Bravais classes, Voronoï cells, Delone symbols

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ABSTRACT

We give the most refined intrinsic classification of three dimensional Euclidean lattices by combining the 14 Bravais classes, the 5 combinatorial types of Voronoï cells and the 24 Delone symbols. After recalling the fundamental concepts of group actions, we define Bravais classes and Voronoï cells in arbitrary dimension. We are quite explicit for the application to two and three dimensions.

The aim of these lectures is to give the most refined intrinsic classification of three dimensional Euclidean lattices. This classification uses two distinct concepts, both used by crystallographers and physicists: the classification by Bravais [1] into 14 symmetry classes; the classification by Fedorov in 1885 of the 5 combinatorial types of their Dirichlet = Voronoï (= Wigner Seitz) cells. The synthesis of these two points of view is given most elegantly by the Delone symbols [4]; it yields a refined classification into 24 classes. The richer paper on this classification is [5] of Delone *et al.* written in Russian and not translated into a Western language.

These lectures are divided into four parts. §1 recalls the fundamental concepts related to the actions of groups and studies an example in Euclidan geometry, using the concepts of the previous section, §2 studies the symmetry of Euclidean lattices of arbitrary dimension n; it defines crytallographic systems and Bravais classes; they are thoroughly studied in dimension $n = 2$. §3 defines Voronoï cells of lattices and recalls their main properties in arbitrary dimension. The generalisation of Selling parameters [10] due to Voronoï [12] is introduced. We apply them to dimension $n = 2$. §4 deals with the Delone classification in dimension $n = 3$, the aim of the lectures.

§1. Fundamental concepts for group actions

§1-1. *Definitions.*

Groups enter in physics through their actions. An action of the group G on the mathematical object M is given by the group homomorphism:

$$G \xrightarrow{\rho} \mathrm{Aut}\, M; \qquad g.m \text{ short for } \rho(g)(m). \qquad 1(1)$$

We generally assume that $\ker\rho = 0$; in that case the action is called *effective*.

Group orbit. The set of transforms of m, that we denote by $G.m$, is the *orbit* of m.

When every $m \in M$ can be transformed into any other $m' \in M$, then M is an orbit of G; equivalently one says that the G action is *transitive*.
M is a disjoint union of its orbits. The set of orbits is called the **orbit space** and we denote it $M|G$. Given the surjective map π, one calls *section* any injective map σ such that $\sigma \circ \pi = I$, the identity map. Here a section of $M \xrightarrow{\pi} M|G$ chooses for any element of $M|G$ a point in M belonging to the orbit; the image of the section is called a *fundamental domain*: it is a subset of M which contains a unique point of each G orbit.
Stabilizer. The set $G_m = \{g \in G,\ g.m = m\}$ of elements of G which leave m fixed, is the *stabilizer* of m; it is a subgroup of G.
It is easy to prove that $G_{g.m} = gG_m g^{-1}$; so *the set of stabilizers of the elements of an orbit is a conjugacy class* $[H]_G$ *of subgroups of* G (H is one of the stabilizers).
Orbit type. Orbits with the same conjugacy class of stabilizers are of the same type. One such type of orbit, with G as stabilizer, are the fixed points. Similarly the orbits with a trivial stabilizer 1 (then all stabilizers of the orbit are 1), are called *principal orbits*.
Example 1) Every subgroup $H < G$ can be a stabilizer of an orbit. Indeed, consider the set $G : H$ of left cosets of H in G with the G action $g.xh = gxH = (gx)H$; by its definition, this action is transitive on $G : H$ and $G_H = H$.
Stratum. In a group action, a stratum is the union of orbits of the same type. Equivalently, *two points belong to the same stratum if, and only if, their stabilizers are conjugate.*
When they exist, the fixed points form one stratum and the principal orbits form another one.
The set of strata is called the **stratum space** and is denoted by $M||G$. Belonging to the same stratum is an equivalence relation for the elements of M or for those of $M|G$. We have the commutative diagram of natural surjective maps (=onto =projections):

$$\begin{array}{ccc} M & \xrightarrow{\pi} & M|G \\ & {\scriptstyle \chi\circ\pi} \searrow & \downarrow \chi \\ & & M||G \end{array} \qquad 1(2)$$

§ **1-2.** *Examples.*

Let us give other examples of group actions:
Example 2) G acts naturally on itself: $G \xrightarrow{\rho} \mathrm{Aut}\, G$ with $\rho(g)(m) = gmg^{-1}$; then $\mathrm{Ker}\, \rho = C(G)$, the center of G, and $\mathrm{Im}\, \rho$ is the group of inner automorphisms of G. The orbit of $x \in G$ is called the "conjugacy class" of x in G; we denote it by $[x]_G$. The stabilizer of $x \in G$ is the subgroup of the elements commuting with x; this subgroup is usually called the "centralizer" of x in G; it is denoted by $C_G(x)$. The stratum of fixed points is $C(G) \equiv C_G(G)$, the center of G.
The action $G \xrightarrow{\rho} \mathrm{Aut}\, M$ defines naturally an action of G on the subsets of M. We

might select only a family of remarkable subsets; for instance, example 2 can be extended to

Example 3) G acts on its subroups by conjugation. We denote the set of subgroups of G by $\{\leq G\}$. The orbit $G.H$ of H is the conjugacy class $[H]_G$ of the subgroups of G conjugated to H; the stabilizer G_H of H is the set $\{g \in G, gHg^{-1} = H\}$. If $G_H = G$, H is by definition an invariant subgroup of G (it is usual to write this relation: $H \triangleleft G$). In the general case, the stabilizer G_H is called the *normalizer* of H in G; it is usually denoted by $N_G(H)$. Remark that it is the largest G-subgroup which contains H as invariant subgroup.

We denote the set of conjugacy classes of subgroups of G by $\{[\leq G]_G\}$. That set is the orbit space of the natural action of G on its subgroups; as an exercise show that it is also the stratum space:

$$\{[\leq G]_G\} = \{\leq G\}|G = \{\leq G\}||G. \qquad 1(3)$$

By definition, in a group action, the set of possible types of G-orbits can be identified to a subset of $\{[\leq G]_G\}$. That can be translated into a natural injection of the stratum space to $\{[\leq G]_G\}$:

$$M||G \xrightarrow{\phi} \{[\leq G]_G\}, \quad \phi \text{ injective.} \qquad 1(4)$$

On the set $\{[\leq G]_G\}$ of conjugacy classes of G subgroups, there is a natural partial ordering, by subgroup inclusion up to a conjugation. Given this partial ordering, the injection ϕ defines a partial ordering on the the stratum space $M||G$. As we shall show the role of this space is essential; indeed, the elements of this space correspond to the different symmetry types of the elements of M. For non finite groups, $|\{[\leq G]_G\}|$ is infinite in general [1] , but in all problems we shall study, $M||G$ is finite. In that case, there exist maximal and minimal strata: the maximal ones correspond to maximal symmetry and the minimal ones to minimal symmetry.As we shall see in the next section, strata spaces are fundamental concepts.

A very simple, but important remark, is that the action $G \xrightarrow{\rho} M$ defines implicitly an action of any strict subgroup $H < G$, by restricting ρ to H (the restriction is denoted by $\rho|_H$). When the action $G \xrightarrow{\rho} M$ is restricted to that of a subgroup H:

$$H < G \xrightarrow{\rho} \text{Aut}\, M: \quad H_m = H \cap G_m. \qquad 1(5)$$

In general the G-orbits split into a disjoint union of H-orbits. When we know the orbits of Aut M on M, this technique of restriction can be applied to study of any group action $G \xrightarrow{\rho} \text{Aut}\, M$ on M by considering the subgroup $\text{Im}\,\rho < \text{Aut}\, M$.

Example 4) G acts on its set of elements, that we denote by a different symbol [2] $\mathcal{G}$, by left mutiplication, i.e. $\forall g \in G$, $\mathcal{G} \ni m \mapsto g.m = gm$; then $\mathcal{G}$ is a principal orbit. Consider the restriction of this G-action to the strict subgroup H. The orbit of $x \in \mathcal{G}$

[1] For instance U_1, the one dimensional unitary group i.e. the multiplicative group of complex numbers of modulus 1, the subgroup of nth roots of 1 is a cyclic group of n elements $\sim Z_n$. Since for different n, the Z_n are not isomorphic, every group containing U_1 has an inifinite set of conjugacy classes of subgroups. For instance, that is the case of $O_n < GL_n(R)$, for $n > 1$.

[2] For instance, for infinite groups, $\mathcal{G}$ might be a manifold, and the action $g.m = gm$ be a diffeomorphism $\in$ Aut M. Then the orbits are submanifolds of M and the orbit space $M|G$ is an orbifold.

is the set of elements Hx. These H-orbits are called *right cosets of H in G*. The set of right H-cosets in G is often denoted by $(G:H)_R$; it is the orbit space:

$$H < G; \quad H \text{ acts on } G \text{ by left multiplication}: \quad \mathcal{G}|H \leftrightarrow (G:H)_R. \qquad 1(6)$$

Remark that the group action of G on $\mathcal{G}$ by right multiplication is defined by $g.x = xg^{-1}$. By restriction to $H < G$, the H-orbits are the left cosets xH and the orbit space can be identified with the $(G:H)_L$, the set of left H-cosets.

Main Example: According to the Erlangen programme of F. Klein, a geometry is the study of the action of a G on one orbit and its subsets. For the lectures, we are interested by Euclidean geometry. The n-dimensional Euclidean group Eu_n is the semi-direct product $Eu_n = R^n \rtimes O_n$, where R^n is the invariant subgroup of translations and O_n the orthogonal group. The Euclidean space $\mathcal{E}_n$ is the principal orbit of R^n or, equivalently, the orbit $\mathcal{E}_n = Eu_n : O_n$. Let $\mathcal{E}_n^{\times 2}$ the set of pairs $x \neq y$ of distinct points of $\mathcal{E}_n$: the action of Eu_n on this set contains a unique stratum [3] with an infinite set of orbits labelled by a positive real number, the Euclidean invariant $d(x,y) > 0$, the distance between x and y.

Similarly, the number of strata in the action of Eu_n on $\mathcal{E}_n^{\times 3}$, the set of triplet x, y, z of distinct points of $\mathcal{E}_n$, is independent of n. The distances ξ, η, ζ between the 3 pairs of points are Euclidean invariant, but they are not arbitrary positive numbers; so we prefer to choose the three invariants λ, μ, ν:

$$\xi = d(y,z) = \frac{1}{2}(\mu+\nu) > 0, \quad \eta = d(z,x) = \frac{1}{2}(\nu+\lambda) > 0, \quad \zeta = d(x,y) = \frac{1}{2}(\lambda+\mu) > 0, \qquad 1(7)$$

so

$$\lambda = -\xi + \eta + \zeta \geq 0, \quad \mu = \xi - \eta + \zeta \geq 0, \quad \nu = \xi + \eta - \zeta \geq 0, \qquad 1(7')$$

with the easy to prove condition that no more than one of these 3 invariants λ, μ, ν vanishes. It is well know that the surface $s(x,y,z)$ of the triangle (x,y,z) is given by:

$$4s(x,y,z)^2 = (\lambda+\mu+\nu)\lambda\mu\nu. \qquad 1(8)$$

We shall determine the stabilizers only in the 2 dimensional case; it corresponds to the Euclidean geometry we have studied in high school. We have to distinguish two cases i) and ii) and several subcases:

i) $\lambda\mu\nu \neq 0$:

a) $(\lambda-\mu)(\nu-\lambda)(\mu-\nu) \neq 0$, i.e. the 3 invariant have different values. The stabilisers are trivial: the orbits of generic triangles (they are 3 parameters of them) are principal.

b) only two of the parameters are equal: that correspond to the two parameter family of orbits of isocele triangles. The stabilisers are the Z_2 groups generated by the reflection through the symmetry axis of the triangle; this conjugacy class is also denoted by C_s in the Schönflies notation used by molecular or solid state physicists.

[3] Let m be the middle of the segment xy, and $\mathcal{E}_{n-1}$ the bisector hyperplane of the pair x, y. As an exercise, show that the conjugacy class of the stabilizers of this stratum is $[O_{n-1} \times Z_2]_{Eu_n}$ where O_{n-1} is the stabilizer of m in the Euclidean group of $\mathcal{E}_{n-1}$ and Z_2 is the 2 element group generated by the reflection (in E_n) through the hyperplane $\mathcal{E}_{n-1}$.

c) $\lambda = \mu = \nu \neq 0$ defines the one parameter family of orbits of equilateral triangle; the stabilizers are $C_{3v} \sim \mathcal{S}_3$ (the permutation group of three objects).
ii) among the three invariants λ, μ, ν exactly one is zero.
a) $(\lambda - \mu)(\nu - \lambda)(\mu - \nu) \neq 0$, i.e. the 3 invariants have different values. The stabilisers are C_s groups generated by the reflection through the axis carrying x, y, z.
b) two invariants are equal and positive, the third one is zero; this means that one point is at the middle of the segment formed by the other two: the stabilizers are $C_{2v} \sim Z_2^2$.

To summarize: we have found 4 strata: the minimal one (trivial stabilizers) which corresponds to generic triangles; the unique strata above it (stabilisers C_s) which contains the orbits of same type for two different kinds of geometric objects: cases i-b) and ii-a); there are two maximal strata with 6 and 4 element stabilisers.

§ **1-3.** *Stabilisers of linear representations of finite or countable groups.*

We shall give now basic results that we will need in §2 and §4 for some linear representations of $GL_n(Z)$. Here we denote the group by G; it acts linearly $\vec{v} \mapsto g.\vec{v}$ on the real finite dimensional vector space V. We denote by V^g the set of vectors left fixed by g; it is a vector subspace of V. Moreover:

$$V^H = \cap_{g \in H} V^g; \quad H < K < G \Rightarrow V^H \geq V^K. \qquad 1(9)$$

We denote by S_H the manifold of vectors of V which have H as a stabilizer.

Lemma 1-1. *In a linear representation of a countable or finite group: H is a stabilizer $\Leftrightarrow S_H$ is dense in V^H.*

If H is not a stabilizer, S_H is empty. We assume that H is a stabilizer, i.e. S_H is not empty. Of course $S_H \subseteq V^H$. Let $\{K_i\}$ the set of stabilizers strictly greater than H; Then V^{K_i} has to be a strict vector subspace of V^H since it has no point of S_H. So S_H is the complement in V^H of $\cup_i V^{K_i}$ a countable (or finite) set of strict subspaces; that proves that S_H is dense in V^H.

