Crystallographic Groups I

The Classical Theory

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Notation

Notation: Group Actions

- Group element γ acting on $x \in X$:

$$x \mapsto \gamma.x$$

- Orbit of Γ through $x \in X$:

$$\Gamma.x = \{\gamma.x \mid \gamma \in \Gamma\}$$

- Stabiliser (isotropy subgroup) of a point $x \in X$:

$$\Gamma_x = \{\gamma \in \Gamma \mid \gamma.x = x\}$$

Notation: Groups

- Affine group:

$$\mathbf{Aff}(\mathbb{R}^n) = \mathbf{GL}_n(\mathbb{R}) \ltimes \mathbb{R}^n$$

- Euclidean group:

$$\mathbf{Iso}(\mathbb{R}^n) = \mathbf{O}_n \ltimes \mathbb{R}^n$$

Notation: Affine Maps

An affine map

$$\gamma : \mathbb{R}^n \to \mathbb{R}^n, \quad x \mapsto A \cdot x + v$$

with linear part

$$\mathrm{L}(\gamma) = A \in \mathbf{GL}_n(\mathbb{R})$$

and translation part

$$\mathrm{T}(\gamma) = v \in \mathbb{R}^n$$

is written in tuple notation

$$\gamma = (A, v),$$

or in (augmented) matrix notation

$$\gamma = \left(\begin{array}{c|c} A & v \\ \hline 0 & 1 \end{array}\right) \in \mathbf{GL}_{n+1}(\mathbb{R}).$$

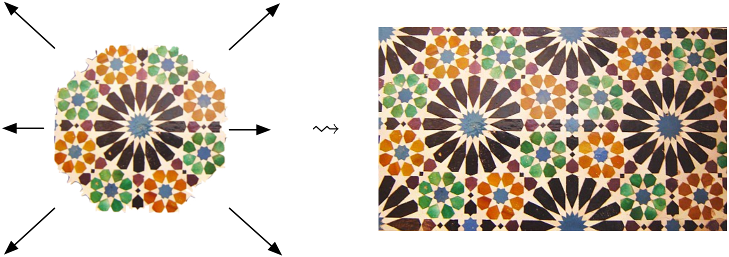
I. Tilings and Crystals

Lattice Patterns

- Start with a single shape in $\mathbb{R}^n$
  $\rightsquigarrow$ rotate, reflect and translate it.
- Consider those shapes whose copies fill up space without gaps or overlaps.
- If the shape is a regular polyhedron, its vertices form a lattice in space.

2D: Ornaments

In dimension $n = 2$, we speak of ornaments
(or tilings, tessellations, wallpapers . . .)

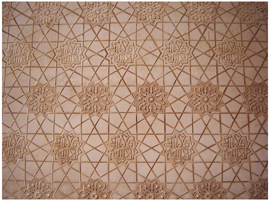


2D: Ornaments

- Ornamental patterns challenged and inspired artists and mathematicians throughout the centuries.
- Ancient Egyptian and medieval Moorish artists created elaborate ornamentations, thereby realising all of the 17 possible symmetry classes.

2D: Ornaments

The Alhambra in Granada (Spain) contains ornamentations realising “most” of the 17 symmetry classes.

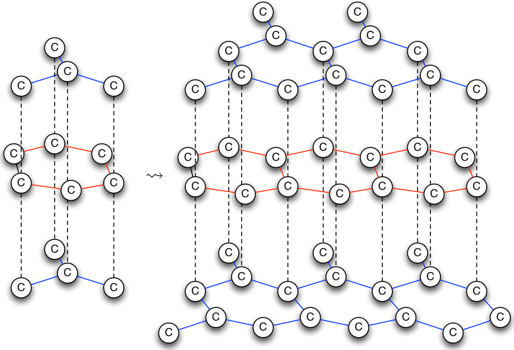



Photographs by John Baez

`http://math.ucr.edu/home/baez/alhambra/`

3D: Crystals

In dimension $n = 3$, we speak of crystals.



