

#### Symmetry in Crystallography

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## Outline

- Which tool ?
- Which space ?
- What physical significance?
- What next?

-

Which tool?

#### Which tool?

### Symmetry $\leftrightarrow$ Invariance $\leftrightarrow$ Group Theory



#### Which tool?

#### Definition

# A group is a set $\mathcal{G}$ , together with an internal law \* that combines any two elements *a* and *b* to form another element, denoted a \* b or simply *a b* that is in $\mathcal{G}$ .

To qualify as a group, the set and the operation,  $(\mathcal{G}, *)$ , must satisfy four requirements :

- Closure : For all a, b in G, the result of the operation, c = a \* b, is also in G.
- Associativity : For all a, b and c in  $\mathcal{G}$ , (a \* b) \* c = a \* (b \* c).
- Identity element :There exists an element e in G, such that for every element a in G, the equation e \* a = a \* e = a holds. Such an element is unique (see below), and thus one speaks of the identity element.
- Inverse element :For each a in G, there exists an element b in G such that a \* b = b \* a = e, where e is the identity element.



#### Which tool?

## Group action theory

The action of a group *G* on a mathematical structure *M* whose automorphism group is Aut(M), is defined by the homomorphism  $\phi$ :

 $G \xrightarrow{\phi} \operatorname{Aut}(M)$  such that  $\forall a, b \in G, \phi(ab) = \phi(a).\phi(b)$ 

Example :

$$\begin{array}{ccccc} e & a & b & c \\ a & e & c & b & \phi \\ b & c & e & a \\ c & b & a & e \end{array} \qquad \left\{ \begin{array}{ccccc} \times 1 & \text{on the set } M = \{1\} \to \phi_0 : 1 & 1 & 1 & 1 \\ \\ \times \pm 1 & \text{on the set } M = \{1, -1\} \to \begin{cases} \phi_1 : 1 & -1 & 1 & -1 \\ \phi_2 : 1 & 1 & -1 & -1 \\ \phi_3 : 1 & -1 & -1 & 1 \end{cases} \right.$$



## Standard representation

 $\mathcal{G} \xrightarrow{\phi} \operatorname{Aut}(\mathbb{R}^n)$ 

where  $Aut(\mathbb{R}^n)$  are the isometries of  $\mathbb{R}^n$ .

$$\mathcal{G} \xrightarrow{\phi} \phi(g) r = (g|t)r = gr + t$$

or in reciprocal space :

Which tool?

$$egin{aligned} \mathcal{G} \xrightarrow{\phi} \phi(oldsymbol{g}) \ket{q} &= (\widehat{g|t}) \ket{q} = \ket{gq} e^{2i\pi gq.t} \ & \ \hline (\widehat{g|t}) &= \sum_{q \in \Lambda^*} \ket{gq} e^{2i\pi gq.t} \langle q \end{vmatrix} \end{aligned}$$

#### Which tool?

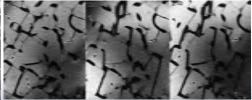


# Other representations : Phases transformations $G \rightarrow H$



 $H \subset G, \; G = \cup g_i H$ 

Variants  $g_i H g_i^{-1}$ , Boundaries  $g_i H$ 



 $ext{Kernel } I = \cap_i g_i H g_i^{-1}, ext{ Quotient group } \Gamma = G/I$ 



#### Group action and crystallography

C. R. Acad. Sc. Paris, t. 307, Série I, p. 905-910, 1988

Which tool?

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Cristallographie/Crystallography

#### Les concepts fondamentaux de la cristallographie

Louis MICHEL et Jan MOZRZYMAS

**Résumé** – Nous introduisons un nouvel ensemble de définitions des concepts de la cristallographie en dimension n. Il est basé sur les propriétés générales des actions de groupe. Enfin nous précisons comment on détermine le système cristallographique et la classe de Bravais d'un groupe cristallographique.