Lemma 1-2. *In a linear representation of a countable or finite group the intersection of two stabilizers is a stabilizer.*

Let P_i the stabiliser of $\vec{r}_i$, $i = 1, 2, \ldots$. Consider the elements of the straight line $\Delta = \{\vec{r}_\lambda\}$ defined by $\vec{r}_1, \vec{r}_2$:

$$\vec{r}_\lambda = \lambda \vec{r}_1 + (1 - \lambda)\vec{r}_2. \qquad 1(10)$$

The stabilizer of any point of the line is $\geq$ the intersection of the stabilizers of two arbitrary points:

$$P_\lambda \geq P_1 \cap P_2, \quad P_1 \geq P_2 \cap P_\lambda, \quad P_2 \geq P_\lambda \cap P_1. \qquad 1(11)$$

Taking the intersection with one of the groups in each intersetion:

$$P_\lambda \cap P_2 \geq P_1 \cap P_2, \quad P_1 \cap P_2 \geq P_2 \cap P_\lambda, \text{ etc....} \qquad 1(12)$$

and similarly for any other stabiliser $P_{\lambda'}$, we obtain the equality of the intersection of any pair of stabilizers of points of Δ:

$$P_1 \cap P_2 = P_2 \cap P_\lambda = \cdots = P_\lambda \cap P_{\lambda'}. \qquad 1(13)$$

Hence it is impossible that all stabilisers be strictly greater that the common intersection of any pair of them, because it would require *all* of them to be different, but the set of different stabilisers is at most countable while the set of P_λ should have the same cardinal as the set of points of Δ, i.e. the power of the continuum. So the common intersection $P_\lambda \cap P_{\lambda'}$ of the stabilisers of any pair of points of Δ is the stabiliser of all points of a dense subset of Δ. We have proven more than the lemma; it is easy to extend that result to any set of vectors spanning a d-dimensional subspace of V:

Corollary 1-1. *In a linear representation of a countable or finite group G on the space V the intersection $P = \cap P_i$ of the stabilizers P_i of a set of vectors $\vec{r}_i$ generating the subspace V_d is a stabilizer; the intersection $V_d \cap S_{[P]}$ of the corresponding stratum $S_{[P]}$ with V_d is dense in this subspace.*

Combining that corollary with lemma 1.2 we obtain:

Corollary 1-2. *In a linear representation of a countable or finite group G on the space V, if P_1 and P_2 are stabilizers, the subspaces V^{P_1} and V^{P_2} span the subspace $V^{P_1 \cap P_2}$ of fixed points of the stabilizer $P_1 \cap P_2$.*

Extending the proof of corollary 1-1 and the results to the whole space V we obtain the existence of a unique minimal stratum, which is open dense and whose stabilizers P is unique since it is the intersection of the stabilisers of all vectors of the space V. By definition it is the kernel of the representation. Hence the theorem:

Theorem 1. *In a linear representation of a countable or finite group G on the space V, there exists a unique minimal stratum, open dense in V; it has a unique stabilizer: the kernel of the representation.*

We end this section by giving a simple theorem that we shall need for a systematic research of the strata. Its proof is obvious.

Theorem 2. *Given an action of G on M, and the inclusion of subgroups $K < H < G$ where K is a stabiliser. Then $M^H \subset \cap_{g\in H} M^{gKg^{-1}}$.*

That is a direct consequence of $K < H \Rightarrow M^H \subset M^K$. Notice that when K is an invariant subgroup of H, the theorem reduces to $M^H \subset M^K$.

For more information on the subject of § 1, see [8] and earlier references given therein.

§ 2. Classification of Euclidan lattice symmetries

This section relies very much on a publication with J. Mozrzymas [9] and the manuscript of a book in preparation with M. Senechal.

§ 2-1. *Manifold $\mathcal{L}_n$ of n-dimensional lattices.*

Let V_n be a n-dimensional orthogonal vector space whose positive definite scalar product is denoted by $(\vec{x}, \vec{y})$; we use the notation $N(\vec{x}) = (\vec{x}, \vec{x})$ for the norm of the vector $\vec{x}$. We simply denote by R^n the additive group of V_n. As we have seen in the main example of § 1, the action of the translation group R^n on the set of elements (a manifold) $\mathcal{V}_n$ of the vector space V_n, transforms it in a Euclidian space $\mathcal{E}_n$. Let o be the origin of V_n. We denote by $x = o + \vec{x}$ the translated of o by $\vec{x}$; every point of $\mathcal{E}_n$ can be obtained by a translation of o. The point y is obtained from x by the translation $\vec{y} - \vec{x}$, i.e. $y = x + \vec{y} - \vec{x}$, so

$$d(x,y)^2 = N(\vec{y} - \vec{x}). \qquad 2(1)$$

We first define the lattices of V_n and simply call them:
Lattice: A lattice L is the subgroup of the translation group of V_n generated by the vectors $\vec{b}_i$ of a V_n basis, i.e. the vectors of L are linear combinations with integral coefficients of the $\vec{b}_i$'s. More abstractly: it is a closed subgroup of R^n of rank n.
The image $L + \vec{x}$ of a lattice L by a any translation $\vec{x} \in R^n$ is an *Euclidean lattice* of $\mathcal{E}_n$. We reduce the study of Euclidean lattices to that of lattices by choosing as origin o a point of the Euclidean lattice.

For convenience, in order to define the matrices of the orthogonal group $O_n =$ Aut V_n, by the relation $rr^\top = r^\top r = I$ we introduce an orthonormal basis $(\vec{e}_\alpha, \vec{e}_\beta) = \delta_{\alpha\beta}$ of V_n. Then an arbitrary basis of V_n is defined by $b_i = \sum_\alpha \tilde{b}_{i\alpha}\vec{e}_\alpha$ where the matrix $\tilde{b}$ has non vanishing determinant, i.e. $\tilde{b} \in GL_n(R)$. Given another basis by the matrix $\tilde{b}'$ there is a unique group element $g \in GL_n(R)$ which transforms the basis $\tilde{b}$ into $\tilde{b}' = g.\tilde{b} = \tilde{b}g^{-1}$. So the set $\mathcal{B}_n$ of bases of V_n is a principal orbit of $GL_n(R)$, i.e. $\mathcal{B}_n$ is the manifold of the elements of $GL_n(R)$.

When is $\tilde{b}'$ another basis of the lattice L generated by $\tilde{b}$? The vectors $\overrightarrow{b'_i}$ must be in the lattice so $\vec{b}'_i = \sum_j m_{ij}\vec{b}_j$, where m is a matrix whose elements m_{ij} are integers. Moreover, the vectors $\overrightarrow{b'_i}$ must form a L basis, so m^{-1} must also be an integral matrix. To summarize the bases of L are of the form $m\tilde{b}$, $m \in GL_n(Z)$. So L can be identified as an orbit of $GL_n(Z)$ acting on $\mathcal{B}_n$ by left multiplication. Using 1(6), we have shown that the manifold $\mathcal{L}_n$ of n-dimensional lattices can be defined as:

$$\mathcal{L}_n = \mathcal{B}_n | GL_n(Z) = (GL_n(R) : GL_n(Z))_R. \qquad 2(2)$$

The matrices of $GL_n(Z)$ have determinant ± 1, so $\det \tilde{b}$ have same absolute value for all bases of the lattice; this value is a characteristic of the lattice; it is simply denoted by:

$$\det(L) = |\det \tilde{b}|. \qquad 2(3)$$

§ **2-2**. *Crystallographic systems.*

The interesting mathematical objects are the intrinsic lattices, i.e. lattices modulo their position in space. The orthogonal group O_n transforms the position of a lattice L into any other position: if L has basis $\tilde{b}$ the lattice $r.L$, $r \in O_n$ is generated by the basis $\tilde{b}r^{-1} = \tilde{b}r^\top$. Hence the manifold of positions of L is the orbit $O_n.L$ and the orbifold $\mathcal{L}_n^o$ of n-dimensional "intrinsic" lattices is the orbit space:

$$\mathcal{L}_n^o = \mathcal{L}_n | O_n. \qquad 2(4)$$

The corresponding strata yield a corresponding classification of lattice symmetry. They are called in [7] (International Tables of Crystallography): Bravais crystallographic systems. Denoting their set in n dimensions by $\{BCS\}_n$ we have the definition [4] as a stratum space:

$$\{\text{Bravais crystallographic systems}\}_n \equiv \{BCS\}_n = \mathcal{L}_n \| O_n. \qquad 2(5)$$

We can give an equivalent and more explicit definition of $\mathcal{L}_n^o$. Indeed, given a basis $\tilde{b} \in GL_n(R)$ of L, we have just shown that the left coset $\tilde{b}O_n \subset GL_n(R)$ is a set of bases generating all lattices belonging to the orbit $O_n.L$ of the positions of L. We also showed (see 2(2)) that the right coset $GL_n(Z)\,\tilde{b} \subset GL_n(R)$ is the set of all bases of L, and therefore represents $L \in \mathcal{L}_n$. Hence the double coset $GL_n(Z)\,\tilde{b}O_n \subset GL_n(R)$ is the set of all bases of all lattices of the orbit $O_n.L$ and therefore represents the "intrinsic" lattice L in $\mathcal{L}_n^o$; that shows that $\mathcal{L}_n^o$ is the set of double cosets:

$$\mathcal{L}_n^o = GL_n(Z) : GL_n(R) : O_n. \qquad 2(6)$$

The set of double cosets can be viewed as an orbit space for the action:

$$(m \times r) \in GL_n(Z) \times O_n, \quad (m \times r).\tilde{b} = m\tilde{b}r^{-1}, \quad \mathcal{L}_n^o = \mathcal{B}|(GL_n(Z) \times O_n), \qquad 2(7)$$

Its symmetry meaning is the following: consider the lattice L generated by the V_n basis $\tilde{b}$ which is tranformed into $\tilde{b}r^{-1}$ by the orthogonal transformation r; if this transformed basis generates the *same* lattice L then, by definition, r is `a symmetry of this lattice` and there must exist $m \in GL_n(Z)$ which transforms the old L basis $\tilde{b}$ into the new one $\tilde{b}r^{-1}$. To summarize:

$$(m \times r) \in (GL_n(Z) \times O_n)_{\tilde{b}} \Leftrightarrow m\tilde{b} = \tilde{b}r^{-1} \quad \Leftrightarrow \quad m = \tilde{b}r^{-1}\tilde{b}^{-1} \Leftrightarrow r = \tilde{b}^{-1}m^{-1}\tilde{b} \quad 2(8)$$

We define the canonical, projective homomorphisms of groups:

$$GL_n(Z) \times O_n \xrightarrow{\pi_z} GL_n(Z), \ \pi_z(m \times r) = m; \quad GL_n(Z) \times O_n \xrightarrow{\pi_o} O_n, \ \pi_o(m \times r) = r. \qquad 2(9)$$

Because $GL_n(R)$ acts freely by left or right multiplication on itself, the stabilizer of any basis, $(GL_n(Z) \times O_n)_{\tilde{b}}$ is a "diagonal" subgroup of $GL_n(Z) \times O_n$, i.e. it contains no element of the kind $m \times 1$ or $1 \times r$ outside the identity 1×1. That implies that the stabilizer and its two canonical projections are isomorphic:

$$(O_n \times GL_n(Z))_{\tilde{b}} \sim \pi_z((O_n \times GL_n(Z))_{\tilde{b}}) \sim \pi_o((O_n \times GL_n(Z))_{\tilde{b}}), \qquad 2(10)$$

It is important to distinguish these two isomorphic groups; that is why we use for them different notations which specify to which group they are subgroups:

$$P_L = \pi_o((O_n \times GL_n(Z))_{\tilde{b}} < O_n, \quad P_L^z = \pi_z((O_n \times GL_n(Z))_{\tilde{b}}) < GL_n(Z). \qquad 2(11)$$

Similarly we shall use different names for them: we call $P_L = \pi_o((O_n \times GL_n(Z))_{\tilde{b}}$ the *holohedry* of L and $P_L^z = \pi_z((O_n \times GL_n(Z))_{\tilde{b}})$ its *Bravais group*.

[4] Bravais did not define the Bravais crystallographic systems. [2] uses "French crystallographic systems"; indeed this concept was defined and used by the French school of crystallography. Weiss [13] in 1816 was the first to introduce a concept of "crystallographic systems"; but this concept, different from that of BCS, does not generalize easily to arbitrary dimension. However both concepts coincide in dimension 2. In dimension 3 both give 7 crystallographic systems: but only 5 of them coincide. Strangely enough, ITC merge the two pairs of different crysallographic systems into one "family" (as they called it).

Lemma 2-1. *The holohedry and the Bravais group of a lattice are isomorphic finite groups.*

The isomorphy has already been proven. The last equality of 2(8) shows that the holohedry is the intersection in $GL_n(R)$ of the compact subgroup O_n and of the discrete subgroup $\tilde{b}^{-1}\, GL_n(Z)\, \tilde{b}$. As a compact and discrete group, it is finite.
We recall that the symmetry through the origin is a symmetry of any lattice; so

$$-I_n \in P_L, \qquad -I_n \in P_L^z. \tag{2(12)}$$

We do know that the symmetry types are given by a conjugacy class of subgroup. As we have seen in 2(4):
the conjugacy class $[P_L]_{O_n}$ defines the Bravais crystallographic system of L.
We shall explain that:
the conjugacy class $[P_L^z]_{GL_n(Z)}$ defines the Bravais class of L

§ **2-3.** *Bravais classes.*

Equation 2(6) is basic for describing the orbifold of n-dimensional intrinsic lattices. We have defined the Bravais crystallographic systems by studying the action of O_n on the manifold of cosets $GL_n(Z) : GL_n(R)$. Now we study the other interpretation: the action of $GL_n(Z)$ on the manifold of cosets $GL_n(R) : O_n$.

The real symmetric $n \times n$ matrices form a vector space V_N of dimension $N = n/(n+1)/2$. This space has a natural scalar product $(a, b) = \operatorname{tr} ab$. The subset of positive matrices form a convex cone $\mathcal{C}^+(\mathcal{Q}_n)$ since the sum of two positive matrices is a positive matrix. The real symmetric positive $n \times n$ matrices, e.g. $\tilde{b}\tilde{b}^\top$ have a unique real symmetric positive square root [5] that we denote by $\sqrt{\tilde{b}\tilde{b}^\top}$ so any $\tilde{b} \in GL_n(R)$ has unique left and right polar decompositions:

$$\tilde{b} = \sqrt{\tilde{b}\tilde{b}^\top}\, r = r\sqrt{\tilde{b}^\top \tilde{b}}, \quad r \in O_n. \tag{2(13)}$$

To verify that $r \in O_n$, compute $rr^\top$ and $r^\top r$. The first equality of the polar decomposition identifies the left coset factorisation $GL_n(R) : O_n$ with $\mathcal{C}^+(\mathcal{Q}_n)$. When the basis $\tilde{b}$ generates the lattice L, the matrix elements of $q = \tilde{b}\tilde{b}^\top$ are $q_{ij} = (\vec{b}_i, \vec{b}_j)$ often called the Grammian of $\tilde{b}$. These scalar products are O_n invariants; with 2(7) we verify again that O_n acts trivially on $\tilde{b}\tilde{b}^\top$ while the action of $GL_n(Z)$ is

$$m \in GL_n(Z),\ q = \tilde{b}\tilde{b}^\top \in \mathcal{C}^+(\mathcal{Q}_n), \quad m.q = mqm^\top. \tag{2(15)}$$

The strata of this action of $GL_n(Z)$ on $\mathcal{C}^+(\mathcal{Q}_n)$ are the Bravais classes of lattices. Denoting by $\{BC\}_n$ the set of Bravais classes of n-dimensional lattices, this definition can be written:

$$\{\text{Bravais classes}\}_n \equiv \{BC\}_n = \mathcal{C}^+(\mathcal{Q}_n) \| GL_n(Z)\,. \tag{2(16)}$$

[5] In other words, for $q \in \mathcal{C}^+(\mathcal{Q}_n)$ the maps $q \mapsto \sqrt{q}$ and $q \mapsto q^2$ are diffeomorphisms of $\mathcal{C}^+(\mathcal{Q}_n)$.

In his memoir Bravais [1] gave a different but equivalent definition of the classes and he determined the 14 Bravais classes of $\{BC\}_3$ correcting the classification of Frankenheim into 15 classes. The action of $GL_n(Z)$ on $\mathcal{C}^+(\mathcal{Q}_n)$ was studied from the 1780's by mathematicians (Lagrange, Gauss, Jacobi, Hermite, etc....) as "arithmetic theory of quadratic forms" without mentioning for a century the traduction in terms of lattices.