The primitive cell on the left generates the crystal lattice of graphite on the right.

Classification by Symmetries

To each ornamental or crystallographic pattern X we can assign its symmetry group Γ:

- Γ is a subgroup of $\mathbf{Iso}(\mathbb{R}^n) = \mathbf{O}_n \ltimes \mathbb{R}^n$.
- $\Gamma.X = X$.
- If $\gamma.X = X$, then $\gamma \in \Gamma$.

Classify ornaments and crystals by classifying their symmetry groups!

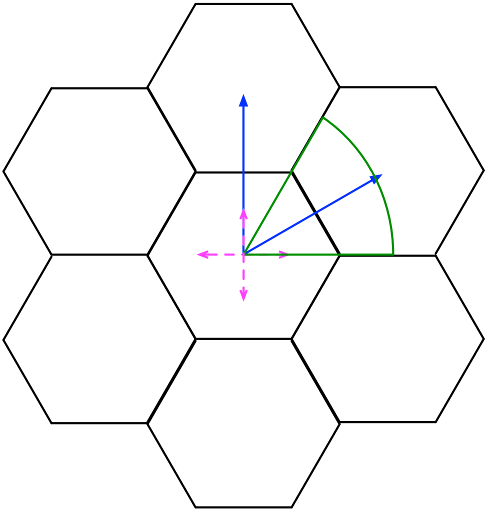
Fundamental Domains

Crystal patterns are generated by transformations of a fundamental domain F_Γ:

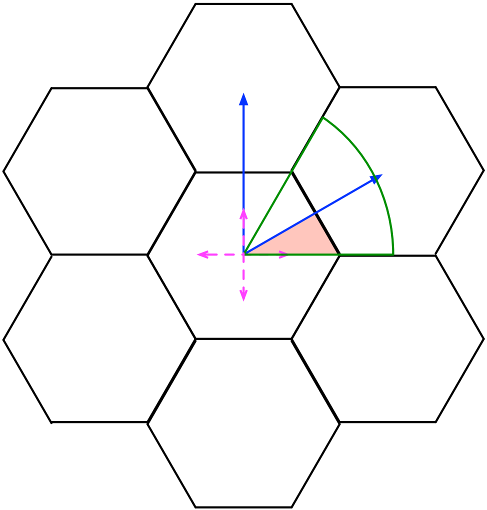
- F_Γ is open in $\mathbb{R}^n$,
- $\Gamma.\overline{F}_\Gamma = \mathbb{R}^n$,
- each Γ-orbit intersects F_Γ at most once.

Note: Often, fundamental domains are much smaller than the generating pattern of an ornament or a crystal.