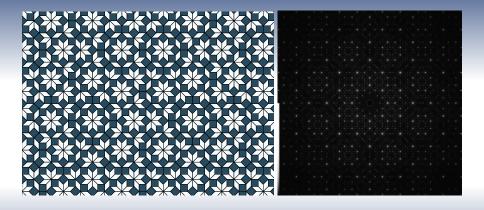
Let *g*.*m* stands for  $\phi(g)m$ , the transform of  $m \in M$  by  $g \in G$ :

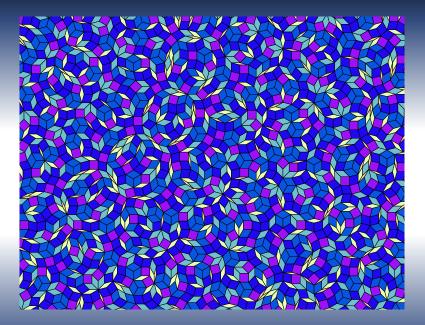
- the orbit G.m is the set of the transforms of m by G;
- the elements of *G* which leave *m* ∈ *M* unchanged make a subgroup *G<sub>m</sub>* called the stabilizer or little group of *m*
- By restriction, the action  $G \xrightarrow{\phi} Aut(M)$  defines an action on M for any subgroup H of G; then  $H_m = H \cap G_m$ .

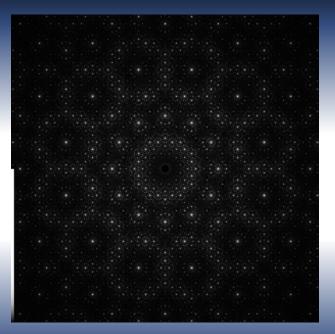


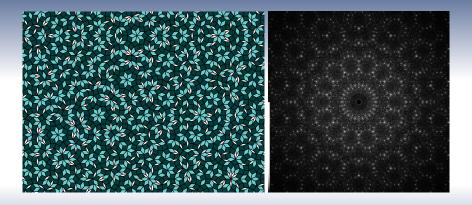
#### Which space?

- A. Bienenstock and P.P. Ewald, Acta Cryst 15, 1253 (1962)
- J.W. Jeffery Acta Cryst 16 1239 (1963)
- D.S. Rokhsar, D.C. Wright and N. D. Mermin, Acta Cryst A44 197 (1988)
- D.A. Rabson, N.D. Mermin, D.S. Rokhsar and D.C. Wright, Rev. Mod. Phys. (July 1991)
- D. Mermin in *Quasicrystals : the state of the art*, Edts D.P. DiVincenzo and P.J. Steinhardt, Series on Directions in Condensed Matter Physics 16 (1999), p 137–195









#### Which space?



# Symmetry is best defined in reciprocal space

#### D. Mermin

Any geometric operation that transforms a solid into another one with identical correlation functions to any finite order *n* can be qualified as a symmetry operation of the solid in the sense that the operation leads to a solid that is physically indistinguishable from the first one. For a crystal of lattice  $\Lambda$ :

$$\varrho(r) = \sum_{q_i \in \Lambda^*} \rho(q_i) e^{2i\pi q_i \cdot r}$$

the correlation function to order N is defined by :

$$c_N(r_1, r_2, \ldots, r_N) = \int \varrho(r - r_1) \ldots \varrho(r - r_N) d^3r$$

#### Which space?



## Symmetry is best defined in reciprocal space

Correlation functions are best expressed in Fourier space :

$$\int \varrho(r-r_1)\dots\varrho(r-r_N)d^3r = \sum_{q_1,\dots,q_n} \rho(q_1)\dots\rho(q_N)e^{-2i\pi(q_1,r_1+\dots+q_n,r_n)}$$
$$\times \int e^{2i\pi(q_1+\dots+q_N)\cdot r}d^3r$$

The integral is non zero only for wave vectors  $q_1, \ldots, q_N$  such that  $q_1 + \ldots + q_N = 0$ .

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What physical significance?

## Indiscernability principle

There is an indiscernability between two densities  $\varrho(r)$  and  $\varrho'(r)$  if all the correlation functions to any finite order are equal between the two structures making them physically undistinguishable. This imposes the product of the Fourier coefficients on a closed path to be equal :

 $\rho(q_1) \dots \rho(q_N) = \rho'(q_1) \dots \rho'(q_N), \text{ with } q_1 + \dots + q_N = 0$ 



What physical significance?

#### Remarkable phases relations (1)

Because the density  $\rho(r)$  takes real values,  $\rho(-q) = \overline{\rho}(q)$  and thus :

$$|\rho(q)|^2 = \rho(q)\rho(-q) = \rho'(q)\rho'(-q) = |\rho'(q)|^2$$

Two undistinguishable densities have Fourier coefficients that differ only by a phase factor :

$$\rho'(q) = \rho(q)e^{2i\pi\chi(q)}$$
(1)

