Crystallographic groups

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I. Introduction

Definition

- We consider groups of affine transformations acting on $\mathbb{R}^n$ by

$$x \mapsto xA + b$$

- A crystallographic group is a group G of affine transformations of $\mathbb{R}^n$,
  - Containing the translation group $\mathbb{Z}^n$ as a normal subgroup.
  - Whose quotient $G/\mathbb{Z}^n$ is a finite group

  The quotient $G/\mathbb{Z}^n$ is called a point group and denoted by $Point(G)$.
- Some examples:
  - $G_1 = \mathbb{Z}^n$ acting on $\mathbb{R}^n$ by translations, $Point(G_1) = \{Id\}$
  - The group G_2:

$$x \mapsto x + t \text{ and} x \mapsto -x + t \text{ with } t \in \mathbb{Z}^n$$

    has $Point(G_2) = \{Id, -Id\}$.
- The group $Point(G)$ acts on the torus $\mathbb{R}^n/\mathbb{Z}^n$.

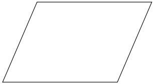
Matrix expressions

- Computationally it is better to write the vectors $x, y \in \mathbb{R}^n$ as $x' = (1, x)$, $y' = (1, y)$ and the pair (A, b) as the matrix $A' = \begin{pmatrix} 1 & b \\ 0 & A \end{pmatrix}$.
  So, we rewrite $y = xA + b$ as $y' = x'A'$.
- If G is a crystallographic group and the elements of G are matrices $\begin{pmatrix} 1 & b \\ 0 & A \end{pmatrix}$ then the point group $Point(G)$ is formed by all those matrices A.
- The point group is a finite subgroup of $\mathrm{GL}_n(\mathbb{Z})$.

II. Examples

Wallpaper groups

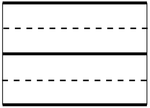
1. Wallpaper groups without rotations:



*p*1

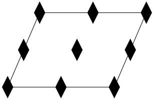
pm

pg

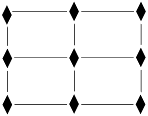


cm

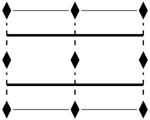
2. Wallpaper groups with rotations of order 2:



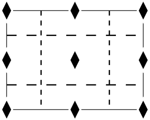
*p*2



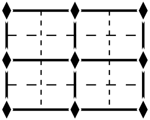
*p*2*mm*



*p*2*mg*



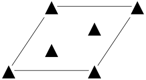
*p*2*gg*



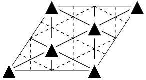
*c*2*mm*

Wallpaper groups

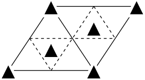
1. Wallpaper groups with rotations of order 3:



$p3$

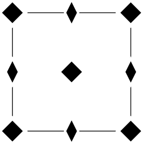


$p3m1$

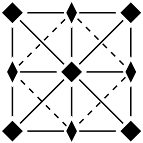


$p31m$

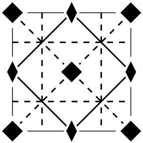
2. Wallpaper groups with rotations of order 4:



$p4$

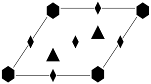


$p4mm$

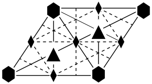


$p4gm$

3. Wallpaper groups with rotations of order 6:



$p6$



$p6mm$

The space groups

- The 3-dimensional crystallographic groups ("Space groups") have been classified by E.S. Fedorov, A.M. Schonflies and W. Barlow.
- There are 219 classes up to equivalence and 230 classes if one distinguish up to reflections.
- 32 types of point groups.
- They have a special naming system and many other things explained in "International Tables for Crystallography".
- Another competing nomenclature:
  - J.H. Conway, O. Delgado Friedrichs, D.H. Huson, W.P. Thurston, *On three-dimensional space groups*. Beiträge Algebra Geom. **42-2** (2001) 475–507.