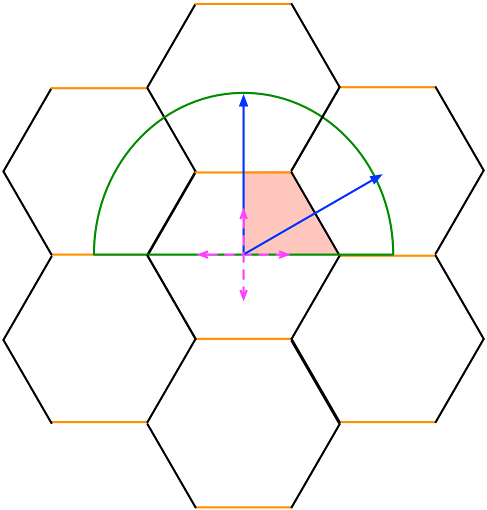
Example: Hexagonal Pattern



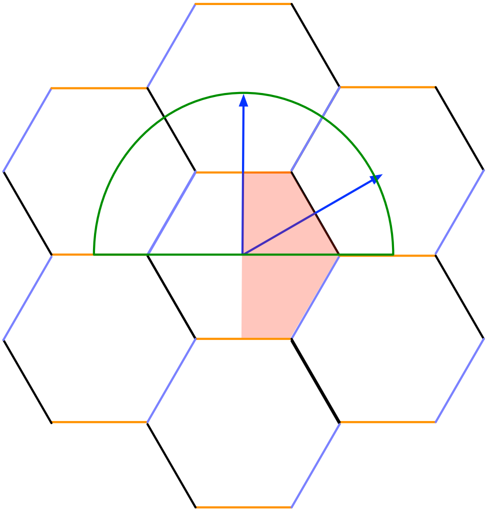
Example: Hexagonal Pattern



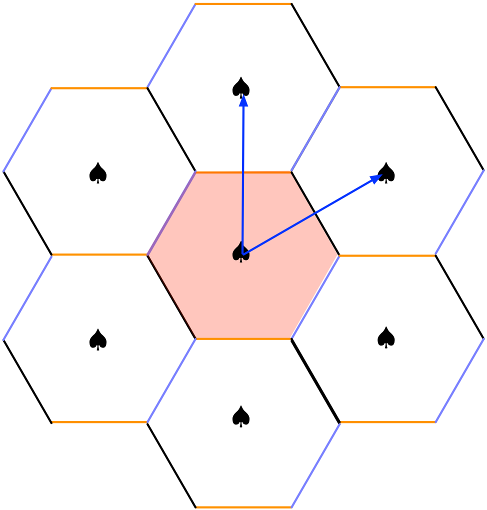
Example: Hexagonal Pattern



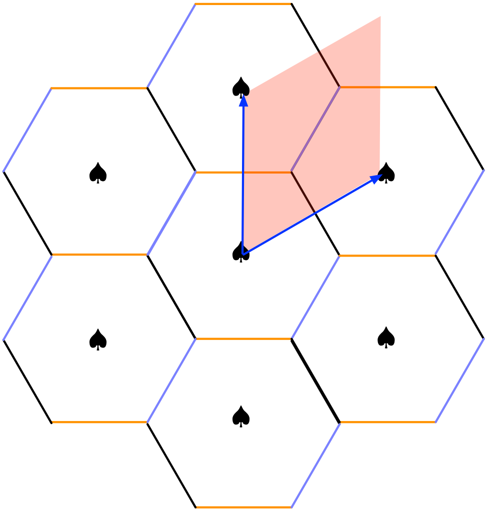
Example: Hexagonal Pattern



Example: Hexagonal Pattern



Example: Hexagonal Pattern?



References I

- J.J. Burckhardt, Die Bewegungsgruppen der Kristallographie, Birkhäuser, 1947
- J.H. Conway, H. Burgiel, C. Goodman-Strauss, The Symmetries of Things, A.K. Peters, 2008
- B. Grünbaum, What Symmetry Groups Are Present in the Alhambra?, Notices Amer. Math. Soc. 53, 2006, no. 6
- B. Grünbaum & G.C. Shephard, Tilings and Patterns, W.H. Freeman and Company, 1989
- D. Schattschneider, The Plane Symmetry Groups: Their Recognition and Notation, Amer. Math. Monthly 85, 1978, no. 6
- H. Weyl, Symmetry, Princeton University Press, 1952

II. Bieberbach's Theorems
and Classifications of Crystallographic Groups

Crystallographic Groups

The symmetry group Γ of a crystal

- is discrete (as a subset of $\mathbf{Iso}(\mathbb{R}^n)$),
- is cocompact, i.e. $\mathbb{R}^n/\Gamma$ is compact.
  (equivalent: $\overline{F}_\Gamma$ is compact.)

Γ is called a crystallographic group.

If Γ is also torsion-free, i.e. for all $\gamma \in \Gamma$ holds

$$\left[\gamma^k = \text{id for some } k \geq 1\right] \quad \Rightarrow \quad \gamma = \text{id},$$

then Γ is called a Bieberbach group.

Classification by Symmetries

When should two crystallographic groups Γ_1 and Γ_2 be considered equivalent?

