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Fundamental concepts for the study of crystal symmetry

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Abstract

Fundamental concepts for the study of crystal symmetry are systematically introduced on the basis of group action analysis.

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1. Introduction

In solids, every atom vibrates around an average position; the amplitude of the vibrations is related to the temperature. To a good approximation these average positions are fixed. We denote by $\mathscr{S}$ the set of points in the d-dimensional[1] Euclidean space $\mathscr{E}_d$ which represent these positions. In condensed matter the interatomic distances are of the same order of magnitude as the size of the atoms, so we cannot neglect their sizes; it is therefore natural to assume that there is a minimum distance $d = 2r$ between any pair of points of $\mathscr{S}$. In the study of solids in bulk, surface effects are neglected; the natural idealization is to suppress the surface by the assumption that the set $\mathscr{S}$ extends to infinity. However this is not enough since it leaves the possibility to have internal holes with a well-defined surface; there must be some upper bound for the distance between "neighboring" points which is of the order of magnitude of the atomic size. This can be obtained by the following condition: R is the upper bound of the radii of the "empty spheres", those which do not contain points of $\mathscr{S}$ in their interior. The mathematical theory of these (r, R) sets has been elaborated by Delone and its school, mainly in Soviet Union (Delaunay, 1932a, b; Delone et al., 1974). Here we call them Delone sets. Each such set defines two dual orthogonal tessellations of the Euclidean space. We summarize these mathematical results in Section 2. Of course it can be skipped since we are interested only in *periodic crystals*. However, the discovery of aperiodic crystals (Shechtman et al., 1984) requires a broader mathematical frame for a unified study of crystals. This frame seems to be provided by the theory of Delone sets; we wanted to mention it to the reader and show how classical crystallography is the study of a very rich particular case.

The other sections of this chapter study *periodic crystals*, i.e. those whose symmetry contains a lattice of translations L. These lattices and their symmetry are studied in Section 3. It will lead to the definition of basic concepts: the crystallographic systems and the Bravais classes; they are both examples of strata. It will also lead to the concept of Brillouin zone, fundamental for the study of many types of experiments.

Translation lattices L define pavings of space by a "fundamental domain" repeated by the translations. Among the possible domains, one is intrinsic (i.e. basis independent): it is studied later, in Section 5. The crystal structure is defined by the positions of the atoms in a fundamental domain. Only the crystals of chemical elements can have a unique atom in a fundamental domain.[2] Such type of space groups are semi-direct products of Bravais groups of lattices by the translation lattice itself. There are 14 of them among the 230 space groups of dimension three; every other space group is one of their subgroups. The list of the 230 space groups has been determined in 1892 by a mineralogist, Fedorov (1885), and a mathematician, Schoenflies (1891), working independently.[3] Presently the "International Tables of Crystallography" (ITC, 1996) (abbreviated hereafter as ITC) is the standard reference for the data on the structure of these groups. They are labelled in ITC by a symbol (using at most seven letters or digits and two typographic characters $^{-}$, /) which gives the

[1] As usual, when statements do not depend on the value of the dimension, we call it d.

[2] That is not the general case. Diamond and graphite, two crystallographic states of carbon, have respectively 2 and 6 atoms per fundamental domain.

[3] By comparing their results before publication, each one made very few corrections to the results of the other one.

structure of each space group! This remarkable notation system is universally used by crystallographers but not yet by some physicists. The translation lattice L is an infinite Abelian group which is an invariant subgroup of any space group G. The quotient group[4] $P = G/L$ is called the point group; it is a finite group.