Affine Coxeter groups

- A Coxeter group $G(m)$ is a group generated by $g_1, \dots, g_M$, whose set of relations is

$$g_i^2 = 1 \text{ and } (g_i g_j)^{m_{ij}} = 1 \text{ with } m_{ji} = m_{ij} \geq 2$$

- The Coxeter matrix $Gram(m)$ is the symmetric matrix

$$Gram(m) = (\cos(\frac{\pi}{m_{ij}}))_{1 \leq i,j \leq M}$$

- The generators $g_1, \dots, g_M$ are reflections for the scalar product $Gram(m)$ in a M dimensional space $\mathbb{R}^M$ along a fundamental simplex S defined by M linear inequalities.
- If the matrix $Gram(m)$ is positive definite then the group $G(m)$ is finite and the classification is known.
- If the matrix $Gram(m)$ is positive then the group $G(m)$ is a crystallographic group and the classification is known.

Finite Coxeter groups

- List of finite irreducible Coxeter groups

names	order	linear representations
A_n	$(n+1)!$	$\mathrm{GL}_n(\mathbb{Z})$
B_n	$2^n n!$	$\mathrm{GL}_n(\mathbb{Z})$
D_n	$2^{n-1} n!$	$\mathrm{GL}_n(\mathbb{Z})$
E_6	51840	$\mathrm{GL}_6(\mathbb{Z})$
F_4	1152	$\mathrm{GL}_4(\mathbb{Z})$
E_7	2903040	$\mathrm{GL}_7(\mathbb{Z})$
E_8	696729600	$\mathrm{GL}_8(\mathbb{Z})$
H_3	120	$\mathrm{GL}_3(\mathbb{Q}(\sqrt{5}))$
H_4	14400	$\mathrm{GL}_4(\mathbb{Q}(\sqrt{5}))$
$\mathrm{I}_2(m)$	$2m$	$\mathrm{GL}_2(\mathbb{R})$

- Only ones, which can occur as subgroups of $\mathrm{GL}_n(\mathbb{Z})$ are A_n, B_n, D_n, E_n, F_4, $I_2(6)$.

Root lattices

- A lattice L is a subset of $\mathbb{R}^n$ of the form $\mathbb{Z}v_1 + \cdots + \mathbb{Z}v_n$. The group of isometries preserving it is called $Aut(L)$.
- It is the point group of a lattice L
- A *root lattice* is a lattice spanned by the roots of a finite irreducible Coxeter group.
- The root lattices are:

Coxeter groups	Root lattices	$\lvert Aut(L)\rvert$
A_n	A_n	$2(n+1)!$
B_n	B_n and C_n	$2^n n!$
D_n	D_n	$2^{n-1} n!$ (if $n \neq 4$)
F_4	F_4	1152
E_6	E_6	103680
E_7	E_7	2903040
E_8	E_8	696729600

Lattices having Coxeter groups as point groups

- If L is a lattice then the dual L^* is defined as

$$L^* = \{x \in \mathbb{R}^n \mid \langle x, y \rangle \in \mathbb{Z} \text{ for } y \in L\}$$

- Results:

Coxeter groups	lattices
A_n	Coxeter lattices A_n^r
D_n	D_n, D_n^* and D_n^+ if n is even
F_4	F_4
E_6	E_6 and E_6^*
E_7	E_7 and E_7^*
E_8	E_8

- A Coxeter lattice A_n^r is defined if r divides $n+1$.

Crystallographic Coxeter groups

- Crystallographic Coxeter groups

Cryst group	point group
$\tilde{A}_n$	A_n
$\tilde{B}_n$	B_n
$\tilde{C}_n$	B_n
$\tilde{D}_n$	D_n
$\tilde{E}_6$	E_6
$\tilde{E}_7$	E_7
$\tilde{E}_8$	E_8
$\tilde{F}_4$	F_4