We have seen in §1 after equation 1(4) that there is a natural partial order on any stratum space. We now prove that there exists an order preserving surjective map

$$\{BC\}_n \xrightarrow{\varphi} \{BCS\}_n, \quad \varphi \text{ surjective,} \tag{2(16)}$$

from the partially ordered set of Bravais classes onto the partially ordered set of Bravais cristallographic systems: it is the restriction on $\{BC\}_n$ of the natural map ϕ (whose existence we shall prove) from the set the conjugated classes of finite subgroups of $GL_n(Z)$ to the similar set for O_n.

Lemma 2-2. *There is a natural bijective map ι between the conjugacy classes of finite subgroups of $GL_n(R)$ and of O_n.*

It is well known that any finite subgroup of $GL_n(R)$ is conjugate to a subgroup of $O_n < GL_n(R)$; so we are left to prove that two subgroups of O_n which are conjugated in $GL_n(R)$ are conjugated in O_n: indeed assume $g, g' \in O_n$ conjugate by $s \in GL_n(R)$: $g' = sgs^{-1}$; let $s = rt$, $r \in O_n$, $t = \sqrt{s^\top s}$ the polar decomposition (see 2(13)) of s; then $I = g'^\top g' = (s^\top)^{-1} g^\top t^2 g s^{-1}$, i.e. $t^2 = g^{-1} t g g^{-1} t g$; since the positve square root of t^2 is unique, $t = g^{-1} t g$ and $g' = sgs^{-1}$ becomes $g' = rgr^{-1}$. (end of the lemma proof)
Since $GL_n(Z) < GL_n(R)$, two subgroups conjugate in $GL_n(Z)$ are conjugate in $GL_n(R)$.
Let ϕ' be this natural surjective map: $\{[\leq GL_n(Z)]_{GL_n(Z)}\} \xrightarrow{\phi'} \{[\leq GL_n(R)]_{GL_n(R)}\}$.
Then φ of 2(16) is the restriction of $\phi = \iota \circ \phi'$ to $\{BC\} \subset \{[\leq GL_n(Z)]_{GL_n(Z)}\}$.

Arithmetic classes is the short hand used by crystallographers for "conjugacy classes of finite subgroups of $GL_n(Z)$". It was proven by C. Jordan that $\{AC\}_n$, the set of arithmetic classes of $GL_n(Z)$, is finite for all n. For $n = 1, 2, 3, 4$ this number is respectively $2, 13, 73, 710$. Strangely, many mathematics books give 70 instead of 73. Hence for any dimension the number of Bravais classes ($\{BC\}_n \subset \{AC\}_n$) and (since φ in 2(16) is surjective) the number of Bravais crystallographic systems are finite. For $n = 1, 2, 3, 4$ these numbers are respectively $1, 5, 14, 64$ for Bravais classes, $1, 4, 7, 32$ for Bravais crystallographic systems.

Remark

Beware that for some holohedries P_L, all the different conjugacy classes $[P_L]_{GL_n(Z)}$ of the ϕ pre-image $\phi^{-1}([P_L]_{O_n})$ are not necessarily Bravais classes (of course at least one of them is). This happens for every dimension $n > 2$. We shall see later the example for $n = 3$.

We have still several concepts to introduce about Bravais classes and Bravais groups.

Dual lattice: The dual L^* of $L < V_n$ is the set of vectors of V_n whose scalar products with all vectors of L are integral. From this definition we deduce that L^* is a lattice. If $\check{b}$ is a basis of L the dual basis $\check{b}^*$, defined by:

$$(\vec{b}_i^*, \vec{b}_j) = \delta_{ij} \Leftrightarrow \check{b}^* = \check{b}^{-1\top} \tag{2(17)}$$

is a basis of L^*. This implies for the corresponding quadratic forms:

$$q(L^*) = q(L)^inv \Leftarrow L^{**} = L \qquad 2(18)$$

When $L^* = L$, we say that the lattice is *self dual*. That is equivalent to $q(L) \in SL_n(Z)$ (easy proof left to the reader). Considering the inverse of each side of the equation $q = mqm^\top$ we obtain for the Bravais group of the dual lattice:

$$P^z_{L^*} = (P^z_L)^{-1\top} \qquad 2(19)$$

i.e. every matrix $m \in P^z_L$ is replaced by $m^{-1\top}$. We call this group the contragredient [6] of P^z_L. When two contragredient Bravais groups belong to the same Bravais class, we say that this Bravais class is self dual. When the two Bravais classes are distinct, we say that they are in duality; show that the map φ of 2(16) sends them into the same Bravais crystallographic system (but the converse is not true!).

Given a finite subgroup $F < GL_n(Z)$ one can define on the $n(n+1)/2$-dimensional vector space $\mathcal{Q}_n$ of n variable quadratic forms. the linear operator σ_F:

$$q \mapsto \sigma_F(q) = |F|^{-1} \sum_{m \in F} mqm^\top . \qquad 2(20)$$

It maps the orbits of F on their barycenter; one easily verifies that $\sigma_F^2 = \sigma_F$, i.e. it is a projector and $\operatorname{Im}\sigma_F$ is a subspace of $\mathcal{Q}_n$ containing all F-invariant quadratic forms. 2(20) shows that σ_F projects any F-orbit on its barycenter. Since the sum of positive quadratic forms is a positive quadratic form, when q in 2(20) is positive, $\sigma_F(\mathcal{C}_+(\mathcal{Q}_n)) \subset \mathcal{C}_+(\mathcal{Q}_n)$. More precisely, if we denote by V^F and $\mathcal{C}_+(\mathcal{Q}_n)^F$ (notation defined in 1(9)), respectively the vector subspace of F invariant quadratic forms and the cone of positive quadratic forms invariant by F:

$$V^F = \operatorname{Im}\sigma_F, \qquad \sigma_F(\mathcal{C}_+(\mathcal{Q}_n)) = V^F \cap \mathcal{C}_+(\mathcal{Q}_n) = \mathcal{C}_+(\mathcal{Q}_n)^F . \qquad 2(21)$$

We know from lemma 1-1 that F is a Bravais group if it is the stabilizer of an open dense subset of $\mathcal{C}_+(\mathcal{Q}_n)^F$. The union of these subsets for all F in the conjugacy class defining the Bravais class, is the corresponding stratum. Hence:

$$\text{dimension of the Bravais class } [P]_{GL_n(Z)} \text{ stratum } = \dim \mathcal{C}_+(\mathcal{Q}_n)^P . \qquad 2(22)$$

We know from theorem 1 that there is a unique minimal stratum, the generic open dense one, whose stabiliser is the kernel K of the linear action of $GL_n(Z)$, that the set of $m \in GL_n(Z)$ such that for all $q(L)$, $mqm^\top = q$; so $m \pm I$, i.e. $m \in Z_2(-I) \sim C(GL_n(Z))$, the center of $GL_n(Z)$.

Since for every dimension n, the number $|\{AC\}_n|$ of arithmetic classes is finite (Jordan theorem), this partially ordered set has maximal elements. The maximal finite subgroups of $GL_n(Z)$ leave invariant the barycenters of their orbits, and since they are maximal, they are the stabilizers of these points. Hence every maximal arithmetic class is a maximal Bravais class. Moreover, if P is a Bravais group of a maximal Bravais class, all lattices represented by points of $\mathcal{C}_+(\mathcal{Q}_n)^P$ have P as the Bravais group.

[6] The concept of dual groups is already defined in mathematics with a very different meaning, so it should not be used here.

We give the simplest examples of maximal Bravais classes in arbitrary dimension. Consider the lattice whose vectors are, in the orthonormal basis $(\vec{e}_i, \vec{e}_j) = \delta_{ij}$

$$L = \{\sum_i \mu_i \vec{e}_i,\ \mu_i \in Z\}. \qquad 2(23)$$

Its quadratic form is $q(L) = I_n$. Its Bravais group is the set of $m \in GL_n(Z)$ such that $mIm^\top = mm^\top = 1$. This is $O_n(Z)$, the orthogonal group on the integers; it is easy to show that it is the symmetry group of the cube (or of its dual, the regular cross polytope) in n dimension and has the structure:

$$O_n \cap GL_n(Z) = O_n(Z) \sim Z_2^n \rtimes \mathcal{S}_n. \qquad 2(24)$$

That group is generated by n^2 reflections through hyperplanes; it is maximal [7]. $O_n(Z)$ is also a symmetry group of a sub lattice of index 2 of L; it is D_n^r, the lattice generated by the roots of the D_n simple Lie algebra:

$$L = \{\sum_i \mu_i \vec{e}_i,\ \mu_i \in Z,\ \sum_i \mu_i \in 2Z\}. \qquad 2(25)$$

and of the dual lattice D_n^w (the weight lattice of D_n whose each vector coordinates satisfy:

$$L = \{\sum_i \mu_i \vec{e}_i,\ \text{all } \mu_i \in Z \text{ or } \in Z + \frac{1}{2}\}. \qquad 2(26)$$

For $2 < n \neq 4$ these 3 lattices belong to three distinct maximal Bravais classes, inverse image of the Cubic BCS $[O_n(Z)]_{O_n}$. For $n = 2$ there is a unique Bravais lattice and for $n = 4$, the Bravais groups of D_4^r and D_4^w is F_4, the symmetry group of a self-dual regular polytope which has no correspondent in the other dimensions.

There is a systematic method for finding the set of Bravais classes as subset of the partially ordered set $\{AC\}_n$ of arithmetic classes. Consider a complete ascending chain of finite subgroups of $GL_n(Z)$ starting from $F_0 = Z_2(-I)$; it is finite and ends with a maximal finite subgroup F_m of $GL_n(Z)$. In such a chain $F_0 < F_1 < F_2 < \ldots$ the corresponding $\dim(\mathrm{Im}\,\sigma_{F_k})$ satifies $\dim(\mathrm{Im}\,\sigma_{F_k}) \geq \dim(\mathrm{Im}\,\sigma_{F_{k+1}})$; the relation is $>$ (respectively $=$) implies F_k is (resp. is not) a Bravais group.

Let $\{ZAC\}_n$ be the set of cyclic arithmetic classes; its image (as conjugacy classes in $GL_n(R)$) by ϕ' (the map defined immediatly after the proof of lemma 2-2) is the set of cyclic geometrical classes; this set can be easily computed by an elegant method given by Hermann [6]. I will not explain it here, and neither explain the use of the first cohomology of finite groups to obtain $\{ZAC\}_n$ from the Hermann list. The conjugacy classes in O_n of the generators of the cyclic geometrical classes are labelled explicitly for $n = 2, 3$ in the [7] under the name *geometric elements*. We will call here the conjugacy classes in $GL_n(Z)$ of the generators of the $\{ZAC\}_n$, *arithmetic elements* and give their list for $n = 2, 3$; the [7] labels them. As we will see for $n = 2, 3$, knowing the set $\{ZAC\}_n$ of cyclic arithmetic classes it is easy to find which ones are Bravais classes.

[7] Indeed in any linear group, all reflections are conjugate into themselves, so O_n is an invariant subgroup of any subgroups of $GL_n(Z)$ containing it. So the largest subgroup containing is its normaliser $N_{GL_n(Z)}(O_n(Z))$. Let n be an element of that group and $r \in O_n(Z)$. Then $nrn^{-1} \in O_n(Z)$, i.e. $(nrn^{-1})(nrn^{-1})^\top = 1$, which is equivalent to $n^\top nr = rn^\top r$. Since $GL_n(Z)$ is irreducible on the complex, $n^\top n$ is a positive diagonal matrix of $GL_n(Z)$ so $n^\top n = I$ i.e. $n \in O_n(Z)$.

§ 2-4. $\{BC\}_2$ *and fundamental domains in* $C^+(\mathcal{Q}_2)$.

In Schönflies notations the finite subgroups of O_2 are $C_n \sim Z_n$ (cyclic group generated by a rotation of $2\pi/n$), C_s the group generated by a reflection and C_{nv}, the $2n$ element group generated by the reflections through two axes with an angle of π/n. The trace of the matrix representing a rotation by θ is $2\cos\theta$: that is an integer only for $\theta = 2\pi/n$ with $n = 1, 2, 3, 4, 6$

In dimension $n = 2$, any real matrix s with $\operatorname{tr} s = 0$, $\det s = -1$ has eigenvalues $1, -1$, so it is conjugate to the Pauli matrix σ_3 which represents a reflection through the x-axis in the orthogonal plane xoy. We shall show that the matrices:

$$pm = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad cm = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad 2(27)$$

are not conjugate in $GL_2(Z)$; so they belong to two different arithmetic classes which are denoted in [7] pm and cm respectively; the common m is an abbreviation of "mirror" (= reflection) in these tables. Let t a conjugation matrix $\sigma_1 = t\sigma_3 t^{-1}$; then $I + \sigma_1 = t(I + \sigma_3)t^{-1}$. It is absurd to assume that $t \in GL_n(Z)$ because that implies that conjugated integral matrices have same gcd (= greatest common divisor) for their set of elements, but $\gcd(I + \sigma_1) = 1$ while $\gcd(I + \sigma_3) = 2$. Note that the two matrices are conjugated in $GL_2(Q)$, the general linear group on the rational; indeed

$$\sigma_1 = t\sigma_3 t^{-1}, \quad \text{with } t = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \; t^{-1} = \tfrac{1}{2} t^{\top}. \qquad 2(28)$$

As we recall in 2(12), $-I$ belongs to every holohedry and Bravais group. So that proof shows also that the two groups:

$$\{\pm I, \pm\sigma_3\} \in pmm, \quad \{\pm I, \pm\sigma_1\} \in cmm, \qquad 2(29)$$

belong to two different arithmetic classes; we denote them by pmm and cmm, the notations of [7].

Any two dimensional representation of an Abelian group is reducible; but on Z the representation might be *indecomposable* into a direct sum of two irreducible representation; choosing as first vector of coordinates, the one which spans an invariant space, we can put the matrices into a upper triangular form. For instance for pm and cm of 2(27):

$$t_3 = \begin{pmatrix} 1 & -y \\ 0 & 1 \end{pmatrix} \; t_1 = \begin{pmatrix} 1+y & -y \\ -1 & 1 \end{pmatrix}; \; t_3\sigma_3 t_3^{-1} = \begin{pmatrix} 1 & 2y \\ 0 & -1 \end{pmatrix}, \; t_1\sigma_1 t_1^{-1} = \begin{pmatrix} 1 & 2y+1 \\ 0 & -1 \end{pmatrix}. \qquad 2(30)$$

That establishes that σ_1 is not diagonalizable and that there exist only two arithmetic classes of reflections. This result extends to every dimension $n > 2$.