Many physical phenomena depend on a less-refined classification of the symmetry of crystal. For example, most of their macroscopic properties depend only on the 32 geometrical classes, i.e. the conjugacy classes in O_3 of the point groups P. These classes have been listed by Frankenheim (1826a, b, 1842) and Hessel (1830) just before the introduction of the word group by Galois (1846). Mechanical, optical, electric and magnetic properties of the crystals are described by tensors invariant by P. These tensors are given by the invariants of the "vector" representation[5] of P; the rings of these invariants have been given in terms of 3–6 generators in Chapter I, Tables 4, 5. Some microscopic properties of crystals may depend only on P, but in a more refined manner which takes into account the action of P on the translation lattice L; this action can be written in terms of matrices whose elements are integers. Such phenomena depend only on the 73 *arithmetic classes*,[6] i.e. the distinct conjugacy classes of the point groups as subgroups of $GL(3, Z)$; they correspond to 73 different actions of the point groups on the Brillouin zone. Arithmetic classes are studied in Section 4. Their ring of invariants on the Brillouin zone is the main subject of Chapter V. In Section 4 we also show that for stationary states (i.e. invariant by time translations) of these microscopic phenomena, time reversal $\mathscr{T}$ reduces the number of relevant arithmetic classes to 24.

Section 5 gives some insight into the structure of the Voronoï cell in d-dimension before describing the two and five types occurring for $d = 2, 3$, respectively. In the reciprocal space, this is the Brillouin cell: it is a geometrical realization of the Brillouin zone. We transpose in this geometrical description the results obtained in the preceeding section on the high symmetry points of the Brillouin zone.

Section 6 gives in a one page Table 7 a very useful application of the general methods given in Chapter I, to these 24 classes. Indeed Table 7 gives the positions on BZ of *the extrema common to all invariant continuous functions on the Brillouin zone* and indicates the nature of these extrema for "Morse-simple functions" (the function with the minimum possible number of extrema);[7] these functions occur most often in the simple physical models.

Of course many physical properties of crystals depend on the more refined classification of their symmetry by the 230 space groups. Is it possible to predict for these types of properties some general results by brute force, i.e. verifying them for the 230 space groups! Another method, (which we prefer for the sake of culture) is to prove such result as a mathematical theorem, whose proof is based on properties specific to space groups; more often the proof will have to consider several cases, each containing only a subclass of space groups. This is illustrated in Chapter VI for the study of the symmetry and topology of the electron energy bands.

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[4] In English one sometimes uses the expression "factor" group. This is misleading because P is generally not a subgroup of G. Moreover quotient structure are obtained by a very general construction in mathematics that we use here for the particular case of groups.

[5] The linear representation of P on the physical space.

[6] Of course this very fundamental concept is defined in ITC, p. 719. It is strangely absent from most physics text books. We will quote some classic papers where it is used.

[7] These recents results have been published (Michel, 1996; Michel, 1997b) but not in a physical journal.

Section 7 gives an elementary and original approach of the important concepts relevant to the rich diversity of space groups. This section will also help the understanding and use of the international tables (ITC, 1996). Section 8 recalls the structure of the unirreps of the space groups G; they are built by induction from the "allowed" unirreps of the stabilizers G_k of the action of G on the Brillouin zone. The images of these allowed G_k unirreps are also those of the group $P_z(k)$ (Herring, 1942), whose structure is much simpler.

There are many introductory books on crystallography, e.g. Buerger (1956); shorter introductions are also included in most solid state books and in some books of applications of group theory to physics. None overlaps very much with this chapter.[8] Our aim is to emphasize fundamental concepts used little or not at all in these introductions, but so necessary for physics of crystals; these concepts are introduced and explained in a direct and completly original method.[9] Moreover this chapter prepares the reader to use effectively ITC;[10] using tables can fully satisfy technicians (they will soon be replaced by softwares). But would physicists accept to use tables of trigonometric functions without knowing their analytic properties and the geometry; Chapter IV tries to give them the deeper knowledge they need on crystallography. Most of the concepts studied in this chapter are necessary for understanding Chapters V and VI which contain essentially original results; but the reader can skip details and come back to them when they are referred to in the last two chapters or when he needs them later in his own work!

2. The Delone sets $\mathscr{S}(r, R)$ of points

Definition. *A Delone set of points* $\mathscr{S}(r, R)$ in a d-dimensional Euclidean space $\mathscr{E}_d$ is defined by two real numbers: $2r$ the lower bound of the distance between two points of the set and R the upper bound of the radius of the spherical balls of $\mathscr{E}_d$ which contain no point of $\mathscr{S}$ in their interior.[11]

The existence of the bound R implies that the set is infinite. The existence of the bound $2r$ implies that the number of points in any bounded domain is finite (otherwise there would be an accumulation point). From now on we use the shorthand "ball" for a spherical ball; its surface is a $(d-1)$-dimensional sphere. It is well known that in $\mathscr{E}_d$ one needs $d+1$ points in general position[12] for determining a $(d-1)$-sphere.

