2 \\ \mathbb{Z}^2\oplus\mathbb{Z}/2\oplus\mathbb{Z}/4 & n=3 \\ \mathbb{Z}/2\oplus\mathbb{Z}/4 & n=4 \\ \mathbb{Z}/2\oplus\mathbb{Z}/2 & n=5 \\ \mathbb{Z} & n=6 \\ 0 & n>6\,. \end{cases}$$

We also have a calculation for a class of aperiodic examples (Sturmian^{3}s).

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- Computer aided calculations for substitution tilings/cut and project tilings?