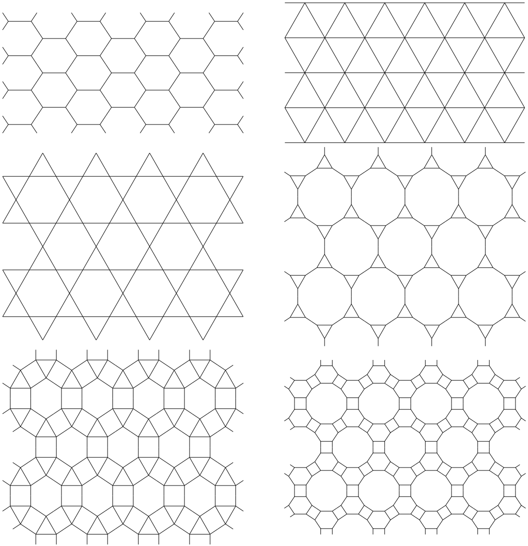
III. Wyckoff positions

Definitions

- Let G be a crystallographic group.
  - If $v \in \mathbb{R}^n$, G is a crystallographic group then the stabilizer $Stab_G(v)$ is a finite subgroup of G identified with a subgroup of the point group.
  - If H is a finite subgroup of G, then the set of point stabilized by H form a plane P_H in $\mathbb{R}^n$.
  - The orbit of P_H under G corresponds to the conjugacy class of H under G and is called the Wyckoff position.
- If G has no non-trivial Wyckoff position, then G is called a Bieberbach group, that is every point has a trivial stabilizer and the quotient $\mathbb{R}^n/G$ is a manifold.
- The interest of Wyckoff positions is to be able to describe crystallographic structures with less parameters, i.e., less measures are needed.

A two dimensional case

- From the crystallographic group $\tilde{A}_2$



Computational method

- It is generally hard to compute the Wyckoff positions.
- Basic algorithm given a space group G:
  - Compute the conjugacy classes of subgroups of $Pt(G)$.
  - For every conjugacy class H find a minimal generating set $h_1, \dots, h_m$
  - Take a lifting $\tilde{h}_i$ of the h_i and compute the solution set of $\tilde{h}_i(x) = x + t_i$ with $t_i \in \mathbb{Z}^n$ up to the transaltion group $\mathbb{Z}^n$.
- Implemented in the GAP package `cryst`
- See also
  - J. Fuksa, P. Engel, *Derivation of Wyckoff positions of N-dimensional space groups. Theoretical considerations.*, Acta Cryst. Sect. **A-6** 50 (1994) 778–792.

IV. Lattice symmetry

Symmetry of lattices

- A symmetry of a lattice L is an isometry u of $\mathbb{R}^n$ preserving 0 such that $L = u(L)$.
- If one selects a basis $\mathbf{v}$ of L and consider the Gram matrix $G_{\mathbf{v}}$, then a u corresponds to a matrix $P \in \mathrm{GL}_n(\mathbb{Z})$ such that $G_{\mathbf{v}} = PG_{\mathbf{v}}P^T$.
- If $A \in S^n_{>0}$, then the symmetry group

$$\mathrm{Aut}(A) = \{P \in \mathrm{GL}_n(\mathbb{Z}) \mid A = PAP^T\}$$

is finite.

AUTO/ISOM

- We actually want to compute Aut(A).
- The method is to find a characteristic finite set $\mathcal{V}$ of vectors, which is invariant under Aut(A), which $\mathbb{Z}$-span $\mathbb{Z}^n$.
  For such a set we have $\mathcal{V}P = \mathcal{V}$.
- A technique is to compute the vectors v of norm $vAv^T \leq \lambda$ for a well specified λ. `AUTO` is then the program computing automorphism group of lattices.
- `ISOM` is the program for testing lattices up to isomorphism.
- Sometimes, instead of `ISOM`/`AUTO` it is better to use `nauty` with the same vector family and the edge colored graph on $\mathcal{V}$ defined by the colors $v_i M v_j^T$.
- See for more details
  - W. Plesken, B. Souvignier, *Computing isometries of lattices*. Computational algebra and number theory (London, 1993). J. Symbolic Comput. 24 (1997), no. 3-4, 327–334.