The rotation by π is represented by the matrix $-I_2$ in the center of $GL_2(Z)$. Since the product of two reflections is a rotation, one can prove from our result on reflections that the rotations of order 3, 4, 6 form a unique arithmetic class for each order. So, in the [7] notation:

$$n = 2 \qquad \text{arithmetic elements}: \; pm, cm, p2, p3, p4, p6. \qquad 2(31)$$

As in [7], we use the same notation for the cyclic arithmetic class generated by these arithmetic elements. As we said, the class $p2$ is the center of $GL_2(Z)$ i.e. the kernel of the linear representation of $GL_2(Z)$ on the 3 dimensional space $\mathcal{Q}_2$ of 2 variable quadratic forms, so the Bravais group of the minimal stratum (which is dense open in $\mathcal{C}_+(\mathcal{Q}_n)$). In $\mathcal{Q}_2$ we choose the basis of the three matrices I_2, σ_3, σ_1:

$$\mathcal{Q}_2 \ni q = tI_2 + x\sigma_3 + y\sigma_1 = \begin{pmatrix} t+x & y \\ y & t-x \end{pmatrix}, \quad \det q = t^2 - x^2 - y^2 \qquad 2(32)$$

In the linear action $q \mapsto mqm^\top$ of $GL_2(Z)$ on $\mathcal{Q}_2$, the only invariant is $\det q$ since $\det m \det m^\top = 1$. So the effective action of the adjoint group $GL_2(Z)/Z_2$ is identical to the action of the Lorentz group (without time reversal) on the 3 dimensional space time (of coordinates t, x, y). This Lorentz group is $O(1,2) \sim S^{\pm}L_2(R)/Z_2$, where $S^{\pm}L_2(R)$ is the subgroup of $GL_2(R)$ containing the matrices of determinant ± 1. Remark that $\mathcal{C}_+(\mathcal{Q}_2)$ is the interior of the future light cone:

$$q > 0 \Leftrightarrow t > 0,\ t^2 - x^2 - y^2 > 0. \qquad 2(32')$$

Using §1-3 it is easy to find the Bravais classes of dimension 2. For example, from 2(29): $\mathcal{C}_+(\mathcal{Q}_2)^{pm} = \mathcal{C}_+(\mathcal{Q}_2)^{pmm}$ is the plane $(t, x, 0)$. Then we have to study the stabilizers of the points of this plane. We consider only those representing matrices $q > 0$, i.e. $-t < x < t$. The elements m of the stabilizers satisfy:

$$m = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \ ad - bc = \varepsilon = \pm 1; \quad m(tI + x\sigma_3)m^\top = \varepsilon(tI + x\sigma_3). \qquad 2(33)$$

We find that the integers a, b, c, d must be the solutions of the 3 equations (use $t+x > 0$, $t - x > 0$) :

$$(a - d\varepsilon) = 0, \quad t(b + c\varepsilon) - x(b - c\varepsilon) = 0, \quad -bc\varepsilon = 1 - a^2. \qquad 2(34)$$

If x/t is irrational, $b = c = 0$ so the only solutions are $m \in pmm$. From corollary 1-1 we deduce that pmm is a Bravais group. The second equation of 2(34) yields $b = -\varepsilon c(t+x)/(t-x)$ so either $b = c = 0$, or $0 < -bc\varepsilon$; from the third equation $a = 0\ (= d)$ and $b = -c\varepsilon$ which implies, from the second equation $x = 0$. So all points of $\mathcal{C}_+(\mathcal{Q}_2)$ in the plane $(t, x, 0)$ have pmm as stabiliser except those in the half-line $t > 0, x = y = 0$: those are invariant by the group generated by pmm and σ_1. That is the group $O_2(Z)$ of symmetry of the square; it is denoted by $p4m$ in [7]. We have proven in footnote 7 that it is a maximal finite subgroup of $GL_2(Z)$ so it is a Bravais group: the stabliser of all points $t > 0 = x = y$.

By a similar computation we find that cmm fixes all positive quadratic forms of the plane $(t, 0, y)$ and it is a Bravais group. Indeed

$$m(tI + x\sigma_1)m^\top = \varepsilon(tI + x\sigma_1),\ \varepsilon = 1 \Leftarrow b + c = 0,\ 2by + (a-d)t = 0,\ b^2 + ad = 1, \quad 2(35)$$

so when y/t is irrational, $b = c = 0$, $a = d$, i.e. $m = \pm I$. We now prove that there are only tree possible non generic lines in this plane. Indeed, to obtain 2(31) we had shown that the only rotation are of order 4,3,6, i.e. $\operatorname{tr} m = a + d = 0, -1, 1$. Assume $a + d = 0$ then from the 3rd equation of 2(35) $b^2 - a^2 = 1$ the only integer solutions are with $a = 0 = d$ which implies from the 2nd equation $y = 0$, so we find again the line $(t, 0, 0)$ (stabiliser $O_2(Z) = p4m$). Assume $a + d = \pm 1$; from the equation of 2(35) we obtain $4y^2 = t^2$ and for these 2 points (which are exchanged by pm) are fixed by a group generated by one rotation of the arithmetic class $p6$ and cmm. Their arithmetic class is called $p6m$ in the [7]. For instance for $x = 0 < t = -2y$ the two new solutions of 2(35) are the reflections of the arithmetic class cm:

$$\begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}. \qquad 2(36)$$

The two planes they fix are

$$2y + 1 \pm x = 0. \qquad 2(37)$$

To summarize we have established the existence in dimension $n = 2$ the existence of 5 Bravais classes which satisfy the partial order relation:

$$\begin{array}{ccccc} & & pmm & \longrightarrow & p4m \\ & \nearrow & & \nearrow & \\ p2 & \longrightarrow & cmm & \longrightarrow & p6m \end{array} \qquad 2(38)$$

From our results we are also able to choose a fundamental domain of the action of $GL_2(Z)$ on $\mathcal{C}_+(\mathcal{Q}_2)$. We arbitrarily choose one of the cone defined by three planes (each one fixed by a reflection), such that the inside have only points in the generic stratum $p2$. We choose arbitrarily:

$$P_1 : y = 0, \quad P_2 : x = 0, \quad P_3 : 2y + 1 - x = 0. \qquad 2(39)$$

The open face, carried by P_1 represents the Bravais class pmm while the two open faces carried by P_2 and P_3 represent the same set of lattices of cmm, but in two different bases; hence one of these 2 faces has to be removed in order to obtain a strict fundamental domain instead of its topological closure. The half lines (with $t > 0$) in the intersections $P_1 \cap P_2$, $P_2 \cap P_3$, $P_1 \cap P_3$, represent respectively the maximal Bavais classes pmm, cmm, and a generator of the closed cone $\overline{\mathcal{C}_+}(\mathcal{Q}_2)$, i.e. a rank one semi-positive quadratic forms in $\mathcal{Q}_2$, which can also be interpreted as one dimensional lattices. The fundamental domain we have chosen is that of the positive quadratic forms q_{ij} satisfying the relations:

$$q_{21} = q_{12}, \quad 0 < q_{22} \leq q_{11}, \quad 0 \leq -q_{12} \leq \frac{1}{2} q_{22}. \qquad 2(40)$$

That fundamental domain could have been obtained without an analysis into Bravais classes; indeed it was first given by Lagrange in 1773.

We draw figure 1-2 to show the the action of $GL_2(Z)$ on $\mathcal{C}_+(\mathcal{Q}_2)$. As we already pointed it out, this action is obtained as a restriction to the subgroup $GL_2(Z)$ of the orthochronous Lorentz group. To draw a two dimensional picture we make a stereographic projection from the tip of the future ligth cone $\mathcal{C}_+(\mathcal{Q}_2)$ onto its intersection with the plane H of equation $t = 1$ (see 2(32)):

$$0 < t, \qquad \xi^2 + \eta^2 \leq 1, \qquad \mathcal{C}_+(\mathcal{Q}_2) \ni (t, t\xi, t\eta) \mapsto \xi, \eta. \qquad 2(40')$$

The two dimensional space V_2 of the lattice is the "spinor space" the bijective map between non vanishing spinors up to sign, and the light vectors was emphasised by E. Cartan (e.g. [3]); explicity, when $n = 2$

$$V_2 \ni \pm v = \pm\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \leftrightarrow v \vee v = q(v) = \begin{pmatrix}\alpha^2 & \alpha\beta\\ \alpha\beta & \beta^2\end{pmatrix}. \qquad 2(41)$$

The v with integral components form a lattice $L \in V_2$; among them, those with relatively prime coordinates are called the *visible* vectors of L. They form one orbit of $GL_2(Z)$. In figure 1-2 the points of the circle $\xi^2 + \eta^2 = 1$, images of visible vectors ℓ are denoted by the coordinate of ℓ. Four among them have a label L, L', K, K':

$$\pm v = \pm\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \leftrightarrow V = (\xi, \eta)$$

$$\begin{aligned} &\pm\begin{pmatrix}1\\ 0\end{pmatrix} \leftrightarrow L = (1,0), \quad &&\pm\begin{pmatrix}0\\ 1\end{pmatrix} \leftrightarrow L' = (0,1), \\ &\pm\begin{pmatrix}1\\ 1\end{pmatrix} \leftrightarrow K = (0,1), \quad &&\pm\begin{pmatrix}1\\ -1\end{pmatrix} \leftrightarrow K' = (0,-1). \end{aligned} \qquad 2(42)$$

The reflection σ_3 acts on H as the symmetry through LL' and the reflection σ_1 acts on H as the symmetry through KK'. That explains the symmetry of the figure 1-2 which shows the strata of the actions of $GL_2(Z)$ on the disc $\xi^2 + \eta^2 \leq 1$. The computation of this figure yields another determination of the five Bravais classes.
We represent the $GL_2(Z)$-orbit of LL' and KK' by the full and the dotted lines respectively. Notice that the stabilizer of a $v \in V_2$ which is, up to a factor, an element of L, is infinite, indeed

$$v = \begin{pmatrix}\alpha\\ 0\end{pmatrix}, \quad GL_2(Z)_v = \{\pm\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}, \pm\begin{pmatrix}1 & b'\\ 0 & -1\end{pmatrix}, \; b, b' \in Z\}. \qquad 2(43)$$

So from the points of the unit circle of H corresponding to the points of $L < V_2$, an infinite number of lines is produced, and they can be proved to be alternatively dotted or full.
The dotted lines represent the q's of $\mathcal{C}_+(\mathcal{Q}_2)^{pmm}$ and the full lines those of $\mathcal{C}_+(\mathcal{Q}_2)^{cmm}$. So, except for their intersection points, they represent q's belonging to the Bravais classes pmm and cmm. The intersections of these lines have to correspond to maximal Bravais classes. Indeed LL' and KK' intersect at a point s which represents q's belonging to the Bravais class $p4m$ (square lattices) and this is also the case of all intersections of a dotted line and a full line (they are labelled s in the figure). The two points h of KK' are at the intersection of three dotted lines; so by $GL_2(Z)$ transformations we know that through each intersection of two full lines passes a third one.

We have labelled these triple points by h; they represents the hexagonal lattices, i.e. those belonging to the maximal Bravais class $p6m$.
The points of the interior of the disc and outside the lines, represent the generic lattices, those of the minimal Bravais class $p2$.

Notice that *in the interior of the disc*, every dotted line contains only one point s and each full line one s and two h's. Each triangle (whose sides are carried by two full lines and one dotted line, whose vertices are s, h and one point of the boundary circle) represent a fundamental domain of the $GL_2(Z)$ action. The Lagrange fundamental domain given in 2(39) corresponds to the triangle of vertices $L : (\xi = 1, \eta = 0)$, $s : (\xi = 0, \eta = 0)$, $h : (\xi = 0, \eta = -\frac{1}{2})$.

§**2-5.** *Selling method in two dimensions.*

In 1874 Selling published a paper [10] on the arithmetic classification of the quadratic forms (not necessarily positive) in 2 and 3 dimensions; it has introduced an elegant symmetry into the problem. We will give in next section the generalization to any dimension for positive forms made by Voronoï [12]; here we already use Voronoï notations.
Consider the quadratic form:

$$Q(\vec{x}) = \lambda_{01}x_1^2 + \lambda_{02}x_2^2 + \lambda_{12}(x_1 - x_2)^2 = (\vec{x}, q\vec{x}). \qquad 2(44)$$

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \qquad q = \begin{pmatrix} \lambda_{01} + \lambda_{12} & -\lambda_{12} \\ -\lambda_{12} & \lambda_{02} + \lambda_{12} \end{pmatrix}. \qquad 2(45)$$

$$\det(q) = \lambda_{01}\lambda_{02} + \lambda_{01}\lambda_{12} + \lambda_{02}\lambda_{12}. \qquad 2(46)$$

We make here the assumptions:

$$0 \leq i, j \leq 2,\ \lambda_{ij} = \lambda_{ji} \geq 0,\ \text{at most one}\ \lambda_{ij} = 0\,. \qquad 2(47)$$

That implies $q > 0$. The converse is not true, i.e. there are positive forms which do not satisfy 2(44) and 2(47); indeed those assumptions correspond to the large triangle $LL'K'$ in figure 1-2; since it contains a fundamental domain, every positive quadratic form of two variables can be transformed by $GL_2(Z)$ into a form satisfying 2(45), 2(47). It represents a lattice generated by the vectors $\vec{b}_1, \vec{b}_2$ which satisfy:

$$q_{11} = (\vec{b}_1, \vec{b}_1) = \lambda_{01} + \lambda_{12}, \quad q_{22} = (\vec{b}_2, \vec{b}_2) = \lambda_{02} + \lambda_{12}, \quad q_{12} = (\vec{b}_1, \vec{b}_2) = -\lambda_{12}. \quad 2(48)$$

Examples of the action of $m \in GL_2(Z)$ on q, $q \mapsto mqm^\top$:

$$m:\ r = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix},\ r^3 = I, \quad \lambda_{01} \to \lambda_{12}, \quad \lambda_{12} \to \lambda_{02}, \quad \lambda_{02} \to \lambda_{01}. \qquad 2(49)$$

$$m:\ s = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ s^2 = I,\ sr = r^{-1}s, \quad \lambda_{01} \leftrightarrow \lambda_{02}, \qquad 2(50)$$

so r, s generate the permutation group $\mathcal{S}_3$ of the λ's. With $-I_2$, which acts trivially on q, they generate the $GL_2(Z)$ subgroup $p6m \sim C_{6v}$.

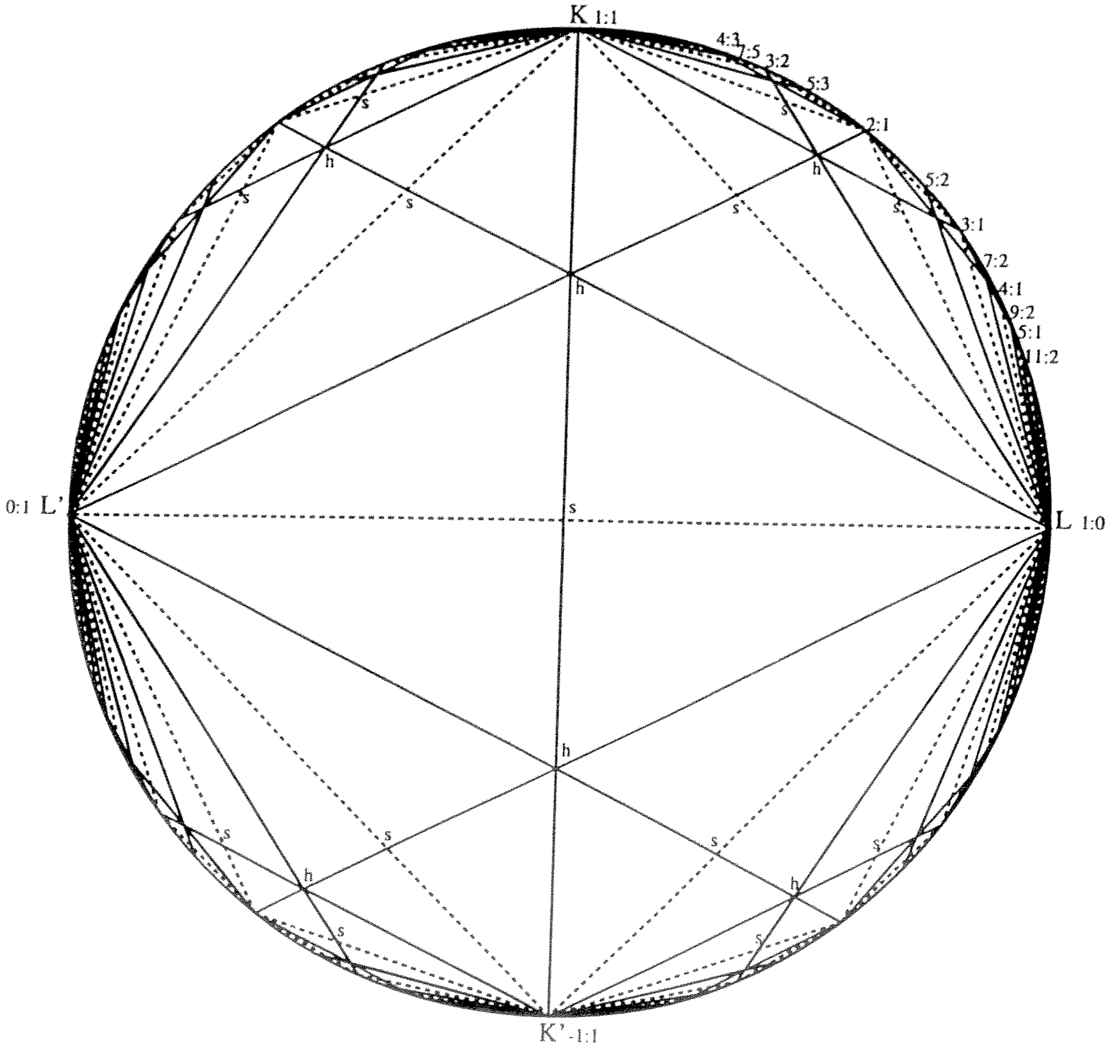


Figure 1-2. Stereographic projection of $\overline{\mathcal{C}_+}(\mathcal{Q}_2)$.