- Conjugation by $g \in \textbf{Iso}(\mathbb{R}^n)$ is too restrictive!
- Choose affine equivalence:

$$\Gamma_1 \sim \Gamma_2 \quad :\Leftrightarrow \quad \Gamma_1 = g \cdot \Gamma_2 \cdot g^{-1} \text{ for some } g \in \textbf{Aff}(\mathbb{R}^n)$$

As we will see later, this is a good choice!

Classification for $n = 2$

Theorem (Fedorov, 1891)

There exist 17 (classes of) crystallographic groups in dimension 2.

Commonly known as wallpaper groups.

Classification for $n = 3$

Theorem (Fedorov & Schoenfließ, 1891)
There exist 230 (classes of) crystallographic groups in dimension 3*.*

Wait. . . is it 230 or 219?

Answer:
Depends on whether conjugation by g with $\det(\mathrm{L}(g)) < 0$ is allowed or not.

- Mathematicians: Yes! $\Rightarrow$ 219 groups.
- Chemists/physicists: No! $\Rightarrow$ 230 groups.

Bieberbach Groups for $n = 2$

Among the 17 wallpaper groups,
there are only 2 Bieberbach groups:
The fundamental groups of the torus and the Klein bottle.

Example: Torus Group

The fundamental group of the torus is generated by the two translations

$$\gamma_1 = \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \gamma_2 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

Clearly, this group is torsion-free.

Example: Klein Bottle Group

The fundamental group of the Klein bottle is generated by a glide-reflection and a translation,

$$\gamma_1 = \left(\begin{array}{cc|c} 1 & 0 & 1/2 \\ 0 & -1 & 1/2 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \gamma_2 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1/2 \\ \hline 0 & 0 & 1 \end{array}\right).$$

This group is also torsion-free (examine the first row in a group word!).

Example: Non-Bieberbach Crystallographic Group

The symmetry group of the hexagonal pattern on slide 14 is generated by

$$\text{(reflections)} \quad \sigma_1 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \sigma_2 = \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\text{(rotation)} \quad \varrho = \left(\begin{array}{cc|c} \sqrt{3}/2 & -1/2 & 0 \\ 1/2 & \sqrt{3}/2 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\text{(translations)} \quad \tau_1 = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \tau_2 = \left(\begin{array}{cc|c} 1 & 0 & (\sqrt{6}+\sqrt{2})/4 \\ 0 & 1 & (\sqrt{6}-\sqrt{2})/4 \\ \hline 0 & 0 & 1 \end{array}\right).$$

The elements σ_1, σ_2 and ϱ are of finite order.
So this is not a Bieberbach group.

Bieberbach Groups for $n = 3$

Theorem (Hantzsche & Wendt, 1935)

Among the 219 space groups, there are only 10 Bieberbach groups.

Hilbert's 18^{th} Problem

"Is there in n-dimensional Euclidean space [. . .] only a finite number of essentially different kinds of groups of motions with a [compact] fundamental region?"

Bieberbach's First Theorem

Theorem (Bieberbach, 1911)
Let $\Gamma \subset \mathbf{Iso}(\mathbb{R}^n)$ *be a crystallographic group.*
Then:

- $\mathrm{L}(\Gamma)$ *is finite.*
- $\Gamma \cap \mathbb{R}^n$ *is a lattice which spans* $\mathbb{R}^n$*.*

With respect to a basis in $\Gamma \cap \mathbb{R}^n$*, the linear group* $\mathrm{L}(\Gamma)$ *is faithfully represented by matrices in* $\mathbf{GL}_n(\mathbb{Z})$*.*

In modern parlance:
$\Gamma \cap \mathbb{R}^n \cong \mathbb{Z}^n$ *is of finite index in* Γ*, that is,*
Γ *is a group extension*

$$\mathbf{0} \to \mathbb{Z}^n \to \Gamma \to \Theta \to \mathbf{1}$$

of $\mathbb{Z}^n$ *by some finite group* $\Theta \cong \mathrm{L}(\Gamma)$*.*

Bieberbach's Second Theorem

Theorem (Bieberbach, 1912)