Then :

$$ho'(-q)
ho'(q)=
ho(-q)e^{2i\pi\chi(-q)}
ho(q)e^{2i\pi\chi(q)}=
ho(-q)
ho(q)$$

and thus :

$$\chi(-\boldsymbol{q}) = -\chi(\boldsymbol{q})$$



## Remarkable phases relations (2)

Next, considering the closed path {  $q_1, q_2, -(q_1 + q_2)$ }, we observe that :

$$egin{aligned} &
ho'(q_1)
ho'(q_2)
ho'(-(q_1+q_2)) = 
ho(q_1)e^{2i\pi\chi(q_1)}
ho(q_2)e^{2i\pi\chi(q_2)}\ & imes
ho(-(q_1+q_2))e^{2i\pi\chi(-(q_1+q_2))}\ &= 
ho(q_1)
ho(q_2)
ho(-(q_1+q_2)) \end{aligned}$$

and therefore :

$$\chi(q_1) + \chi(q_2) + \chi(-(q_1 + q_2)) = \chi(q_1) + \chi(q_2) - \chi(q_1 + q_2) = 0$$

so that :

$$\chi(q_1+q_2)=\chi(q_1)+\chi(q_2)$$

The phase factors between the Fourier coefficients of two undistinguishable densities are linear forms in q. (2)



#### What physical significance?

## Remarkable phases relations (3)

Considering now  $\widehat{\mathbf{g}}$  an operation of the point group of the crystal, the indiscernability principle imposes :

$$\rho(\widehat{\mathbf{g}}\boldsymbol{q}) = \boldsymbol{e}^{2i\pi\Phi_g(\boldsymbol{q})}\rho(\boldsymbol{q})$$
(3)

Using similar arguments as previously with the closed paths  $\{\widehat{\mathbf{g}}q, -\widehat{\mathbf{g}}q\}$  and  $\{\widehat{\mathbf{g}}q_1, \widehat{\mathbf{g}}q_2, -\widehat{\mathbf{g}}(q_1 + q_2)\}$  and noting that  $\widehat{\mathbf{g}}(q_1 + q_2) = \widehat{\mathbf{g}}q_1 + \widehat{\mathbf{g}}q_2$  we obtain :

$$\Phi_g(-q) = -\Phi_g(q), \quad \Phi_g(q_1 + q_2) = \Phi_g(q_1) + \Phi_g(q_2)$$
(4)



#### What physical significance?

## Remarkable phases relations (4)

Also, explicit writing of the product  $\widehat{\mathbf{gh}}$  of two operations  $\widehat{\mathbf{h}}$  and  $\widehat{\mathbf{g}}$  of the indiscernability group leads to the group compatibility relation :

$$\Phi_{gh}(q) = \Phi_g(\widehat{\mathbf{h}}q) + \Phi_h(q)$$
(5)

and, finally, two distributions related by :

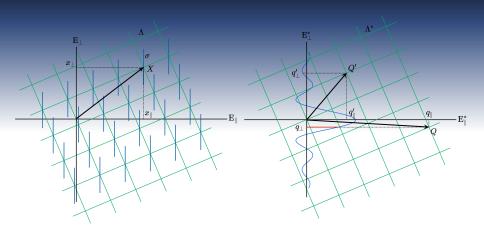
$$\Phi'_{g}(q) = \Phi_{g}(q) + \chi(\widehat{\mathbf{g}}q) - \chi(q)$$
(6)

are equivalent (gauge invariance).



#### N-dim crystallography

- P. M. de Wolff, Acta Cryst., A33, 493 (1977)
- A. Janner and T. Janssen, Phys. Rev. B, 15, 643 (1977)
- T. Janssen, Acta Cryst. A, 42, 261-271 (1986).
- D. Levine and P. J. Steinhardt, Phys. Rev. Lett. 53 (26), 2477-2480 (1984)
- M. Duneau M and A. Katz, Phys. Rev. Lett. 2688 (1985)
- P. A. Kalugin, A. Y. Kitayev and L. S. Levitov J. Physique Lett. 46 L-601-607 (1985);
- V. Elser, Acta Cryst A 42 36-43 (1986)
- P. Bak, Phys. Rev. B 32, 5764 (1985)



$$\begin{split} \varrho &= (\sigma * \Lambda) \cdot \mu_{\parallel} & \qquad \widetilde{\varrho} &= (\widetilde{\sigma} \cdot \Lambda^*) * \mu_{\perp} * \\ \mu_{\parallel} &= \mathbf{1}_{\parallel} \otimes \delta_{\perp}, & \qquad \mu_{\perp} * &= \widetilde{\mu_{\parallel}} &= \delta_{\parallel} * \otimes \mathbf{1}_{\perp} * \end{split}$$

Symmetry in Crystallography



What physical significance?