Each point inside the circle represents a ray of positive quadratic forms q's (i.e. defined up to a positive factor). The q's belonging to the Bravais classes *pmm*, *cmm*, *p4m*, *p6m* are represented respectively by the dotted lines, the full lines, the points s (intersections of a dotted line and a full line: square lattices), h (intersections of three full line: hexagonal lattices). The dense open set of the other points of the interior of the disc represents the generic q's; they belong to the minimal Bravais class $p2$. See the text for the meaning of the pairs $p : q$ of relatively prime integers. Each triangle represents the topological closure of a fundamental domain in the action of $GL_2(Z)$ on $\overline{\mathcal{C}_+}(\mathcal{Q}_2)$.

Selling showed that syntactic permutation symmetry and he made it obvious with the adjunction of the vector $\vec{b}_0$ defined by:

$$\vec{b}_0 + \vec{b}_1 + \vec{b}_2 = 0 \quad i,j = 0,1,2;\ i \neq j:\ (\vec{b}_i, \vec{b}_j) = -\lambda_{ij}; \quad (\vec{b}_i, \vec{b}_i) = \sum_{j \neq i} \lambda_{ij}. \qquad 2(51)$$

The quadratic forms invariant by any one of the three elements s, rs, r^2s of $GL_2(Z)$ (corresponding to the odd permutations of $\mathcal{S}_3$ and generating this group) are represented in figure 1-2 by the 3 full lines (partly) inside the triangle $LL'K'$; hence one can also see in the figure that the group $\mathcal{S}_3$ they generate is the symmetry group of that triangle. The sides of the triangle $LL'K'$ are dotted lines and they correpond to the three cases where one only of the three parameters λ_{ij} vanishes. So the method of Selling yields again the classification of Bravais classes. It just depends also on the number of parameters λ_{ij} which are equal. A short hand for listing the cases is to use triangular symbols whose vertices are labelled by $0, 1, 2$ and the sides by the λ_{ij} parameters.

first case: $\lambda_{01}\lambda_{02}\lambda_{12} \neq 0$:

 *p*2, *generic Bravais class*;

 *cmm*

 *p*6*m*

second case: one only of $\lambda_{01}, \lambda_{02}, \lambda_{12}$ vanishes [8]:

 *pmm*

 *p*4*m*.

There is an analogy with the "main example" of § 1-2 with the change of notation λ, μ, ν into $\lambda_{01}, \lambda_{02}, \lambda_{12}$. The difference is that while in § 1-2 the sum of two parameters is twice the distance between two of the 3 distinct points (which do not form necessarily a triangle), here it is the square of the lengths of the side of the (genuine) triangle defined by $\vec{b}_0 + \vec{b}_1 + \vec{b}_2 = 0$. For the two problems the symmetry group is the same; it is the Euclidean group in two dimension since our study of lattice symmetry generalizes immediately to Euclidean lattices (see § 2-1). For each problem the cases to consider are the same because they are determined by the syntactic symmetry of the three parameters and the effective symmetry groups of each case are identical with the difference that here the action is not effective, so one must enlarge the group with $-I$. For the lattices, if we had used the symmetry classification by Bravais crystallographic systems, we would have had also four strata only; the classification by 5 Bravais classes is more refined and distinguishes between the two Bravais classes *pmm* and *cmm* of the same Bravais crystallographic system *mm*. We will show in § 4 that the most refined classification of lattices in dimension 3 by group symmetry (with 14 Bravais classes) can be refined by using more invariant concepts. We shall introduce them in the next section.

[8] Using the $\mathcal{S}_3$ symmetry, one can choose $\lambda_{12} = 0$ so the quadratic form is diagonal and invariant by σ_3.

§ 3. Voronoï cells, Voronoï and Delone tessellations of lattices

This section deals with these topics for Euclidean lattices in arbitrary dimension n. As general reference we use the last Voronoï's paper in two parts [11], [12], and the monography in preparation with M. Senechal.

§ 3-1. *Voronoï paving. Corona and face vectors of Voronoï cells.*

Given an Euclidean lattice L in dimension n, we define the *Voronoï cell* $\mathcal{D}_L(o)$ of $o \in L$ as the topological closure of the set of points of the Euclidean space $\mathcal{E}_n$ which are nearer to o than to any other point ℓ of the lattice. Explicitly:

$$o \in L,\ \mathcal{D}_L(o) = \{x \in \mathcal{E}_n,\ \forall \ell \in L,\ d(x,o) \leq d(x,\ell)\}. \qquad 3(1)$$

The interior is defined by replacing $\leq$ with $<$ in 3(1). The points of the space common to at least two cells belong to their boundaries. The Voronoï cells of L form an orbit of the translation group of L; they also form a paving of $\mathcal{E}_n$. We recall that the points of the lattices and the middle between any pair of those points are symmetry centers of the lattice. So o is the symmetry center of $\mathcal{D}_L(o)$.

Let us take $o \in L$ as origin of the space. We will write simply $\mathcal{D}_L$ for the Voronoï cell of the origin of the lattice $L < R$. From 3(1) we can write:

$$\mathcal{D}_L = \{\vec{x} \in R^n,\ \forall \vec{\ell} \in L,\ N(\vec{x}) \leq N(\vec{x} - \vec{\ell})\}. \qquad 3(2)$$

Since the lattice L is a subgroup of R^n, if we consider the coset $\vec{x} + L \equiv \vec{x} - L = \{\vec{x} - \vec{\ell},\ \vec{\ell} \in L\}$, we can interpret 3(2) as:

$$\vec{x} \in \mathcal{D}_L \Leftrightarrow \vec{x} \textit{ is shortest in its coset } R^n/L. \qquad 3(3)$$

$$\left\{ \begin{array}{ll} \vec{x} \text{ unique shortest vector} & \vec{x} \in \text{interior of } \mathcal{D}_L \\ \vec{x} \text{ not unique shortest vector} & \vec{x} \in \partial\mathcal{D}_L \text{ the boundary} \end{array} \right\} \qquad 3(4)$$

so $\mathcal{D}$ is a fundamental domain of the translation group L; its volume is by definition that of the lattice:

$$\mathrm{vol}\mathcal{D}_L = \mathrm{vol}(L). \qquad 3(5)$$

We can also translate 3(2) into:

$$\mathcal{D}_L = \{\vec{x} \in R^n,\ \forall \vec{\ell} \in L,\ (\vec{x}, \vec{\ell}) \leq \frac{1}{2}(\vec{\ell}, \vec{\ell})\}. \qquad 3(6)$$

That shows that $\mathcal{D}_L$ is the intersection of the half-spaces containing o and bounded by the hyperplanes bisectors of the segments $o\ell$, $\ell \in L$. That implies that $\mathcal{D}_L$ is convex. Since $\mathcal{D}_L$ has been defined in terms of norm or scalar product of vectors, the symmetry group P_L^z of the lattice is symmetry group of the Voronoï cell $\mathcal{D}_L$.

Corona vectors. We say that $0 \neq \vec{c} \in L$ is a corona vector if the Voronoï cell centered at $c = o + \vec{c} \neq o$ has common points with the Voronoï cell at the origin; then $c' = o + \frac{1}{2}\vec{c}$, the middle of oc is one of these common points; moreover

c' is the symmetry center of $\mathcal{D}_L(o) \cap \mathcal{D}_L(c)$.

Denoting by $2L$ the lattice whose vectors are 2ℓ, $\ell \in L$ and denoting $\mathcal{D}_{2L}$ as $2\mathcal{D}_L$, we can give two equivalent definitions of C, the set of corona vectors of L:

$$C = \{\vec{c} \in L,\ \mathcal{D}_L(o) \cap \mathcal{D}_L(c) \neq \emptyset\} \Leftrightarrow C = L \cap \partial 2\mathcal{D}_L. \qquad 3(7)$$

From 3(3) we deduce the lemma

Lemma 3-1. *The corona vectors are the shortest lattice vectors in their $L/2L$ cosets,*

Equivalently:

$$\vec{c} \in C \Leftrightarrow \forall 0 \leq \vec{\ell} \in L, \quad N(\vec{c} + 2\vec{\ell}) - N(\vec{c}) \geq 0 \Leftrightarrow \vec{c}.\vec{\ell} + N(\vec{\ell}) \geq 0. \qquad 3(8)$$

Remark $\vec{c} \in C \Rightarrow -\vec{c} \in C$. So, for the number of corona vectors, we have the inequality:

$$2(2^n - 1) \leq |C|. \qquad 3(9)$$

In 3(8), let us replace 2 by $m > 2$:

$$\vec{c} \in C, m > 2, \quad \forall 0 \leq \vec{\ell} \in L, \quad m^{-1}(N(\vec{c} + m\vec{\ell}) - N(\vec{c})) =$$

$$= 2(\vec{c}.\vec{\ell} + N(\vec{\ell})) + (m-2)N(\vec{\ell}) > 0. \qquad 3(10)$$

This shows that a corona vector is **the** shortest vector in its coset L/mL, $m > 2$. So for $m = 3$ and $\vec{c} \neq 0$, we obtain:

$$|C| \leq 3^n - 1. \qquad 3(11)$$

That proves that the number of supporting hyperplanes of $\partial\mathcal{D}_L$ is finite. Moreover these hyperplanes cannot be all parallel to a direction since vol$\mathcal{D}_L$ finite. So

$\mathcal{D}_L$ is a polytope of center o.

Face vectors. When the bisector plane of the corona vector $\vec{c}$ supports a face of dimension $n-1$ of $\mathcal{D}_L$, we say that $\vec{c}$ is a face vector. We denote by F the set of face vectors:

$$F = \{\vec{f} \in C, \quad \dim(\mathcal{D}_L \cap \mathcal{D}_L(f)) = n - 1\} \subset C. \qquad 3(12)$$

The equation of the plane bisector of a lattice vector $\vec{f}$ is $(\vec{f}, \vec{x}) = \frac{1}{2}N(\vec{f})$; so we can give a definition of $\mathcal{D}_L$ knowing F:

$$\mathcal{D}_L = \{\vec{x},\ \forall \vec{f} \in F,\ |\vec{f}.\vec{x})| \leq \frac{1}{2}N(\vec{f})\}. \qquad 3(13)$$

Theorem 3-1 (Voronoï). *A lattice vector $\vec{f}$ is a face vector if and only if $\pm\vec{f}$ are strictly shorter than the other vectors of their $L/2L$ coset.*

Proof of "if". Assume that in the same $L/2L$ coset there are other corona vectors $\pm\vec{c}$, $N(\vec{c}) = N(\vec{f})$; so $\vec{\ell} = \frac{1}{2}(\vec{f} + \vec{c}) \in L$. Then one computes $2(\vec{f}, \vec{\ell}) = N(\vec{f}) + (\vec{f}, \vec{c}) = 2N(\vec{\ell})$; comparing with equation 3(13) that means that $\frac{1}{2}\vec{f}$ is in the face of center $\frac{1}{2}c$. With $N(\vec{f}) = N(\vec{c})$, that implies $\vec{f} = \vec{c}$.

Proof of "only if". Assume that $\pm c$ are stricly shorter in their $L/2L$ coset and that the corona vector is not a face vector: $\frac{1}{2}c$ belongs to the boundary of a face of center

$\frac{1}{2}f$; so $(f,c) = N(f)$. The middle of the vector $c' = 2f - c$ is in the same face (it is the symmetric of $\frac{1}{2}c$ through the face center); so c' is a corona vector in the same $L/2L$ coset as c. However $N(c') = N(c) + 4N(f) - 4(f,c) = N(c)$ which contradicts the hypothesis.

This theorem proves that the number of faces is $\leq 2(2^n - 1)$. A lower bound is $2n$; indeed, at least n pairs of parallel hyperplanes are necessary to envelop a bounded domain. Gathering these results and those of 3(9) and 3(11):

$$2n \leq |F| \leq 2(2^n - 1) \leq |C| \leq 3^n - 1. \qquad 3(14)$$

We will prove the following equivalences:

$$|F| = 2(2^n - 1) \Leftrightarrow |C| = 2(2^n - 1); \quad 2n = |F| \Leftrightarrow |C| = 3^n - 1. \qquad 3(15)$$

From the theorem 3-1, if $|F|$ is maximum, $F = C$ and conversely. In dimension n, remark that if a Voronoï cell has $2n$ faces, each hyperplane of a parallel pair has to be perpendicular to the hyperplanes of the other pairs. That means that one can take as basis n orthogonal face vectors; in that basis the quadratic form $q(L)$ is diagonal. If its elements are all different, the Bravais group $P_L^z \sim Z_2^n$ contains all diagonal matrices with elements ± 1; its Bravais class is usually called "orthorhombic P-lattice". When the multiplicites of equal elements in the diagonal $q(L)$ are n_i, the Bravais group is the direct product $\times_i O_{n_i}(Z)$. As we have seen, in the particular case where $q(L)$ is proportional to the unit matrix, the Bravais group is $O_n(Z)$ and the Voronoï cell is an n-dimensional cube. For all the cases in which $|F| = 2n$, the center of all d-dimensional facets is the middle of a corona vector; so $|C| = 3^n - 1$.
For the dimensions 2,3, 3(14) reads:

$$n = 2,\ 4 \leq |F| \leq 6 \leq |C| \leq 8; \qquad n = 3,\ 6 \leq |F| \leq 14 \leq |C| \leq 26. \qquad 3(15')$$

§ **3-2.** *Delone tessellations. Primitive lattices.*

A vertex of a Voronoï cell is at the intersection of at least n bisector hyperplanes corresponding to (at least) $n+1$ points of L. Those form the L subset

$$L \supset \mathcal{P}_v = \{\ell \in L,\ v \text{ is a vertex of } \mathcal{D}_L(\ell)\}. \qquad 3(16)$$

The vertex v is equidistant from all points of $\mathcal{P}_v$; in other words: all points of $\mathcal{P}_v$ are on a sphere of center v.
Definition: The Delone cell[9] $\Delta_L(v)$ is the convex hull of $\mathcal{P}_v$.
Since they are on a sphere, the points of $\mathcal{P}_v$ are the vertices of $\Delta_L(v)$ and this polytope is inscribed in a sphere of center v. We leave to the reader to prove that the Delone cells of L form a tessellation of the space $\mathcal{E}_n$ and of the following result:
the Voronoï and the Delone tessellations of the lattice L are dual of each other; i.e. for every integer d $0 \leq d \leq n$, to every d-dimensional facet Φ_d of the Delone tessellation corresponds a unique $n-d$-dimensional facet F_{n-d} of the Voronoï tessellation and

[9] Voronoï [11] has defined these cells and began to study them for arbitrary lattices. They have been studied more thoroughly by Delone.

