On symmetries of quasicrystals

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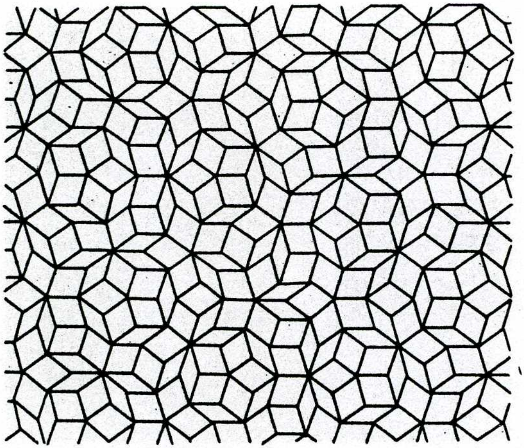
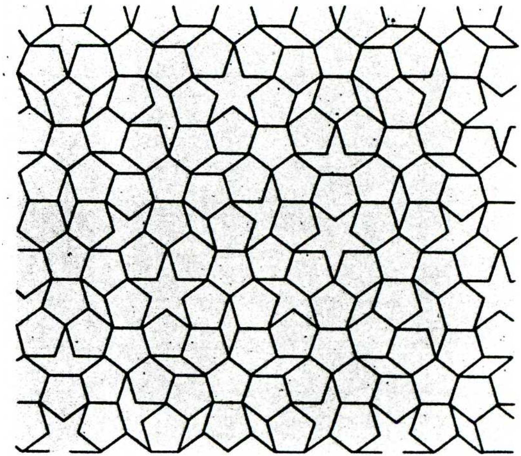
Outline

Symmetries of crystals play a substantial role in the geometric theory of crystals, helping to classify all possible combinations for positions occupied by atoms in materials. A complete classification of symmetries of crystals was known since thirties in the last century. But in 1984 a new alloy $Al_{0,86}Mn_{0,14}$ was discovered with a symmetry which was forbidden in the symmetry theory of crystals. The new metallic alloys are called quasicrystals.





A crystal K is located in a finite dimensional Euclidean space E. An *isometry* of E is a map $\Phi : E \to E$ preserving a distance between any two vectors. All isometries of E form a group $\mathrm{Iso}\, E$ with the operation of multiplication of transformations.
It is known that a transformation Φ of an Euclidean space E is an isometry if and only if there exists an orthogonal linear operator $\phi = d(\Phi)$, the *differential* of Φ, and a vector $a \in E$ such that $\Phi(x) = \phi(x) + \Phi(0)$ for all $x \in E$.

For a subset $K \subset E$ its symmetry group $\operatorname{Sym} K$ consists of all isometries Φ of the space E such that $\Phi(K) = K$.

A Delaunay set in an Euclidean space E is subset K in E such that its symmetry group $\mathrm{Sym}\, K$ satisfies the following conditions:

1) for any point $A \in E$ there exists a real number $d(A) > 0$ such that for any $\Phi \in \mathrm{Sym}\, K$ an inequality $\|\Phi(A) - A\| < d(A)$ implies $\Phi(A) = A$;

2) there exists a fixed real number $D > 0$ such that for any two points $A \in K$ and $B \in E$ there exists a transformation $\Psi \in \mathrm{Sym}\, K$ for which $\|\Psi(A) - B\| < D$.

A discrete subgroup L of an additive group of the Euclidean space E is a *lattice* if $E = \mathbb{R} \otimes_{\mathbb{Z}} L$.

Theorem (Schönflies–Bieberbach)

Let $\Gamma = \mathrm{Sym}\, K$ *be a symmetry group of a Delaunay set* $K \subset E$ *and* $N = N(\Gamma)$ *a subset of all transfers in* $\mathrm{Sym}\, K$. *Then* $N \triangleleft \Gamma$ *and the factorgroup* $\Delta = \mathrm{Sym}\, K/N \simeq d(\mathrm{Sym})$ *is finite. The orbit* L *of the origin 0 of the group* N *is a lattice in* E *invariant under the action of the finite group* Δ.