V. Bravais space and normalizer

Space of invariant forms

- Given a subgroup G of $\mathrm{GL}_n(\mathbb{Z})$, define

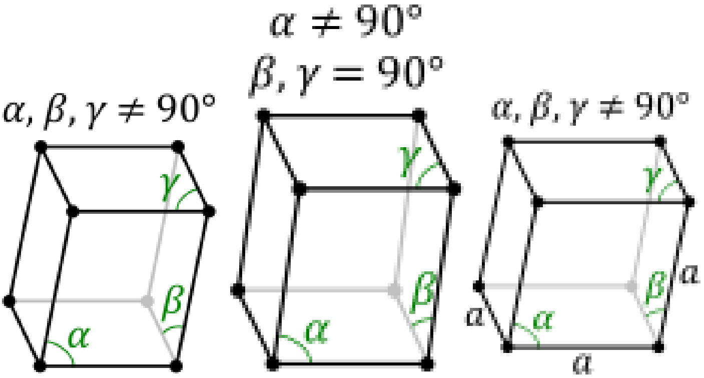
$$\mathcal{SP}(G) = \{\ X \in S^n \ \text{ such that } \ gXg^T = X \ \text{ for all } \ g \in G\ \}$$

- If G is finite then $dim\mathcal{SP}(G) > 0$.
- Given a linear space $\mathcal{SP}$ of S^n, define

$$Aut(\mathcal{SP}) = \left\{ \begin{array}{c} g \in \mathrm{GL}_n(\mathbb{Z}) \ \text{ such that } \\ gXg^T = X \ \text{ for all } \ X \in \mathcal{SP} \end{array} \right\}$$

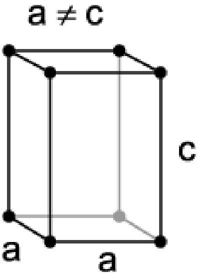
- A Bravais group satisfies to $Aut(\mathcal{SP}(G)) = G$ and $\mathcal{SP}(G)$ is its Bravais space.
- Every finite group is contained in a Bravais group $G \subset Aut(\mathcal{SP}(G))$.

The 3-dimensional Bravais spaces

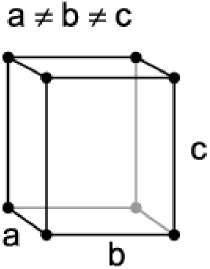


Triclinic (dimension 6) | Monoclinic (dimension 4) | Rhombohedral (dimension 4)

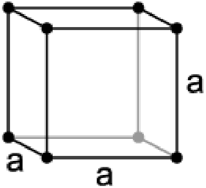
The 3-dimensional Bravais spaces



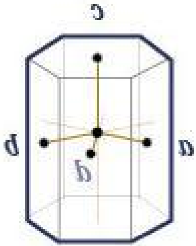
Tetragonal
(dimension 2)



Orthorhombic
(dimension 3)



Cubic
(dimension 1)



Hexagonal
(dimension 2)

Normalizer

- If G is a group H a subgroup of G then the normalizer is

$$\{g \in G \mid gHg^{-1} = H\}$$

- Thm. (Zassenhaus) If G is a finite subgroup of $\mathrm{GL}_n(\mathbb{Z})$ then one has the equality

$$\{g \in \mathrm{GL}_n(\mathbb{Z}) \mid g\mathcal{SP}(G)g^T = \mathcal{SP}(G)\} = N_{\mathrm{GL}_n(\mathbb{Z})}(G)$$

  So, for example if $G = \{\pm I_n\}$
  - $\mathcal{SP}(G) = S^n$
  - $N_{\mathrm{GL}_n(\mathbb{Z})}(G) = \mathrm{GL}_n(\mathbb{Z})$
- The normalizer is important since it is the automorphism group of the bravais space.

G-perfect matrices

- A matrix $A \in \mathcal{SP}(G)$ is G-perfect if:

$$B \in \mathcal{SP}(G) \text{ and } xBx^T = min(A) \text{ for all } x \in Min(A)$$

  implies $B = A$.
- If A is G-perfect then:
  - Partition $Min(A)$ into $Min(A) = O_1 \cup O_2 \cup \cdots \cup O_r$,
  - with $O_i = \cup_{g \in G} x.g$ for some $x \in Min(A)$ (O_i is an orbit).
  - Define $p_i = \sum_{x \in O_i} x^T x$
  - Define the G-perfect domain by

$$Dom_G(A) = \{\sum_{i=1}^{r} \lambda_i p_i \text{ with } \lambda_i \geq 0\}$$

- A matrix $A \in \mathcal{SP}(G)$ is G-extreme if it is a local maximum in $\mathcal{SP}(G)$ of the packing density.
- G-extreme $\Rightarrow$ G-perfect.