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[8] The overlap is much greater with Burckhardt (1966), Schwarzenberger (1980), Engel (1998), and the elegant and more elementary Senechal (1991).

[9] This method does not require more sophisticated mathematics as, for instance, cohomology theory, which is of course very useful for a deeper knowledge.

[10] Strangely, in the action of the space groups on the Euclidean space, these tables give only the geometric class of the stabilizer and not their arithmetic class. However they give very useful information on the subgroups of space groups. They do not study the Brillouin zone.

[11] There exists for each dimension d a lower bound for R/r; e.g. it is 1 in the trivial case $d = 1$. For $d = 2$ it is probably obtained by the two-dimensional hexagonal lattice $R/r = (2/\sqrt{3}) = 1.13397\ldots$ I do not know what is known in higher dimensions. There are many results for the special case of lattices; many references are in Conway and Sloane (1988).

[12] That means that any subset of $k+1$ points, $1 < k \leq d$, is not contained in a linear manifold of dimension $< k$. We use the shorthand "k-plane" for a k-dimensional linear submanifold of $\mathscr{E}_d$. We also recall that $k+1$ points in general position are the vertices of a *simplex*.

Definition. *A hole* of $\mathscr{S}$ is a d-dimensional ball which contains no point of $\mathscr{S}$ in its interior and has on its surface at least $d+1$ points; among them there must be a subset of $d+1$ points in general position. Of course, in a Delone set $\mathscr{S}$, any subset of $d+1$ points in general position does not determine a hole (the sphere it defines may contain set points in its interior). Let us consider the complete set of holes of $\mathscr{S}$. We denote by $\mathscr{V}$ the set of their centers (two centers cannot coincide) and for a given $v \in \mathscr{V}$, we denote by Δ_v the convex hull of the set points on the surface of the corresponding sphere; this d-dimensional convex polyhedron is called a *Delone cell*. Beware that Δ_v may not contain v (this does not happen for $d=2$ but it is easy to make counter-examples in dimension 3).

Proposition 2a. *In the Euclidean space $\mathscr{E}_d$ the Delone cells of a Delone set $\mathscr{S}$ form a tesselation* ($=$ *a facet-to-facet paving*) *denoted by Δ_S.*

Indeed, consider a facet (i.e. a $(d-1)$-face) Φ of Δ_v. We denote by $\mathscr{H}_\Phi$ the $(d-1)$-plane containing Φ. It determines two half-spaces. We denote by $\mathscr{H}_\Phi^+$ the one containing Δ_v and by $\mathscr{H}_\Phi^-$ the other one. We denote by Γ the $(d-2)$-dimensional sphere intersection of the $(d-1)$-dimensional sphere of the hole with $\mathscr{H}_\Phi$. The set of $(d-1)$-spheres containing Γ is called a linear sheave of spheres. The centers of its spheres are on the straight line Λ perpendicular to $\mathscr{H}_\Phi$ at the center of Γ. Let us consider the continuous family of spheres S_x of the sheave whose center $x \in \Lambda$ moves continuously from v in the direction of $\mathscr{H}_\Phi^-$. The vertices of the Δ_v's in the interior of $\mathscr{H}_\Phi^+$ do not belong to these spheres; so we can find a new hole whose sphere center is denoted by v'. Then $\Delta_v \cap \Delta_{v'} = \Phi$. Continuing this construction for all facets of all Delone cells, we obtain the full tessellation.

Definition. A Delone set is *primitive* when all its Delone cells are simplexes ($=$ convex hull of $d+1$ points in general position).

The set of balls of radius r centered at the points of the Delone set $\mathscr{S}$ is called *the sphere packing* on $\mathscr{S}$. The only possible intersection between these balls are contact points between two tangent balls at the middle of the segment formed by two set points at the minimum distance $2r$. We denote by $d(p,q)$ the distance between two points of $\mathscr{E}_d$.