The finite group Δ is called a *point* group.

Theorem

Let a point group Δ be a subgroup in $O(2,\mathbb{R})$. Then Δ is either a cyclic group $\langle a\rangle_n$ or a dihedral group $\mathbf{D}_n$, where n = 1, 2, 3, 4, 6.

A subgroup Γ in the group of affine transformation Aff E of a finite dimensional real space E is *crystallographic* if

1) Γ is *completely discontinuous* in the sense that for any compact D in E there exist finitely many elements $\gamma \in \Gamma$ with nonempty intersection $\gamma(D) \cap D$;

2) there exists a compact K_0 in E such that $E = \cup_{\gamma \in \Gamma} \gamma(K_0)$.

It is easy to see that the group Γ from Theorem 1 is crystallographic because we can take the unit cube of a basis of the lattice L as K_0.
Generalizing Theorem 1 Auslander raised the following problem.

Conjecture

Let Γ be a crystallographic group of affine transformations of a space E. The Γ has a normal solvable subgroup N of a finite index.

A survey of results on Conjecture 1 can be found in

- Abels Herbert, Geometricae Dedicata. – 2001. – 87. – p. 309-333.

The answer is positive in dimensions 2 and 3, see

- Fried D., Goldman W. D., Adv. in Math. – 1983. – 47. – 1-49.

There are several approaches to the study of mathematical models of quasicrystals and to the definition of their symmetry groups. One of the most common is the *cut and project* model.

Let V, U be real finite dimensional vector spaces $\dim U = d$ and M a lattice in $E = U \oplus V$. Then the factorgroup E/M is compact. The space E is a *hyperspace*, U — a *physical* space and V — a *phase* space. Consider the diagram of projections and embeddings

$$\begin{array}{ccccc} U & \xleftarrow{\ \pi\ } & E & \xrightarrow{\ \rho\ } & V \\ & & \cup & & \\ & & M & & \end{array}$$

It is assumed that $\pi\,|_M$ is injective and $\rho(M)$ is dense in V.

A nonempty compact subset $W \subset V$ is a *window* if W is a completion of its interior. Since $\rho(M)$ is dense in V, the set $\rho(M) \cap W$ is dense in W. In particular there exists a point $A \in M$ and a base $e_1, \ldots, e_n$ of the lattice M such that the image under the projection ρ of the unit cube

$$K = \{A + \mu_1 e_1 + \cdots + \mu_n e_n \mid 0 \leqslant \mu_i \leqslant 1\} \tag{1}$$

belongs to W. Thus the space V is spanned by elements $\rho(e_1), \ldots, \rho(e_n)$. We shall fix the choice of W, A, $e_1, \ldots, e_n$.

Put $Q = \rho^{-1}(W) \cap M$. The set $\pi(Q)$ is a *quasicrystal* in the physical space U.
Note the π maps Q injectively into U. Hence π induces a bijection between Q and $\pi(Q)$.

Theorem

Let Q, W, U, E be as above and S a finite subset in Q such that $\rho(S)$ is contained in the interior of W. For any real number $T > 0$ there exists a vector $x \in M$ such that the length of $\pi(x)$ is greater than T and $S + x \in Q$.

If Ψ is an affine transformation of the hyperspace E then there exists an invertible linear operator ψ in E such that

$$\Psi(B + x) = \psi(x) + b, \quad b \in E,$$

for all $B, x \in E$. The operator ψ is the *differential* $d\Psi$ of the map Ψ. The map $d : \Psi \to d\Psi$ is a group homomorphism $d : \mathrm{Aff}\, E \to GL(E)$ where GL(E) is the group of all invertible linear operators in E.

Let $W \subset V$ be a window. Define a *proper symmetry group* $\mathrm{Sym}_W\, Q$ of a quasicrystal Q as the group of all affine transformation of the hyperspace E which map the set Q bijectively onto itself.