$\Phi_d \perp F_{n-d}$; and conversely: to every d-dimensional facet F_d of the Voronoï tessellation corresponds a unique $n-d$-dimensional orthogonal facet Φ_{n-d} of the Delone tessellation.

In the Euclidean space $\mathcal{E}_n$, a sphere is defined by $n+1$ points in general position (so they are vertices of a simplex). If more than $n+1$ points are on a sphere they are not metrically in general position.

Definition: *A lattice L is primitive* [10] if, and only if, every vertex of its Voronoï tessellation belongs to exactly $n+1$ cells or, equivalently, if, and only if, every one of its Delone cells is a simplex.

Lemma 3-2a. *In the Voronoï tesselation of a primitive lattice, every d-dimensional facet F_d belongs to exactly $n+1-d$ adjacent Voronoï cells.*

Indeed every vertex of this facet is the intersection of n bissector hyperplanes and this facet is supported by the intersection of a subset of $n-d$ hyperplanes; they separate $n+1-d$ adjacent cells.

The Voronoï cells belonging to the Voronoï tessellation of a primitive lattice set are called *primitive Voronoï cells.* There is a necessary condition to be satisfied by primitive Voronoï cells.

Lemma 3-2b. *An n-dimensional primitive cell must have* $2(2^n-1)$ *faces (or, equivalently, $F = C$).*

If this condition is not satified there is a corona vector $\vec{c}$ which is not a face vector. For instance if $\frac{1}{2}\vec{c}$ is the center of a d-facet ($d < n-1$) which is the intersection $\mathcal{D}_L(c) \cap \mathcal{D}_L(o)$; it contains at least $d+1$ vertices. At any one of them, there is a cell whose intersection with $\mathcal{D}_L(o)$ has dimension $d < n-1$, so there are more than n cells meeting $\mathcal{D}_L(o)$ at this vertex v; so the cells are not primitive since more than $n+1$ meet at v. That ends the proof of the lemma.

The set of d-faces, $0 \leq d < n$, of a lattice Vororonoï tesselation can be decomposed into orbits of the translations. Let us study the intersection of these orbits with a given Voronoï cell $\mathcal{D}_L(o)$. Let F_d be one of its d-face; we have seen in the proof of lemma 3-2a that it is the intersection of $n-d$ faces; let $\{\vec{\ell}_\alpha\}$, $1 \leq \alpha \leq n-d$ the set of their face vectors; they give the centers $o + \vec{\ell}_\alpha$ of the $n-d$ other Voronoï cells which share this d-face with $\mathcal{D}_L(o)$. Each translation $-\vec{\ell}_\alpha$ transforms $\mathcal{D}_L(o+\vec{\ell}_\alpha)$ into $\mathcal{D}_L(o)$ and therefore F_d into $\vec{\ell}_\alpha + F_d$, another d-face of the Voronoï cell $D_L(o)$. That proves the

Lemma II 3-2c. *A primitive Voronoï cell contains exactly $n+1-d$ d-faces which can be obtained form each other by a translation of L.*

We can now study the orbits of the group of translations and symmetry through points and their intersections with D_L. We will show that, except for $d = n-1$, the orbits of this group split into two orbits of translations. Indeed consider a d-facet F_d of $\mathcal{D}_L$ and F'_d its symmetric throught the origin. If they were on the same translation orbit, there would exists a translation $-\vec{\ell}$ transforming F_d into F'_d; but we have shown

[10] One could have said generic, but Voronoï used the word primitive when he introduced this notion for lattices. Moreover, we are mainly interested by Euclidean lattices; for them we have already defined the generic ones: those with the smallest possible symmetry. The primitive and the generic lattices form two open dense sets of $\mathcal{L}_n$ which do not coincide.

in the proof of the preceeding lemma that $\vec{\ell}$ is a face vector; so this is possible only if $d = n - 1$. When $d < n - 1$, F_d and F'_d belong to two distinct translation orbits. We will call *family of d-faces* the set of d-faces of D_L on the same orbit of the translation and symmetry through points group of the lattice. So we have proven

Lemma II 3-2d. *In a primitive Voronoï cell, the number of d-faces, $0 \leq d < n-1$, is a multiple of $2(n+1-d)$, which is the number of d-faces in the same family.*

In the particular case $d = 0$ that proof shows that, for a primitive lattice, the set Υ of the vertices of the Voronoï tesselation forms a crystal of lattice L with $|V|/(n+1)$ points by fundamental domain. The Delone tesselation is another aspect of the same crystal structure. The set Υ can be decomposed into L-orbits. Let $\Upsilon \xrightarrow{\pi} \Upsilon|L$ the canonical projection on the orbit space. A section [11] $\Upsilon|L \xrightarrow{\sigma} \Upsilon$ is a choice of one vertex (or one Delone cell) per orbit. The total volume of these chosen Delone cells must be equal to the volume of the unit cell of the lattice

$$\sum_{v_\alpha \in \mathrm{Im}\,\sigma} \mathrm{vol}\,\Delta(v_\alpha) = |\det(L)| = \mathrm{vol}\,\mathcal{D}_L. \qquad 3(17)$$

Any vertex of the Voronoï cell of a primitive lattice L belongs to exactly n faces; their face vectors are linearly independent so they form a basis of the space. Do they form a basis of the lattice L? Not necessarily: they may generate only a sublattice L'. So we define:

Definition: A primitive lattice or a Voronoï cell are called principal if for each vertex of the cell, the face vectors of the n faces meeting at this vertex form a basis of the lattice.

That definition implies an important property of the Delone cells of principal primitive lattices: they have all the same volume. Indeed, they are simplexes defined by the n edges of their vertex o, i.e. the n face vectors $\vec{f_\alpha}$ forming a basis of the lattice; so the volume [12] of each Delone cell is $(n!)^{-1} \det f_\alpha = (n!)^{-1} \det L$.

Lemma 3-2e. *A principal primitive Voronoï cell has $(n+1)!$ vertices.*

When all Delone cells have the same volume, we can replace the sum in the left hand side of equation 3(17) by the product by $|V|/(n+1)$, the number of vertices by fundamental domain in the crystal Υ of Delone cells of a primitive lattice. That equation becomes $|V| = (n+1)(\det L)/\,\mathrm{vol}\,\Delta(v) = (n+1)n!$.

Corollary 3-2e. *A principal primitive Voronoï cell has $(n+1)!\,n/2$ edges.*

Indeed, in a primitive lattice, n edges meet at each vertex and each edge has two vertices.

[11] It has to satisfy $\sigma \circ \pi = I_\Upsilon$, the identity map on Υ.

[12] Here is a proof of the formula given the volume of a n-dimensional simplex defined by a vertex at the origin and n vectors. First assume that these vectors are mutually orthogonal and have same length r. The volume is of the form $K_n r^n = \int_0^r K_{n-1}(d\rho^{n-1}/d\rho)(r-\rho)d\rho$; so $K_n = n^{-1}K_{n-1}$, i.e. for vectors of unit length, the volume of this simplex is $K_n = (n!)^{-1}$. The group $GL_n(R)$ acts transitively on the bases of the vector space: the matrix which transforms an orthonormal basis into the basis $\{f_i\}$ has for determinant $\det f_i$ so the volume of the simplex is $(n!)^{-1} \det f_i$.

Voronoï found that there are non principal primitive cells only for $n > 4$ and that there exist some for $n = 5$; they have one family less of vertices, that is $|V| = 708$ instead of 720.

We denote by $N_d(n)$ the number of d-faces of the Voronoï cell of a n dimensional primitive lattice. They satisfy the relation imposed by the Euler-Poincaré characteristic:

$$\sum_{0 \le d \le n-1} N_d(n) = 1 + (-1)^n. \tag{3(18)}$$

With our knowledge of $N_d(n)$ for $d = 0, 1, n-1$ we know all these numbers up to $n = 4$ for primitive cells:

$$N_0(2) = N_1(2) = 6, \quad N_0(3) = 24, \ N_1(3) = 36, \ N_2(3) = 14;$$
$$N_0(4) = 120, \ N_1(4) = 240, \ N_2(4) = 150, \ N_3(4) = 30. \tag{3(19)}$$

§**3-3.** *Voronoï cells in two dimensions.*

First we notice that for the quadratic form q of 2(45), when the 3 Selling parameters are strictly positive, the six vectors $\pm b_i$, $i = 0, 1, 2$ are face vectors. Indeed 2(44) shows that their norms are sums of two λ's and the norm of any other vector is a linear function of the 3 lambda's with some (or all) coefficients strictly larger. So the Voronoï cell [13] is a centrosymmetric hexagon.
From lemma 3-2d we remark that in dimension 2, all vertices belong to the same family; by an elementary geometry proof that shows that their 6 vectors have same norm, so *a two dimensional Voronoï cell is inscribed in a circle* [14].

We will call $\pm v_i$ the 6 vertices. To precise the notations we indicate their incidence into the edges (that we denote by their face vector):

$$\vec{b}_1, -\vec{v}_2, -\vec{b}_0, \vec{v}_1, \vec{b}_2, -\vec{v}_0, -\vec{b}_1, \vec{v}_2, \vec{b}_0, -\vec{v}_1, -\vec{b}_2, \vec{v}_0, \vec{b}_1. \tag{3(20)}$$

The equation of the support line of the face $\vec{b}_i$ is:

$$(\vec{b}_i, q(\vec{b}_i - 2\vec{x})) = 0. \tag{3(21)}$$

We obtain for instance the coordinates of v_0 by changing $\vec{x}$ into $\vec{v}_0$ in the two equations written for $\vec{b}_1$ and $\vec{b}_2$. Denoting $\det(q)$ computed in 2(46) by D, we find for the coordinates:

$$v_1 = \frac{1}{2}\begin{pmatrix} 1 - \lambda_{02}\lambda_{12}/D \\ 1 + \lambda_{01}\lambda_{12}/D \end{pmatrix}, \ v_2 = \frac{1}{2}\begin{pmatrix} -1 - \lambda_{02}\lambda_{12}/D \\ -1 + \lambda_{01}\lambda_{12}/D \end{pmatrix}, \ v_3 = \frac{1}{2}\begin{pmatrix} 1 - \lambda_{02}\lambda_{12}/D \\ -1 + \lambda_{01}\lambda_{12}/D \end{pmatrix}. \tag{3(22)}$$

Let us denote by e_i the square length of the Voronoï cell edges orthogonal to the face vector $\vec{b}_i$; we find

$$e_0 = N(\vec{v}_1 + v_2) = \lambda_{12}(1 - \lambda_{01}\lambda_{02}/D), \quad e_1 = N(\vec{v}_0 + v_2) = \lambda_{02}(1 - \lambda_{01}\lambda_{12}/D),$$

[13] In dimension 2, the nature of the cells was first determined by Dirichlet (Collected works of Lejeune-Dirichlet t.II, p. 41). That is why we use the symbol $\mathcal{D}$ for them.

[14] Indeed this is also true for rectangles.

$$e_2 = N(\vec{v}_0 + v_1) = \lambda_{01}(1 - \lambda_{02}\lambda_{12}/D), \qquad 3(23)$$

Thus e_i is proportional to λ_{jk}, where i, j, k is a permutation of 0,1,2. So when one of the λ's vanishes, the corresponding edges shrink to zero and the Voronoï cell becomes a rectangle. Indeed, from the syntactic symmetry, we can choose $\lambda_{12} = 0 = e_0$ and $(\vec{b}_1, \vec{b}_2) = 0$, i.e. the face vectors of the non vanishing faces are orthogonal; notice that q is diagonal.

Finally we verify that the six vertices are at the same distance from the origin; indeed

$$N(\vec{v}_i) = \frac{1}{4}(\lambda_{12} + \lambda_{01} + \lambda_{02} - \lambda_{12}\lambda_{01}\lambda_{02}D^{-1}). \qquad 3(24)$$

This is still true when one of the λ's vanishes.

§ **3-4.** *Voronoï generalisation of Selling parameters.*

In [12] Voronoï study the $N = n(n+1)$ parameter family of quadratic forms as a generalisation of 2(44):

$$1 \le i, j \le n, \quad Q(\vec{x}) = \sum_i \lambda_{0i} x_i^2 + \sum_{i<j} \lambda_{ij}(x_i - x_j)^2, \quad \lambda_{0i} \ge 0, \lambda_{ij} \ge 0. \qquad 3(25)$$

The basis vectors $\vec{b}_i$ and the vector $\vec{b}_0$ defined by

$$0 \le \alpha, \beta \le n, \quad \sum_\alpha \vec{b}_\alpha = 0, \qquad 3(26)$$

satisfy

$$(\vec{b}_\alpha, \vec{b}_\alpha) = \sum_{\beta \ne \alpha} \lambda_{\alpha\beta}, \quad \alpha \ne \beta, \; (\vec{b}_\alpha, \vec{b}_\beta) = -\lambda_{\alpha\beta}. \qquad 3(27)$$

Let us consider the vectors $\pm\vec{b}_{\mathcal{K}}$ defined by:

$$\mathcal{N} = \{1, 2, 3, \ldots, n\}, \; \emptyset \ne \mathcal{K} \subseteq \mathcal{N}, \quad \vec{b}_{\mathcal{K}} = \sum_{i \in \mathcal{K}} \vec{b}_i. \qquad 3(28)$$

When all the parameters λ's are strictly positive, a simple generalisation of the argument we gave for $n = 2$, proves that the $2(2^n - 1)$ vectors $\pm\vec{b}_{\mathcal{K}}$ are the face vectors, so the Voronoï cell of the lattice defined by q is primitive. Voronoï showed that for $n = 4$ (and a fortiori for $n > 4$), there are positive quadratic forms which cannot be written in the form 3(25) by a$GL_n(Z)$ transformation. He called those which can be written as 3(25) with all $\lambda_{ij} > 0$, primitive of the first type; he showed that there are two other primitive types for $n = 4$.

In the literature, one calls *zone* a set of parallel edges of a Voronoï cell; for primitive cells it is one or a union of families of $2n$ edges (see lemma 3-2d). Voronoï [12] extended to dimension n what we showed in the previous subsection for dimension 2, i.e. the edges of a family shrink to zero when one of the parameters $\lambda_{ij} \to 0$. That is generally called *zone contraction*; zone contraction may be made on several zones successively up to the step when it becomes impossible (e.g. the cell collapses). Voronoï conjectured that any cell could be obtained from a primitive one by this method, but he added he could not prove it. Indeed there exists a counter-example already for $n = 4$. Let us just remark here

Lemma 3-4. *It is not possible that the n λ's containing a fixed index are all zero.*

Let α be this fixed index. Then 3(27) shows that $N(\vec{b}_\alpha) = 0$. So the vectors $\vec{b}$'s span only a $n-1$-dimensional space and the quadratic form q is degenerate: $\det(q)0$.

It was shown by Selling that every positive quadratic form $\in \mathcal{Q}_3$ can be transformed by $GL_3(Z)$ in the form 3(25); Voronoï proved that is not true for $n = 4$ and he constructed the three combinatorial types of Voronoï cells existing in dimension 4. He called the cells of the quadratic forms of 3(25) with all $\lambda > 0$, in any dimension, the primitive cells of the first type.