Definition. *The Voronoï cell* $\mathscr{D}_S(p)$ at the point $p \in \mathscr{S}$ is the set of points of $\mathscr{E}_d$ whose distance to p is smaller or equal to the distance to any other point of $\mathscr{S}$:

$$p \in \mathscr{S}, \quad \mathscr{D}_S(p) = \{x \in \mathscr{E}_d;\ \forall q \in \mathscr{S},\ d(p,x) \le d(q,x)\}\ . \tag{1}$$

Proposition 2b. *The Voronoï cells of a Delone set are convex polyhedrons*; *each $\mathscr{D}_S(p)$ is contained in the ball, centered in p, of radius R.*

The bisector plane of the segment pq defines two-half spaces and $\mathscr{D}_S(p)$ is in the one containing p. So $\mathscr{D}_S(p)$ is the intersection of all these half-spaces made for all set points $q \neq p$. As an intersection of convex domain, it is convex. It contains the sphere of radius r centered at p. We now show that it is contained in the sphere of radius R centered at p. Indeed, assume that $x \in \mathscr{D}_S(p)$ is outside this

sphere (i.e. $\overline{xp} > H$); since, by definition of $\mathscr{D}_S(p)$, x is nearer to p than any other points of $\mathscr{S}$, the spherical ball of radius R centered at x does not contain points of $\mathscr{S}$ (inside or on its surface). It is absurd to find a hole at x of radius $> R$. We have already remarked that the number of points of $\mathscr{S}$ inside any bounded domain is finite; that is the case of the sphere of radius $2R$ centered at p: so the number of points q whose bisector pq intervenes in the constructions of $\mathscr{D}_S(p)$ is finite. This ends the proof of Proposition 2b.

Corollary 2b. *The Voronoï cells of a Delone set form a tessellation of the Euclidean space.*

The intersection of two Voronoï cells $\mathscr{D}_S(p) \cap \mathscr{D}_S(p')$ is in the bisector plane of pp'. Either it is empty or it is a common facet. Indeed, any point of $\mathscr{E}_d$ is either in the interior of a Voronoï cell or on the boundary of $k \geq 2$ Voronoï cells; when $k = 2$ it is the common face of the two cells.

Let us consider a k'-dimensional face $\Phi_{k'}$ of the Delone cell Δ_v, with $0 \leq k' \leq d$ (when $k' = d$, $\Phi_{k'}$ is the Delone cell). Let F_k, $k + k' = d$ be the k-plane containing v and perpendicular to the supporting k'-plane of $\Phi_{k'}$. The points of F_k are equidistant of the vertices of $\Phi_{k'}$, so F_k contains the common k-dimensional face $\mathscr{F}_k$ of the Voronoï cells at the vertices of $\Phi_{k'}$. In particular, when $k' = d$, then v is the vertex common to the Voronoï cells defined by the vertices of Δ_v (which form a hole). Remark that $|\Phi_{k'}|$, the number of vertices of $\Phi_{k'}$ satisfy $|\Phi_{k'}| \geq k' + 1$; the equality occurs for all k' when the Delone set is primitive. Conversely, by construction of the Voronoï tessellation, the points of F_k, the k-plane supporting a k-face $\mathscr{F}_k$, are equidistant from at least $d + 1 - k$ points of $\mathscr{S}$ and the convex hull of these points (which form a face $\Phi_{k'}$ of Δ_S) is orthogonal to F_k.

To summarize: the vertices of the Delone cells are points of $\mathscr{S}$, i.e. constructing centers of the Voronoï cells of $\mathscr{S}$ and their vertices are the centers of the spheres circumscribed to the Delone cells; more generally in the tessellations Δ_S and $\mathscr{D}_S$ there is an orthogonal duality between their faces. These two tessellations are said to be *dual orthogonal*.

We leave to the reader the straightforward proof of

Proposition 2c. *If the holes of a Delone set $\mathscr{S}(2r, R)$ have the same radius* (*which has to be R*), *the Delone tessellation of $\mathscr{S}$ is the Voronoï tessellation of $\mathscr{V}$ the set of centers of the holes = the set of vertices of the Voronoï cells of $\mathscr{S}$.*

As we shall see in Section 4 this is the case of all two-dimensional lattices and of the three-dimensional lattices belonging to 7 (out of 14) Bravais classes.