Theorem

Let $\Psi \in \mathrm{Sym}_W Q$ and $\Psi(A + x) = \psi(x) + b$ where A is the chosen point in Q and x an arbitrary point in E. Then $b = \Psi(A) \in Q$. The physical U is stable under the differential $\psi = d\Psi$. The lattice M is Ψ-invariant.

Theorem

Let W be a window and $\Psi \in \mathrm{Sym}_W Q$. Then W is invariant under the restriction of the product $\rho\Psi\,|_V$ to the subspace V. The map ρ^* sending Ψ to $\rho\Psi\,|_V$ is a group homomorphism $\mathrm{Sym}_W Q \to \mathrm{Aff}\, V$. The group $\rho^*(\mathrm{Sym}_W Q)$ is relatively compact and isomorphic to the group of its differentials. In particular there exists a scalar product in V such that $\rho^*(\mathrm{Sym}_W Q)$ consisits of isometries of V.
If W is a convex polygon then the group $\rho^*(\mathrm{Sym}_W Q)$ is finite.

Corollary

There exists an interior point $F \in W$ such that $\Psi(F) - F \in U$ for any $\Psi \in \mathrm{Sym}_W Q$.

Following Theorem 4 define the *general symmetry group* Sym of the quasicrystal Q as the subgroup of the group Aff E of affine transformations Ψ of E such that the lattice M is Ψ-invariant and the physical space U is $d\Psi$-invariant.
By Theorem 4 the proper symmetry group $\mathrm{Sym}_W Q$ is a subgroup of Sym. It is easy to see that Sym is a discrete subgroup in Aff E. The groups $d(\mathrm{Sym}_W Q)$, $d(\mathrm{Sym})$ are called *point groups*.

Theorem

The map $\rho^*(\Psi) = \rho\Psi$ *is a group homomorphism* $\rho^* : \mathrm{Sym} \to \mathrm{Aff}\, V$.

Proposition

Suppose that $\Psi \in \mathrm{Aff}\, E$ *and* M, U *are* Ψ*-invariant. Then* $\Psi \in \mathrm{Sym}$.

Corollary

Let G be a subgroup in Sym*. Suppose that for every element $g \in G$ there exists a vector $x \in E$ with compact g-orbit. This is the case when G is either periodic or compact. Then G is isomorphic to a subgroup of its point group.*

The main result of the paper

- V.A. Artamonov, S, Sanchez, Remarks on symmetries of 2Dquasicrystals, Proc. of the Conference on computational and Mathematical Methods in Science and Engineering, (CMMSE-2006), University Rey Juan Carlos, Madrid, Spain, September 21-25, 2006, 59-70.

is a classification of finite subgroups G in the group Sym under the assumption that $\dim U = 2$, $\dim E = 4$. Suppose that G is not a symmetry group of a crystal. Then G is a subdirect product of two dihedral groups $\mathbf{D}_{k_1} \times \mathbf{D}_{k_2}$ where

(1) $k_1 = k_2 = 10$;

(2) $k_1 = 5,\ k_2 = 10$ or $k_1 = 10,\ k_2 = 5$;

(3) $k_1 = k_2 = 8$;

(4) $k_1 = k_2 = 12$.

In each case G belongs to one of the types:

a) a cyclic group $\langle B \rangle$;

b) a direct product to two cyclic groups $\langle B \rangle \times \langle a \rangle$;

c) a semidirect product of a normal subgroup from the previous cases and a cyclic group of order 2;

d) a dihedral group $\mathbf{D}_{10}$.