#### Superspace groups

The agreement of the superspace group approach with the indiscernability criteria is trivial : with no loss of generality, the basic linearity in q of the relations between phases shows that they are associated with scalar products q.t in the superspace :

$$\Phi_g(q) = \widehat{\mathbf{g}} q.t$$
 and  $\chi(q) = q.t$  (7)

Formula (7) are sufficient to fulfill all the phase relations imposed by the indiscernability principle.



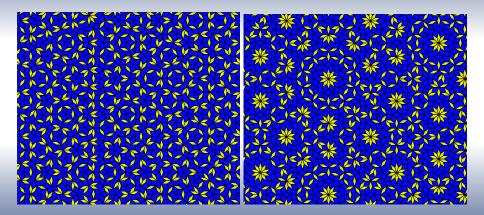
### Superspace groups are indiscernability groups

The indiscernability group of a quasicrystal or incommensurate phase — the Fourier carrier of which is a  $\mathbb{Z}$ -module of rank N — is the N-dim superspace group :

- any two locally isomorphic structures have same correlation functions to any finite order and are therefore physically undistinguishable from each other;
- the operations that transform into each other two locally isomorphic structures (obtained by two distinct but parallel cuts) are indiscernability operations.
- the superspace group is the pertinent symmetry tool to be considered in physics for the purpose of describing the thermodynamical aspect of phases transformations between quasicrystals and crystals.



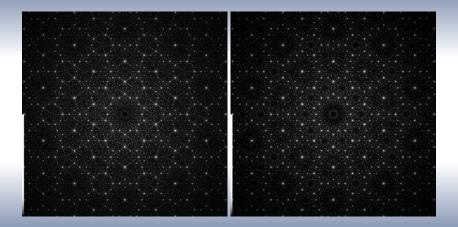
## Standard and generalized Penrose tilings...







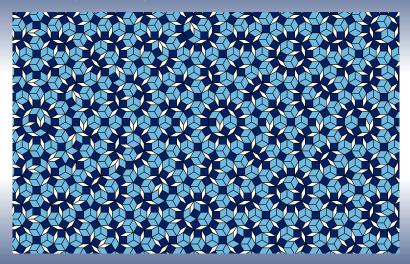
## ... are not equivalent !



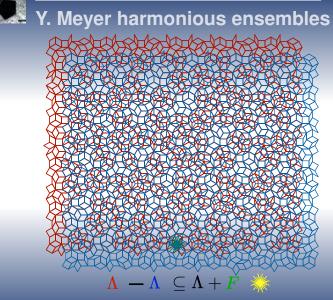




## Symmetry of translation







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# Substitution tilings 1 VT VT VT

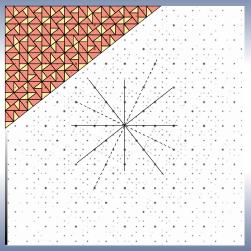
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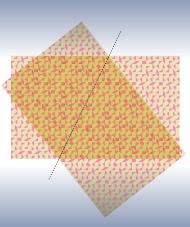


#### Further examples



## Magnetic Action Million Millio

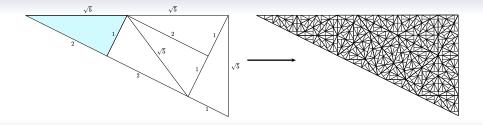


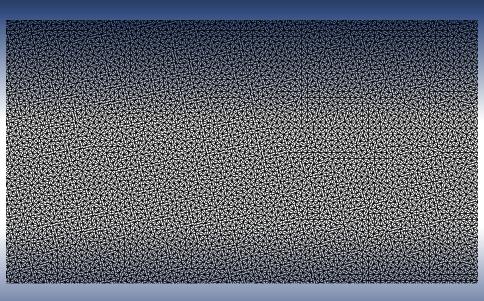


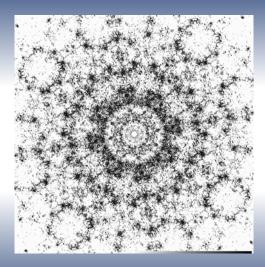


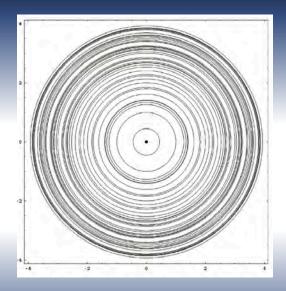
What next?

## 👫 The "Pinwheel" tiling of J. H. Conway









Robert V. Moody, Derek Postnikoff and Nicolae Strungaru, Ann. Henri Poincaré 7 (2006), 711-730