Let $\Gamma_1, \Gamma_2 \subset \mathbf{Iso}(\mathbb{R}^n)$ *be crystallographic groups.*
$\Gamma_1 \cong \Gamma_2$ *if and only if* Γ_1 *and* Γ_2 *are affinely equivalent.*

Proof:

- An isomorphism $\psi : \Gamma_1 \to \Gamma_2$ maps $\Gamma_1 \cap \mathbb{R}^n$ to $\Gamma_2 \cap \mathbb{R}^n$.
- Therefore, $T = \psi|_{\Gamma_1 \cap \mathbb{R}^n} \in \mathbf{GL}_n(\mathbb{R})$.
- The induced map $\psi_{\mathrm{L}} : \mathrm{L}(\Gamma_1) \to \mathrm{L}(\Gamma_2)$ on the linear parts is $\psi_{\mathrm{L}}(A) = T \cdot A \cdot T^{-1}$.
- Finite subgroups of $\mathbf{Iso}(\mathbb{R}^n)$ have a fixed point ("origin").
- Choose $v \in \mathbb{R}^n$ to compensate for the displacement from origin($\mathrm{L}(\Gamma_1)$) to origin($\mathrm{L}(\Gamma_2)$); then

$$\psi = (T, v) \in \mathbf{Aff}(\mathbb{R}^n). \quad \square$$

Bieberbach's Third Theorem

Theorem (Bieberbach, 1912)
For given dimension n, there exist only finitely many (affine equivalence classes of) crystallographic groups.

Proof:

- By Bieberbach 2: Sufficient to prove that there are only finitely many classes of isomorphic crystallographic groups.
- By Bieberbach 1: Γ is an extension $\mathbf{0} \to \mathbb{Z}^n \to \Gamma \to \Theta \to \mathbf{1}$.
- By a Theorem of Jordan/Minkowski: Every finite subgroup of $\mathbf{GL}_n(\mathbb{Z})$ maps injectively to a subgroup of $\mathbf{GL}_n(\mathbb{F}_3)$. So there is only a finite number of non-equivalent finite subgroups.
- Equivalent extensions for a Θ-module $(\mathbb{Z}^n, \varrho)$ are encoded by $\mathrm{H}^2(\Theta, \mathbb{Z}^n, \varrho)$, but this is finite for a finite group Θ.
- Also, only finitely many modules $(\mathbb{Z}^n, \varrho)$ exist for a given finite group Θ.
- Equivalence of extensions implies isomorphism of groups.
  So there are only finitely many isomorphism classes. □

Zassenhaus' Algorithm

Zassenhaus gave a constructive proof for the third Bieberbach Theorem.

In doing so, he also proved a converse to the first:

Theorem (Zassenhaus, 1948)

A group Γ *which is an extension of* $\mathbb{Z}^n$ *by a finite* $\Theta \subset \mathbf{GL}_n(\mathbb{Z})$ *can be embedded in* $\mathbf{Iso}(\mathbb{R}^n)$ *as a crystallographic group.*

Higher Dimensions

$n = 4$:

- Crystallographic: 4783
- Bieberbach: 74

$n = 5$:

- Crystallographic: 222018
- Bieberbach: 1060

$n = 6$:

- Crystallographic: 28927915
- Bieberbach: 38746

The computer algebra system GAP provides tables and algorithms for crystallographic groups.