It seems that the concept of a Delone set is a good tool for unifying the study of periodic and aperiodic crystals (see e.g. Dolbilin et al., 1998). The local symmetry can be studied with the following tools:

Definition. The *star*, respectively (*ℓ-star*) of a point $p \in \mathscr{S}$ is the set of straight line segments joining p to all points of the Delone sets, respectively (all points whose distance to p is $\leq \ell$). Stars (ℓ-stars) are congruent when they can be transformed into each other by an Euclidean transformation. Let us denote by $St(\mathscr{S})$ ($St(\ell, \mathscr{S})$) the set of congruence classes of the stars (ℓ-stars) of $\mathscr{S}$. When $St(\ell, \mathscr{S})$ is finite (as is the case for Penrose tilings) there is some order in $\mathscr{S}$.

The crystal structure is due to some order correlation which does not vanish at infinite distance. Delone sets with their classes of stars $St(\mathscr{S})$ are a possible frame for a comprehensive study of crystals and their symmetry when $St(\ell,\mathscr{S})$ is finite. When all stars form one class, $\mathscr{S}$ is called a *regular Delone set*.

Theorem 2a. *A regular Delone set is a periodic crystal. Equivalently*: $\mathscr{S}$ *is the union of orbits of a translation lattice.*

The statement equivalent to this theorem was proven by Schoenflies (1891) in dimension 3 and extended by Bieberbach (1910, 1912) to an arbitrary dimension. It proves that periodic crystals are a particular (and very important) case of Delone sets.

There is also an important mathematics literature on classification of tessellations, also called tilings with, eventually, matching rules, and their possible local or global symmetries: see e.g. Moody (1995).

The other sections deal only with periodic crystals.

3. Lattice symmetry: crystallographic systems, Bravais classes

3.1. General definitions. Intrinsic lattices

We recall that an orthogonal d-dimensional vector space E_d contains the Abelian group R^d of addition of its vectors and an orthogonal scalar product that we denote by $(\boldsymbol{x},\boldsymbol{y})$; the norm of a vector is $N(\boldsymbol{v}) = (\boldsymbol{v},\boldsymbol{v})$.

Definition. A *lattice* in E_d is the subgroup of R^d generated by a basis $\{\boldsymbol{b}_j\}$ of E_d; i.e. the vectors of L are those with integer coordinates on $\{\boldsymbol{b}_j\}$. Hence the group isomorphism $L \sim Z^d$. Let $\{\boldsymbol{b}'_j\}$ be another basis of L; the new basis vectors must have integer coordinates in the old basis and vice versa, so

$$\boldsymbol{b}'_i = \sum_i m_{ij}\boldsymbol{b}_j, \quad m \in GL(d,Z)\,, \tag{2}$$

indeed the matrix m_{ij} and its inverse must have integer elements, so their determinants have same value which is ± 1. Eq. (2) shows that the set of bases of a lattice L is a principal orbit of $GL(d,Z)$.

In order to deal later with the orthogonal group, we choose an orthonormal basis $(\boldsymbol{e}_i,\boldsymbol{e}_j) = \delta_{ij}$ of E_d. For any basis $\{\boldsymbol{b}_i\}$ of E_d the matrix $\tilde{b}$ of elements $\tilde{b}_{ij} = (\boldsymbol{b}_i,\boldsymbol{e}_j)$ is the matrix of the d components of its d vectors. It is invertible since the basis vectors are linearly independent, so $\tilde{b} \in GL(d,R)$. Conversely, given a matrix of $GL(d,R)$ the elements of its d lines can be considered as the d components of the d vectors of a basis of E_d. So the correspondance $\{\boldsymbol{b}_i\} \leftrightarrow \tilde{b}$ is bijective and it gives a bijective map between the set $\mathscr{B}_d$ of bases of E_d and the set of elements of the group $GL(d,R)$ (notice that this identification gives to $\mathscr{B}_d$ a structure of a manifold). Using Eq. (2), we can identify the set of bases of L as the right coset $GL(d,Z)\tilde{b}$ of $GL(d,Z)$ in $GL(d,R)$ and we can identify $\mathscr{L}_d$, the

set of d-dimensional lattices, as the set of right cosets of $GL(d,Z)$ in $GL(d,R)$. In Chapter I Section 3.1, we have shown that this set of cosets can also be interpreted as the orbit space of the action of $GL(d,Z)$ on $\mathscr{B}_d = GL(d,R)$, i.e.