Theorem

Let G be a finite symmetry group of a quasicrystal such that dimensions of a phase space and of a physical space are equal to 2 and 3 except the case of dimensions 2 and 2. Then G is isomorphic to a subgroup of one of the groups:

(i) *a cyclic group of order* $k = 1 — 6, 8, 10, 12$;

(ii) *a dihedral group* D_k *were* k *is from* (i);

(iii) *direct product of two cyclic groups of order* k *from* (i);

(iv) *direct product of* D_k, *where* k *from* (i) *and a cyclic group of order 2;*

(v) *a direct product of any two groups from the list* $\langle a\rangle_k,\ \langle a\rangle_k \times \langle j\rangle_2,;\ D_k,\ D_k \times \langle j\rangle_2,;\ T;\ T \times \langle j\rangle_2;\ O,\ O \times \langle j\rangle_2,\quad I,\quad I \times \langle j\rangle_2;\ OT$ *where* $k = 1 — 4, 6$.

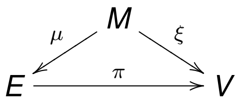
Theorem

Let G be a subgroup in Sym*. Suppose that the group $\rho^*(G)$ is relatively compact. Then there exists a window $W \subset V$ such that $G \subseteq \mathrm{Sym}_W Q$.*

There are other models of quasicrystals.

- Le Ty Qyok Taig, S.A. Piunikhin, V.A. Sadov, Uspehi mat. nauk, 48(1993):1, 41-102.

According to this paper a *quasilattice* in an Euclidean space V is an additive finitely generated abelian subgroup M in V spanning V whose rank is greater than the dimension of V. Hence we have the surjective linear map $\pi : E = \mathbb{R} \otimes_{\mathbb{Z}} M \to V$ making commutative the following diagram



where μ, ξ are embeddings of M into E and into V.
According to this paper the symmetry group of a quasicrystal is the isometry group of V mapping the quasilattice M onto itself.

Theorem

For any symmetry groups G in the previous sense there exists a subgroups $H \subset \mathrm{Aff}\, E$ such that:

1) *the space $\ker \pi$ is H-invariant;*
2) *the lattice $\mu(M) \simeq M$ is also H-invariant;*
3) *the map π induces group isomorphism $\pi^* : H \to G$.*

Another model of a quasicrystal is considered in the paper

- B.N. Fisher, D.A. Rabson, Applications of group cohomology to the classification of quasicrystal symmetries, J. Phys. A:Math. Gen., 36(2003), 10195-10214.

Let L be a quasilattice in an Euclidean (phase) space V. A *quasicrystal* is a function $\hat{\rho} : L \to \mathbb{C}$ where $\mathbb{C}$ is the complex field. It is assumed that L as an abelian group is spanned by the support $\hat{\rho}$ that is by elements $x \in L$, such that $\hat{\rho}(x) \neq 0$. Elements of $\hat{L} = \mathrm{hom}(L, \mathbb{R}/\mathbb{Z})$ are called *gauge* functions on L. Two quasicrystals $\hat{\rho}_1,\ \hat{\rho}_1$ are *indistinguishable* if there exists a gauge function χ on l such that $\hat{\rho}_2(x) = \exp\left(2\pi i \chi(x)\right) \hat{\rho}_1(x)$ for all $x \in L$.

Symmetries of a quasicrystal $\hat{\rho}$ are orthogonal operators g in V such that

1) L is g-invariant,

2) $\hat{\rho} \circ g$ and $\hat{\rho}$ are indistinguishable.

It is easy to see that the function χ_g from 2) nd from the definition of indistinguishability is a 2-cocycle.

A *point group* G in this sense if the group of all symmetries g. A *space group* of a quasicrystal $\hat{\rho}$ is the extension of G by $\hom_{\mathbb{Z}}(L, \mathbb{Z})$. Theorem 9 says the point group are subgroup of general symmetry groups considered introduced in this talk.

Another approach to the definition of symmetries is proposed in

- B. Loridant, Luo Jun., Thuswaldner, Topology of crystallographic tiles, Geom. Dedicata, 122 (2007), 113-144.

Let Γ be as crystallographic group and X a finite subset in physical U spanning V. A quasicrystal $Q = \{gx, | \ g \in \Gamma, \ x \in X\}$. Then Sym $Q \subset$ Aff U is the set of all transformations of U mapping Q onto itself. Clearly $\Gamma \subseteq$ Sym Q.