§ 4. Classification of 3 dimensional lattices

§ 4-1. *The five types of Voronoï cells in dimension 3.*

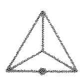
We recall what we already know on the primitive cell for the particular case $n = 3$ (see 3(19)). It has 24 vertices, 36 edges (three meeting at each vertex) and 14 faces. The faces have a symmetry center; s of them have 4 edges and h others have 6 edges. Since an edge is common to two faces,

$$4s + 6h = 72, \quad s + h = 14, \Rightarrow s = 6, \; h = 8. \tag{4(1)}$$

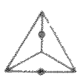
Delone [4],[5] introduced a symbolic representation of the four values $0, 1, 2, 3$ of the indices in $3(26-27)$ as the vertices of a tetrahedron and of the six λ_{ij} as the edges. The tetrahedron has the same symmetry $\mathcal{S}_4$ as the syntactic symmetry of the parameters. For this group, the 6 edges form one orbit, the 15 pairs of edges form 2 orbits of 12 and 3 elements which correspond to pairs of edges with and without a common vertex, respectively; the 20 triplets of edges form 3 orbits, one of the 4 triangles of the face, another of 4 elements (the three edges have a common vertex), the last one of 12 elements (the two possible paths of 3 edges, connecting the two vertices of an edge).

As we explained in the preceeding section, the different types of Voronoï cells are obtained by zone contraction, i.e. by distributing 1,2,3 zeros on the edges of the Delone symbol. It is not possible to put 4 zeroes because any quadratic form in $\mathcal{Q}_3$ with only two λ's has a zero determinant. For the same reason, lemma 3-4 forbids us to put 3 zeroes on 3 edges with a common vertex. From our count of orbits it seems that we have five possibilities; but we will see that the two orbits of three vanishing λ's yield the same type of cell.

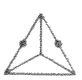
Let us list the different possibilities:



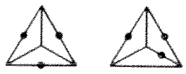
$\lambda_{12} = 0$, all choices are equivalent



$\lambda_{12} = 0$, $\lambda_{23} = 0$, the 2 edges have no common vertex.

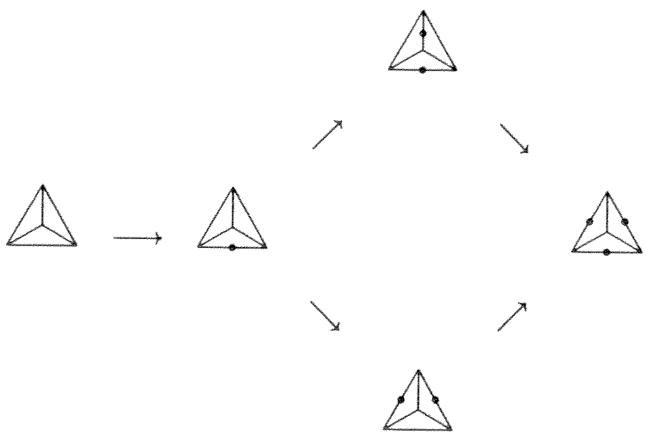


$\lambda_{13} = 0$, $\lambda_{23} = 0$, the quadratic form is a direct sum of a block 2×2 with three parameters (correspond to hexagon) and one diagonal parameter fixing the height of the hexagonal prism.

 $\lambda_{13} = 0$, $\lambda_{23} = 0$, and either $\lambda_{12} = 0$ or $\lambda_{02} = 0$, the quadratic form is again a direct sum of a block 2×2 but with two parameters only; so it yields a rectangle (see §2-3) and both cases yield a rectangular parallelpipede.

With the primitive cell, we have obtained five different combinatorial types of Voronoï cells. The number of non zero parameters for each type of cells is also the dimension of their domain in $\mathcal{C}_+(\mathcal{Q}_2)$.

The map of successive zone contractions is:



4(2)

The table 4-1 gives all relevant information on the cells types.

Let us precise the position of the middle of the corona vectors which are not face vectors for the different lines of table 4-1:
line 2; the middle of the 4 edges common to two hexagons (the 4 hexagons form a belt);
line 3: the 6 vertices of valence 4;
line 4: the middle of the edges of the two hexagonal faces: $20 - 8 = 2 \times 6$;
line 5: the 12 middle of edges and the eight vertices: $26 - 6 = 12 + 8$.
The line 2 cell has a belt of 4 hexagons; on each side of the belt four rhombohedras which meet at a valence 4 vertex. The line 3 cell is called dodecarhombohedra for its 12 faces are rhombohedras.

§**4-2.** *The 14 Bravais classes and the 7 Bravais crystallographic systems.*

We follow here the same strategy as for dimension 2. The proof of crystallographic restriction for the order of rotation to 1,2,3,4,6 is the same. These five kinds of rotations and their product by $-I$ give the 10 "geometric elements" which are listed in [7] under the notation:

$$1,\ 2,\ 3,\ 4,\ 6, (-I) \equiv \bar{1}, (\bar{2}) \equiv m,\ \bar{3},\ \bar{4},\ \bar{6}. \qquad 4(3)$$

(Caution: $\bar{3}$ is of order 6). These 10 geometric elements generate the 32 geometric classes, i.e. the 32 conjugacy classes of subgroups of O_3 satisfying the crystallographic restriction; their list was established independently by Frankenheim in 1826 and Hessel

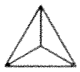
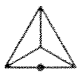
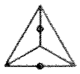
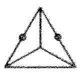
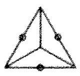
Delone	dim	6 - 4	$\|F\|$	$\|E\|$	$\|V\|$	3 - 4	$\|C\|$	L/2L
	6	8 - 6	14	36	24	24 - 0	14	2 2 2 2 2 2 2
	5	4 - 8	12	28	18	16 - 2	16	2 2 2 2 2 2 4
	4	0 - 12	12	24	14	8 - 6	18	2 2 2 2 2 2 6
	4	2 - 6	8	18	12	12 - 0	20	2 2 2 2 4 4 4
	3	0 - 6	6	12	8	8 - 0	26	2 2 2 4 4 4 8

Table 4-1. Three dimensional Voronoï cells.
Column 1 gives the Delone symbol. Column 2: the dimension of their domain in $\mathcal{C}_+(\mathcal{Q}_2)$. Columns 3, 4: the number of hexagonal and 4-edges faces and $|F|$ the total number of faces. Column 5: $|E|$ the number of edges. Column 6, 7: $|V|$, the total number of vertices and the number of those of valence 3 and 4. Column 8: $|C|$ the number of corona vectors. Column 9: the number of shortest vectors in each of the 7 non trivial $L/2L$ cosets.

1830 (before the invention of the word "group" by Galois). Among them 11 groups contain $-I$ and are therefore candidate to be stabilizers of Bravais crystallographic systems. Among those 11 groups we shall obtain from our study of Bravais classes, the seven of them which are holohedries: they define the 7 Bravais crystallographic systems. We list them here in both notations, Schönflies and [7]:

$$C_i = \bar{1},\ C_{2h} = 2/m,\ D_{2h} = mmm,\ D_{4h} = 4/mmm,$$

$$D_{3d} = \bar{3}m,\ D_{6h} = 6/mmm,\ O_h = m\bar{3}m. \qquad 4(4)$$

The next step in our strategy is to list the "arithmetic elements" that is the conjugacy classes of $GL_3(Z)$ which are mapped by ϕ (defined after the proof of lemma 2-2) into those of O_3. We know from §2-4 that there are two classes of reflections (denoted by [7] as for $n = 2$ but with upper case) Pm, Cm. Multiplying the integral matrices by $-I$, this implies the same dinstinction between $P2$, $C2$. We shall prove below the distinction between $P3$ and $R3$ and therefore $P\bar{3}$ and $R\bar{3}$; we will leave to the reader the corresponding study of the elements of order 4.

$$\begin{array}{cccccccccc} P1 & P2 & P3 & P4 & P6 & P\bar{1} & P\bar{m} & P\bar{3} & P\bar{4} & P\bar{6} \\ & C2 & R3 & I4 & & & C\bar{m} & R\bar{3} & I\bar{4} & P\bar{6} \end{array} \qquad 4(5)$$

Table 4-2. The sixteen arithmetic elements in 3 dimensions.

We continue our strategy for the determination of Bravais classes. Here we first deal with

The maximal Bravais classes

We have proven in § 2-3 that three maximal Bravais classes are the one whose holohedry is $O_3(Z) < O_3$, which is the symmetry group of the cube. The three lattices defined in 2(23),2(25),2(26) have the same holohedry but their Bravais groups are non conjugate. These three groups are denoted in [7] by $Pm\bar{3}m \equiv O_3(Z)$, $Fm\bar{3}m$, $Im\bar{3}m$. Their Bravais domains are 1 dimensional (in $\mathcal{C}^+(\mathcal{Q}_3)$). Indeed one can choose such bases that the set of their quadratic forms are q_P, q_F, q_I defined by [15]:

$$J_{ij} = 1,\ t > 0,\ q(b) = I + b(J - I), \quad q_P = tI = tq(0),\ q_F = tq(\frac{1}{2}),\ q_I = tq(-\frac{1}{3}). \quad 4(6)$$

These 3 Bravais classes $Pm\bar{3}m$, $Fm\bar{3}m$, $Im\bar{3}m$ are mapped by φ of 2(16) on the crytallographic system [16] called *cubic*.

The intersection of the stabilizers of these 3 quadratic form is a stabilizer (lemma 1-2); it fixes the 2-parameter quadratic forms $tq(b)$ whose positivity conditions are $-\frac{1}{2} < b < 1$. This group $R = \langle -I, r, m\rangle$ is generated by the matrices [17]:

$$-I_3,\ r = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ m = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad -\frac{1}{2} < b < 1,\ q_R = tq(b) = \mathcal{C}_+(\mathcal{Q}_3)^R. \quad 4(7)$$

R is a maximal subgroup subgroup of $O_3(Z)$; in it, its index is 4. It is therefore a Bravais group; its Bravais class is denoted by $R\bar{3}m$.

The conjugation of the matrices r, m by the matrix $u \in GL_3(Z)$ gives:

$$u = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad r' = uru^{-1} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix}, \quad m' = umu^{-1} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & -1 & 1 \end{pmatrix}. \quad 4(8)$$

That shows that this representation of the group R is reducible: indeed the first vector of the basis is invariant. However the matrices of the group are in upper triangular form for two diagonal blocks of dimensions 1 and 2.

By a conjugation in $GL_3(Q)$ the matrices r' and m' could be completely decomposed into a direct sum of two integral representations of R (a one dimensional one $\oplus$ a faithful 2-dimensional one) but using arguments similar to those which gave 2(30), one can show that it is impossible to change by a conjugation in $GL_3(Z)$ the value mod2 of the second and third elements of the first line of r' and m'. So this integral reducible representation of R is indecomposable by $GL_3(Z)$.

To construct the two other arithmetic classes mapped by ϕ to the same geometric class $\bar{3}m$ we define the matrices $\hat{r}'$, $\hat{m}'$ which are a decomposable representation of r', m'

[15] The generalisation to dimension n is trivial: replace 3 by n at the end of 4(6).

[16] In dimension 3, for the five Bravais crystallographic systems which coincide with the Weiss crystallographic systems (defined only in dimension 3) we simply say here "crystallographic system".

[17] It is isomorphic to the 12 element dihedral group. To show that is a too poor information for our subject, we note that the isomorphic groups form 4 conjugacy classes in O_3 and 7 in $GL_3(Z)$).

with (for our convenience) a permutation of the two diagonal blocks and we also define the matrice $\hat{m}$" (obtained from $\hat{m}'$ by changing the sign of the 1-dimensional block):

$$\hat{r}' = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \hat{m}' = \begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \hat{m}" = \begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \qquad 4(9)$$

The two groups $R' = \langle -I, \hat{r}', \hat{m}' \rangle$ and $R'' = \langle -I, \hat{r}', \hat{m}" \rangle$ and the group R are in the same conjugacy class [18] of $GL_3(R)$, but they belong to 3 different arithmetic classes denoted in [7]: $R\bar{3}m$, $P\bar{3}m1$, $P\bar{3}1m$.

By an easy computation one finds:

$$a > 0,\ e > 0, \quad q_H = a \begin{pmatrix} 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & \frac{e}{a} \end{pmatrix} = \mathcal{C}_+(\mathcal{Q}_3)^{R'} = \mathcal{C}_+(\mathcal{Q}_3)^{R"} = \mathcal{C}_+(\mathcal{Q}_3)^{H} \subset q_C, \qquad 4(10)$$

where $H = \langle R', R" \rangle$ (q_C will be defined in 4(14)). The 24 element group H is denoted by $P6/mmm$ in [7]. It belongs to a maximal geometric and (therefore) also maximal arithmetic class so it is a maximal Bravais group whose label is $P6/mmm$. That Bravais class is the only one of the corresponding Bravais crystallographic system; it is called *Hexagonal system*. Indeed $P6/mmm$ is the symmetry group of a regular hexagonal prism.

We have given the example of three arithmetic classes mapped by ϕ in the same geometric class, but the lattices they leave invariant belongs to two different Bravais crystallographic system. That is the example mentioned in the "remark" after lemma 2-2.

We continue our strategy by starting from the minimal Bravais class. In dimension 3, the arithmetic class of the group generated by $I, -I$ is denoted $P\bar{1}$ (see 4(3)). As we saw, it is the kernel of the linear action of $GL_3(Z)$ on the 6 dimensional vector space $\mathcal{Q}_3$ and therefore (by theorem 1), it is the minimal Bravais class. Its domain is 6 dimensional. It is the only Bravais class of the *triclinic* crystallographic system.

We now study the action of the reflections. The matrices

$$s_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \in Pm, \quad m = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \in Cm, \qquad 4(11)$$

(m was already defined in 4(7)) are representatives of the two $GL_3(Z)$ conjugacy classes of reflections, denoted by Pm and Cm respectively. We study now the domain in $\mathcal{C}_+(\mathcal{Q}_3)$ invariant by them:

$$a > 0,\ c > 0,\ e > 0,\ ac - b^2 > 0; \quad q_A = \begin{pmatrix} a & b & 0 \\ b & c & 0 \\ 0 & 0 & e \end{pmatrix} = \mathcal{Q}_3^{s_3}, \qquad 4(12)$$

$$a - |b| > 0,\ ae - d^2 > 0,\ (a+b)e - 2d^2 > 0, \quad q_B = \begin{pmatrix} a & b & d \\ b & a & d \\ d & d & e \end{pmatrix} = \mathcal{Q}_3^{m}. \qquad 4(13)$$

[18] One shows they are conjugate in the 48 element normaliser of $H = \langle R', R" \rangle$ in $GL_3(R)$.

These 4 dimensional domains are invariant respectively by the group $A = \langle -I, s_3 \rangle$ and the group $B = \langle -I, m \rangle$. By applying corollary 1-1 we prove that these groups are stabilizers and therefore Bravais groups, whose conjugacy classes are denoted by $P/2m$ and $C/2m$ respectively. We know that (in any dimension) there are only two Bravais classes in this crystallographic system: it is called *monoclinic.*

The group $C = \langle -I, s_3, r \rangle = \langle A, B \rangle$ belongs to the arithmetic class denoted by $Cmmm$. The domain invariant by this group is the intersection of the two domains defined in 4(12-13):

$$a - |b| > 0,\ e > 0, \quad q_C = \begin{pmatrix} a & b & 0 \\ b & a & 0 \\ 0 & 0 & e \end{pmatrix} = q_A \cap q_B \equiv \mathcal{C}_+(\mathcal{Q}_3)^{s_3} \cap \mathcal{C}_+(\mathcal{Q}_3)^{m} \qquad 4(14)$$

Checking that this group is stabilizer of points in the domain, corollary 1-1 proves that $Cmmm$ is a Bravais class. Its holohedry is $mmm = D_{2h} \sim Z_2^3$. That holohedry defines the *orthorhombic* crystallographic system.