References II

- L. Bieberbach, Über die Bewegungsgruppen der Euklidischen Räume, Math. Ann. 70, 1911 & Math. Ann. 72, 1912
- J.J. Burckhardt, Die Bewegungsgruppen der Kristallographie, Birkhäuser, 1947
- L.S. Charlap, Bieberbach Groups and Flat Manifolds, Springer, 1986
- J. Milnor, Hilbert's problem 18: On crystallographic groups, fundamental domains, and on sphere packings, in *John Milnor: Collected Papers I*, Publish or Perish, 1994
- J.A. Wolf, Spaces of Constant Curvature, 6^{th} ed., AMS Chelsea Publishing, 2011
- H. Zassenhaus, Über einen Algorithmus zur Bestimmung der Raumgruppen, Comment. Math. Helv. 21, 1948

III. Flat Manifolds

Why Bieberbach Groups?

Theorem (Killing, 1891)
If M is a complete connected flat Riemannian manifold, then $M = \mathbb{R}^n/\Gamma$, where $\Gamma \subset \mathbf{Iso}(\mathbb{R}^n)$ is the fundamental group of M.

The fundamental group Γ...

- is discrete,
- is torsion-free.
  Proof: Assume $\gamma \in \Gamma \setminus \{\mathrm{id}\}$ satisfies $\gamma^k = \mathrm{id}$, $k > 1$.
  Then $x = -\frac{1}{k-2}\sum_{j=1}^{k-1} v_j$ (or $x = \frac{1}{2}v_1$ for $k = 2$) is a fixed point for $\langle\gamma\rangle$, where $v_j = \mathrm{T}(\gamma^j)$.
  Contradiction to Γ acting simply transitively on the fibre $\pi^{-1}(\pi(x))$. □

Corollary
If $M = \mathbb{R}^n/\Gamma$ is a compact complete connected flat Riemannian manifold, then its fundamental group Γ is a Bieberbach group.

Bieberbach's First Theorem (geometric)

Theorem

Let M be a compact complete connected flat Riemannian manifold.
Then the flat torus is a finite Riemannian cover of M.
The holonomy group Θ of M is finite.

Bieberbach's Second Theorem (geometric)

Theorem

Let M_1 and M_2 be a compact complete connected flat Riemannian manifolds with fundamental groups Γ_1 and Γ_2.
Then $\Gamma_1 \cong \Gamma_2$ if and only if M_1 and M_2 are affinely equivalent.

Bieberbach's Third Theorem (geometric)

Theorem

For a given dimension n, there only finitely many equivalence classes of compact complete connected flat Riemannian manifolds.

Non-Compact Manifolds

Assume Γ is the fundamental group of a non-compact complete connected flat Riemannian manifold M.

One can show that Γ is an embedding of a Bieberbach group $\Gamma \subset \mathbf{Iso}(\mathbb{R}^k)$ into $\mathbf{Iso}(\mathbb{R}^n)$, where $k < n = \dim M$.

In particular:
There exists a real analytic deformation retract of M onto a compact totally geodesic submanifold of dimension k.

References III

- L.S. Charlap, Bieberbach Groups and Flat Manifolds, Springer, 1986
- J.H. Conway, H. Burgiel, C. Goodman-Strauss, The Symmetries of Things, A.K. Peters, 2008
- J. Milnor, Hilbert's problem 18: On crystallographic groups, fundamental domains, and on sphere packings, in *John Milnor: Collected Papers I*, Publish or Perish, 1994
- A. Szczepański, Problems on Bieberbach groups and flat manifolds, Geometriae Dedicata 120, 2006
- J.A. Wolf, Spaces of Constant Curvature, 6th ed., AMS Chelsea Publishing, 2011

IV. Holonomy

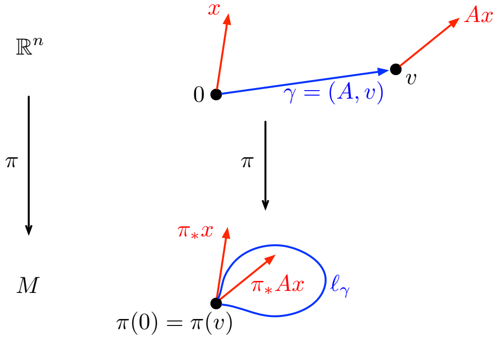
Holonomy Groups of Flat Manifolds

Let $M = \mathbb{R}^n/\Gamma$ be a complete (affinely) flat manifold with fundamental group $\Gamma \subset \mathbf{Aff}(\mathbb{R}^n)$.