Voronoi algorithm and the normalizer

- Thm. (Bergé, Martinet & Sigrist): G-perfect domains realize a polyhedral subdivision of $\mathcal{SP}(G) \cap S^n_{>0}$.
  There is a finite number of G-perfect domains up to $N_{\mathrm{GL}_n(\mathbb{Z})}(G)$.
- We can enumerate all G-perfect matrices with analogs of Voronoi algorithm.
- The generators of the normalizers come from:
  - The automorphism of a G-perfect form, which do not belong to G and preserve $\mathcal{SP}(G)$ globally.
  - The matrices P realizing equivalence of a G-perfect domain.
- See for more details:
  - J. Opgenorth, *Dual cones and the Voronoi algorithm*. Experiment. Math. **10-4** (2001) 599–608.

VI. Classification methods

Having the point groups

- Suppose that we have G a finite subgroup of $\mathrm{GL}_n(\mathbb{Z})$, we want to find the crystallographic groups $\tilde{G}$ having G as point group.
- We write the elements of $\tilde{G}$ as

$$\begin{pmatrix} 1 & t_g + t \\ 0 & g \end{pmatrix} \text{ for } g \in G \text{ and } t \in \mathbb{Z}^n$$

- Actually $t_g \in V = \mathbb{R}^n/\mathbb{Z}^n$ and belongs to

$$Z^1(G, V) = \{t \mid t_1 = 0 \text{ and } t_{gh} = t_g.h + t_h\}$$

- If one adds the function $\delta_g = v.g - v$ to t_g it is simply a translation. Denote $B^1(G, V)$ the space of such functions.
- So, the space of possible t_g coincide with the quotient space

$$H^1(G, V) = Z^1(G, V)/B^1(G, V) \text{ up to } N_{\mathrm{GL}_n(\mathbb{Z})}(G)$$

- $t_g \in \mathbb{Z}^n$ if and only if there is a point of stabilizer G.

The methodology

- The enumeration of crystallographic groups is reduced to the enumeration of finite subgroups of $GL_n(\mathbb{Z})$.
- Two subgroups G_1, G_2 of $GL_n(\mathbb{Z})$ are conjugate if there exist $P \in GL_n(\mathbb{Z})$ such that $G_1 = P G_2 P^{-1}$
- Theorem Given a finite subgroup G of $GL_n(\mathbb{Q})$ there exist a maximal finite subgroup H of $GL_n(\mathbb{Q})$ containing it.
- The method is
  - Enumerate the maximal finite subgroups of $GL_n(\mathbb{Q})$.
  - Then their $\mathbb{Z}$-classes.
  - Then their conjugacy classes of subgroups.
  - Then the corresponding crystallographic groups.
- See for more details

  - J. Opgenorth, W. Plesken and T. Schulz, *Crystallographic algorithms and tables*, Acta Crystallographica Section A, **54-5**, (1998), 517–531.
  - B. Eick and Bernd Souvignier, *Algorithms for crystallographic groups*, International Journal of Quantum Chemistry, **106**, 316–343 (2006).

Zassenhaus/Plesken theory

- Theorem For a fixed dimension n, there exist a finite number of maximal irreducible finite subgroups of $\mathrm{GL}_n(\mathbb{Z})$ up to conjugacy.
- The list is enumerated up to dimension 31:
  - W. Plesken, M. Pohst, *On maximal finite irreducible subgroups of* $\mathrm{GL}_n(\mathbb{Z})$*. I. The five and seven dimensional cases.* Math. Comp. **31-138** (1977) 536–551.
  - G. Nebe and W. Plesken, *Finite rational matrix groups*, Mem. Amer. Math. Soc. **116** (1995), no. 556, viii+144 pp.
  - G. Nebe, *Finite subgroups of* $\mathrm{GL}_{24}(\mathbb{Q})$, Experiment. Math. **5-3** (1996) 163–195.
  - G. Nebe, *Finite subgroups of* $\mathrm{GL}_n(\mathbb{Q})$ *for* $25 \leq n \leq 31$. Comm. Algebra **24-7** (1996) 2341–2397.

THANK

YOU