We know also the existence (in any dimension) of the P-orthorhombic Bravais class denoted by $Pmmm$. A representative group is the group D generated by the diagonal reflections (one element of the unit matrix is changed of sign; example s_3). It fixes the 3-dimensional domain of diagonal quadratic forms:

$$a > 0,\ c > 0,\ e > 0, \quad q_D = \begin{pmatrix} a & 0 & 0 \\ 0 & c & 0 \\ 0 & 0 & e \end{pmatrix} = \mathcal{C}_+(\mathcal{Q}_3)^D. \qquad 4(15)$$

The 2-dmensional domain fixed by the group $Q = \langle C, D \rangle$ is

$$a > 0,\ e > 0, \quad q_Q = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & e \end{pmatrix} = \mathcal{C}_+(\mathcal{Q}_3)^Q = q_C \cap q_D. \qquad 4(16)$$

$Q \sim D_{4h} = 4/mmm$ is a maximal subgroup of $O_h = m\bar{3}m$ of index 3. So it is a Bravais group. Its Bravais class is denoted by $P4/mmm$ and its crystallographic system is called *tetragonal.*

We have already found 11 Bravais classes. By inclusion of the different domains q_X fixed by group representatives of these classes we have also established their partial ordering (see figure 4-2). To find more Bravais classes we will apply Theorem 2 (at the end of §1). In order to do that we first build the normaliser $N = N_{GL_3(Z)}(B)$, $B \in C2/m$. Then we will study the action of N on the 4-dimensional domain $q_B = \mathcal{C}_+(\mathcal{Q}_3)^B$.

We first notice that $B = \langle -I, m \rangle$ is in the center of N: indeed $G \triangleleft N$, so every $n \in N$ has to conjugate the 4 matrices $I, -I, m, -m$ of B into each other; since the matrices of B have different traces, n commute with them. So $N = C_{GL_3(Z)}(B)$, the centralizer of B in $GL_3(Z)$. To compute this centralizer, it is sufficient to find the integral matrices n which satisfy $nr = rn$ and impose their determinant to be ± 1:

$$n = \begin{pmatrix} \alpha & \beta & \delta \\ \beta & \alpha & \delta \\ \delta' & \delta' & \gamma \end{pmatrix}, \quad \det n = (\alpha - \beta)(\gamma(\alpha + \beta) - 2\delta\delta'). \qquad 4(17)$$

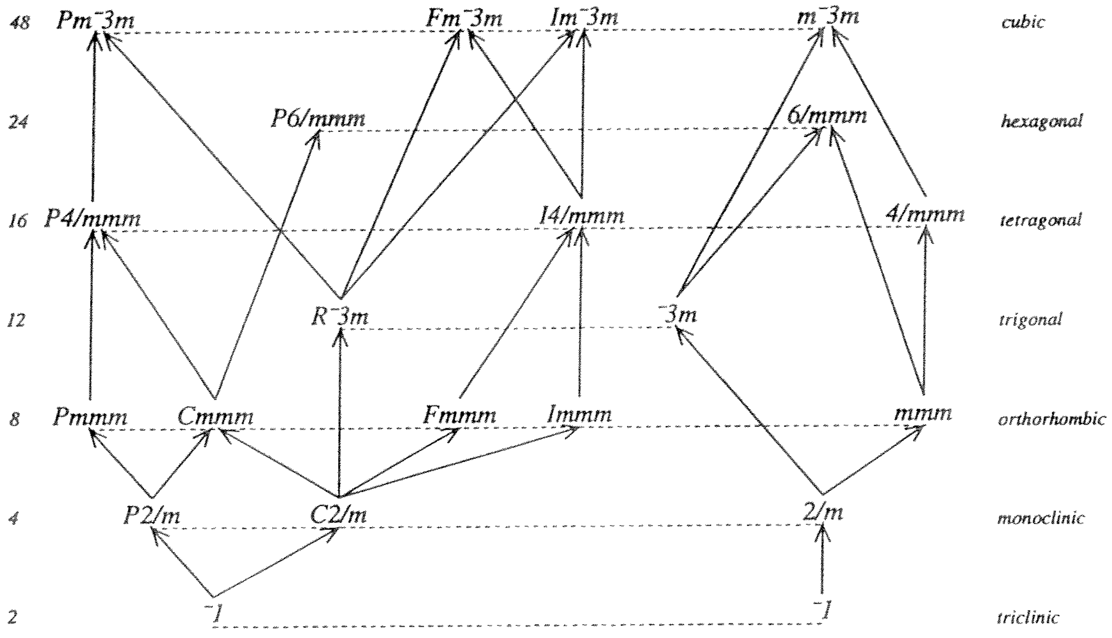


Figure 4-2. Partially ordered set $\{BC\}_3$ and $\{BCS\}_3$ and the map φ.
The left diagram shows the partial order on $\{BC\}_3$, the set of the 14 Bravais classes and the right one shows the partial order on $\{BCS\}_3$, the set of the 7 Bravais crystallographic systems. Their names are given in the last colummn. The first one gives the order of the groups. The dotted horizontal lines represent the order preserving map φ defined in equation 2(16).

Each factor of the determinant should be ± 1:

$$\varepsilon^2 = 1, \eta^2 = 1\,,\ \alpha - \beta = \varepsilon,\ \gamma(\alpha+\beta) - 2\delta\delta' = \eta\ \Rightarrow\ \alpha \pm \beta \text{ is odd},\ \gamma \text{ is odd},\ \det n = \varepsilon\eta. \qquad 4(18)$$

One can check that N is generated by the matrices:

$$-I,\ m,\ s_3,\ d = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix},\ d' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}. \qquad 4(19)$$

As we have seen the group $C\langle -I, s_3, r\rangle$ fixes the 3-dimensional domain $q_C \subset q_B$ (see 4(14)). Since the stabiliser of any lattice is finite, the orbits of N in q_B are infinite. Finite groups of N are crystallographic point groups; therefore each one containig B as strict subgroup will have a linear manifold of fixed points corresponding to a larger Bravais class. To find the finite subgroups of N, we must first determine their elements of finite order. As for $GL_3(Z)$ their order can be only $1, 2, 3, 4, 6$. Elements of order 3 must have for eigen values the three cubic roots of 1, so their trace, $\operatorname{tr} n \equiv \tau = 2\alpha + \gamma$, must be 0. That is impossible as, from 4(18), we know that γ is odd. Hence N *has no* *elements of order 3 or 6* (the square of the latter would be of order 3). Writing from 4(17) the equation $n^2 = 1$ yields the following conditions in supplement of those of 4(18), and combined with them:

$$\gamma^2 + 2\delta\delta' = 1, \quad 2\alpha(\alpha - \varepsilon) + \delta\delta' = 0, \quad \delta(\tau - \varepsilon) = 0 = \delta'(\tau - \varepsilon) \quad \text{with } \tau = \operatorname{tr} n. \quad 4(20).$$

Since the eigenvalues of these matrices are ± 1, their trace can be either -3 or ± 1. In the former case we find easily that $n = -I$. When the trace $\tau = \pm 1$ we must have $\operatorname{tr} n + \det n = 0$ so

$$\tau = 2\alpha + \gamma = -\varepsilon\eta. \qquad 4(21)$$

That, with the first two conditions of 4(20), yields $\eta = -1$. Notice that for elements of N which are squares, $\varepsilon = \eta = 1$, so there are no elements of order 4 in N. That proves that in N, all non trivial elements of finite order are of order 2. Hence all finite subgroups of N have the structure Z_2^k and we know from the study of $GL_3(Z)$ subgroups (or of the geometrical classes), that $k \leq 3$.

It is easy to verify that the largest finite subgroups of N represent 3 of the four conjugacy classes of Z_2^3 subgroups in $GL_3(Z)$; explicitly, representatives of the conjugacy classes $Cmmm$, $Fmmm$ and $Immm$ are [19]:

$$C = \langle m, s_3, -I \rangle \in Cmmm\,, \quad F' = \langle m, w^\top, -I \rangle \in Fmmm\,, \quad I' = \langle m, w, -I \rangle \in Immm, \qquad 4(22)$$

with

$$w = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ -1 & -1 & -1 \end{pmatrix}. \qquad 4(23)$$

It is straightforward to compute the 3-dimensional domains of the groups F' and I'; one obtain the following planes in q_B

$$q_{F'} = q_B \cap (a + b + 2d = 0), \quad q_{I'} = q_B \cap (-e + 2d = 0). \qquad 4(24)$$

One verify with corollary 1-1 that F' and I' are stabilisers. Hence we have found 4 Bravais classes: $Pmmm$,$Cmmm$,$Fmmm$,$Immm$ corresponding to the *orthorhombic* crystallographic system.

Finally, we are led to consider the group $Q' = \langle F', I' \rangle$ with the 2-dimensional domain it fixes. This group is isomorphic to $4/mmm \sim D_{4h}$ maximal subgroup of O_h. It has to belong to a Bravais class, just smaller [20] than the Bravais classes $Fm\bar{3}m$ and $Im\bar{3}m$. That completes our determination of the Bravais classes.

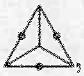
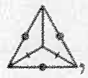
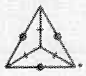
§ 4-3. *The Delone symbols belonging to a Bravais class.*

The type and symmetry properties of a Voronoï cell is completly characterized by the Delone symbol. As we shall see, there are 9 Bravais classes whose all lattices are represented by a unique Delone symbol. Consider for instance the Bravais class

[19] Among the different method for distinguishing the two point groups $Fmmm$ and $Immm$, the fastest one is the computation of their fixed points (i.e. their cohomology group $H^0(P, L)$) by their action on the lattice L: $Fmmm$ has 2 fix points and $Immm$ has 4 of them.

[20] In the basis used, the verification is a little tedious.

$Pmmm$ and the larger ones, $P4/mmm$ and $Pm\bar{3}m$. We have already seen that their Voronoï cells are of the type 6-20 (meaning 6 faces and 20 corona vectors which are not face vectors). They are rectangle parallelohedrons; hence they have 3 zones (= families of parallele edges: they have the same length) corresponding to the three non zero parameters of their Delone symbols. For the tetrahedral lattices in $P4/mmm$ two zones have same length and for the cubic lattices in $Pm\bar{3}m$ the three zones have the same length. To summarize

$Pmmm$: , $P4/mmm$: , $Pm\bar{3}m$: . 4(25)

Similarly for the ordered sequence of Bravais classes: $P2/m$, $Cmmm$ $P6/mmm$ the Voronoï cells are of the type 8-12: they are hexagonal prisms with 4 zones. The length of one gives the height of the prism; it is always arbitrary. The three others correspond to the opposite edges of the two hexagonal faces (they have a symmetry center). The equality of two or three of these zones is seen on the Delone symbols:

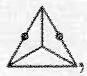
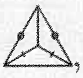
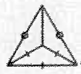
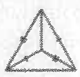
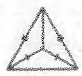
$P2/m$: , $Cmmm$: , $P6/mmm$: . 4(26)

Table 4-2 gives the list of the Delone symbols describing the Voronoï cells of the lattices belonging to a Bravais class. The last column gives the dimensions *up to a dilation*. Indeed all geometrical properties we are studying are invariant by dilations including $\mathcal{C}_+(\mathcal{Q}_3)$ itself! It is convenient to remove the scale by the stereographic projection as we have done it for dimension 2 (see for instance figure 1-2). An equivalent table was first given by Delone in [5].

Consider for instance the generic Bravais class $P\bar{1}$. Its stereographic projection has dimension 5 and as we explained the generic Voronoï cells are primitive with different length for the six zones. When one of the parameters $\lambda \to 0$ there is a 4-dimensional boundary of type 12-4 cells. More precisely there are 6 boundaries (one per λ) supported by hyperplanes, so they form a simplex Σ containing the domain of primitive Voronoï cells. But the largest possible stereographic dimension for the Bravais class domains other than that of $P\bar{1}$ is 3. So their domains are in the intersections of the faces of the simplex Σ; that is on its edges. And the 4 dimensional domain of Voronoï cells of type 12-4 with their five zones all inequal is inside the domain of the minimal (and generic) Bravais class.

As table 4-2 shows there are 5 Delone symbols for describing the cells of the lattices in $P2/m4$=*Mono C*. There are two different ones for primitive cells (type 14-0 with 14 faces: 8 hexagons and 6 tetragons)

a :  b :  4(27)

The symmetry $2/m$ is generated by the symmetry through the origin (all cells have it) and a rotation by π. In case a: the rotation axis passes through the centers of two tetragons (symmetric through the origin); in case b: the rotation axis passes through the middles of two edges (symmetric through the origin), each one common to two hexagons.

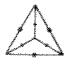
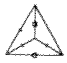
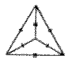
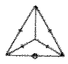
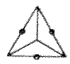
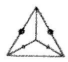
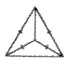
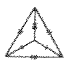
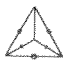
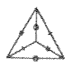
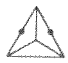
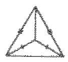
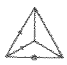
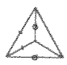
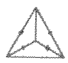
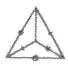
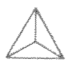
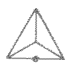
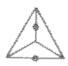
Voronoï	14-0	12-4	12-6	8-12	6-20	dim.
Cubic P						0
Cubic F						0
Cubic I						0
Hexa P						1
Trigo R						1,1
Tetra P						1
Tetra I						1,1
Ortho P						2
Ortho C						2
Ortho F						2
Ortho I						2,2,1
Mono P						3
Mono C						3,3,2
Mono C						3,2
Tricli P						5,4,3

Table 4-2. List of the Delone symbols describing the Voronoï cells of the lattices belonging to a Bravais class.

The first column lists the Bravais classes. The last column gives the dimensions up to a dilation, of the different domains of cells; the first dimension is also that (up to a dilation) of the domain of the Bravais class in $\mathcal{C}_+(\mathcal{Q}_3)$.

§ 5 Acknowledgements

In the last lecture in Zajączkowo , I showed that the 3-dimensional edges of the 5 dimensional simplex Σ (in the stereographic projection of $\mathcal{C}_+(\mathcal{Q}_3)$) that I described in the previous subsection, are paved by two families of tetrahedrons (= 3 dimensional simplexes) corresponding to the two monoclinic Bravais classes. And I exhibited 3-dimensional models of them. Each tetrahedron has a face in the wall of $\mathcal{C}_+(\mathcal{Q}_3)$, the 3 other faces of the one representing $C2/m$ correspond to the $Cmmm$, $Fmmm$, $Immm$ Bravais classes; the edge between the last two named faces representing the class $I4/mmm$. The class $R\bar{3}m$ is represented by a line crossing the interior of the tetrahedron while the other Bravais classes $> C2m$ are represented (with a finite multiplicity) by lines and points on the faces. The interior of the tetrahedron contains two domains of Voronoï cells of types 14-0 and 12-4 with an inner triangle of type 12-6. The tetrahedron of $P2/m$ has one face in $\partial\mathcal{C}_+(\mathcal{Q}_3)$, another correspond to the class $Pmmm$ and the last two $Cmmm$, one being shared with the tetrahedron $C2/m$. The 3 more symmetric Bravais classes appear as an edge ($P4/mmm = Pmmm \cap Cmmm$) or lines ($P6/mmm$ and point ($Pm\bar{3}m$) on the surface.

I have not had the time yet for making a picture of these 2 models which were made in the mechanic shop of the Technion in the fall 1993. I wrote the present text during a stay in the Technion in the fall 1994; I am very grateful to the Physics department of the Technion for its warm, fruitful and quasiperiodic hospitality.

I enjoyed tremenduously the third international school on "Symmetry and structural properties of condensed matter". I thank very warmly the organizers for their invitation.

I thank cordially Professor Marjorie Senechal for many interesting discussions on the topics of these lectures.

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