Theorem

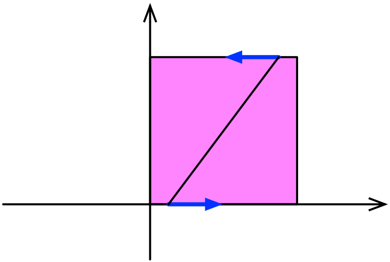
$$\mathbf{Hol}(M) = \mathrm{L}(\Gamma).$$

Proof:



Example: Disconnected Holonomy

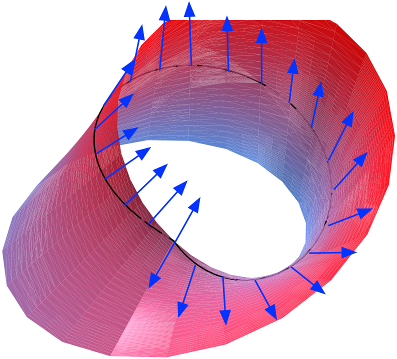
Parallel transport on the Möbius Strip:



$$\Gamma = \left\langle \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right) \right\rangle \quad \text{and} \quad \mathbf{Hol}(M) = \left\langle \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\rangle.$$

Example: Disconnected Holonomy

Parallel transport on the Möbius Strip:



Classification Results

Theorem (Auslander & Kuranishi, 1957)
Let Θ be a finite group. Then there exist a Bieberbach group Γ with $\mathrm{L}(\Gamma) = \Theta$ and a compact complete flat Riemannian manifold M with $\mathbf{Hol}(M) = \Theta$.

For $\Theta \cong \mathbb{Z}/p\mathbb{Z}$ (p prime) a precise classification of the corresponding Bieberbach groups is known.

- Exploit that the faithful Θ-modules are known.
- Isomorphism classes are determined by a finite number of parameters.

References IV

- L.S. Charlap, Bieberbach Groups and Flat Manifolds, Springer, 1986
- A. Szczepański, Problems on Bieberbach groups and flat manifolds, Geometriae Dedicata 120, 2006
- J.A. Wolf, Spaces of Constant Curvature, 6^{th} ed., AMS Chelsea Publishing, 2011

V. Related Topics

Almost Flat Manifolds

Theorem (Gromov 1978, Ruh 1982)
There exists a number $\varepsilon = \varepsilon(n)$ *such that for a compact connected n-dimensional Riemannian manifold* M *satisfying*

$$diam(M)^2 \cdot |K_M| \leq \varepsilon,$$

where K_M *denotes the sectional curvature, there exists a nilpotent Lie group* N *and a discrete subgroup* Γ *of* $\mathbf{Aut}(N) \ltimes N$ *such that*

- M *is diffeomorphic to* N/Γ,
- $\Gamma \cap N$ *has finite index in* Γ,
- Γ *is an extension of a lattice* $\Lambda \subset N$ *by a finite group* Θ.

Such a manifold M is called almost flat.

Quasi-Symmetries

- There exist tilings of the plane constructed from regular polygons that do not arise from group symmetries (Kepler, 1619).
- Bravais proved that no crystal lattice in $\mathbb{R}^3$ has a 5-fold symmetry.
- Shechtman got the Nobel Prize in Chemistry 2011 for the construction of quasi-crystals with a 5-fold symmetry.
- There exists irregular polyhedra whose copies fill up space even though they are not fundamental domains of groups ($n = 2$ by Heesch, 1935, and $n = 3$ by Reinhardt, 1928).

Generalisations

What happens if we assume that Γ...

- acts by pseudo-Riemannian isometries?
- acts by affine transformations?

Everything falls apart!
(No analogues to the Bieberbach Theorems.)

See part II of this talk!