$$\mathscr{L}_d = \mathscr{B}_d \,|\, GL(d,Z) = GL(d,Z)\backslash GL(d,R), \tag{3}$$

where, as sets, $\mathscr{B}_d = GL(d,R)$. The orthogonal group O_d is the group of automorphisms of E_d. The elements of O_d transform the lattice L in a family of lattices which are simply different orientations in E_d of the same "intrinsic" lattice L. For instance, given $r \in O_d$, if $\tilde{b}$ is the matrix representing a generating basis of the lattice L, $\tilde{b}r^{-1} = \tilde{b}r^{\top}$ represents a basis generating $r \cdot L$, the lattice L transformed by r. An intrinsic lattice is defined by the Gram matrix of its generating basis; its elements are

$$(\boldsymbol{b}_i, \boldsymbol{b}_j) = (\tilde{b}\tilde{b}^{\top})_{ij} \ . \tag{4}$$

We can also identify an intrinsic lattice of L to the orbit $O_d \cdot L$. So L_d^i, the set of intrinsic lattices, is the set of such orbits. Since the action of $r \in O_d$ is $\tilde{b} \mapsto \tilde{b}r^{-1}$, from Eq. (3) we can also identify $\mathscr{L}_d^i$ with the double cosets of $GL(d,Z)$ and O_d in $GL(d,R)$. To summarize

$$\mathscr{L}_d^i = \mathscr{L}_d \,|\, O_d = GL(d,Z)\backslash GL(d,R)/O_d, \qquad \{BCS\}_d = \mathscr{L}_d /\!/ O_d \ . \tag{5}$$

Bravais (1850) did consider the types of intrinsic lattices and the strata[13] of O_d on $\mathscr{L}_d$ are called Bravais crystallographic systems in ITC p. 722.

The stabilizer $(O_d)_L$ is the *point group* of L and its conjugacy class in O_d is called the *holohedry* of L that we shall denote by P (or P_L). The orthogonal transformation r is a symmetry of L if $\tilde{b}r^{-1}$ is another basis of L; then, from Eq. (2), there exists

$$m \in GL(d,Z), \quad m\tilde{b} = \tilde{b}r^{-1} \Leftrightarrow m = \tilde{b}r^{-1}\tilde{b}^{-1} \Leftrightarrow r = \tilde{b}^{-1}m^{-1}\tilde{b} \ . \tag{6}$$

Equivalently (we use the lower index b to remind the dependence on the basis)

$$P_b^z = \tilde{b}P_b\tilde{b}^{-1} \subset GL(d,Z), \quad P_b = O_d \cap \tilde{b}^{-1}GL(d,Z)\tilde{b} \subset O_d \ . \tag{7}$$

As the intersection of a compact and a discrete subgroups of $GL(d,R)$, the point group P_b is a finite group. P_b^z is called the *Bravais group* of L and its conjugacy class P^z in $GL(d,Z)$ is the *Bravais class* of L. In other words one can say that the Bravais group P^z gives the action of the point group on the lattice while the holohedry gives simply the action of the point group on the space. This suggests that there is a natural surjective map $\{BC\}_d \overset{\phi'}{\hookrightarrow} \{BCS\}_d$.

We also remark that $-I_d$, the matrix representing the symmetry through the origin, is an element of P and P^z (in every basis); indeed if $\ell \in L$, then $-\ell \in L$.

The matrix $q_b = \tilde{b}\tilde{b}^{\top}$ defined in Eq. (4) is a symmetric positive matrix. We denoted it by q because it represents a positive quadratic form $q_b(x) = \sum_{ij} x_i (q_b)_{ij} x_j$. The set $\mathscr{Q}_d$ of $d \times d$ symmetric real matrices ($= d$ variable quadratic forms) forms a $N = d(d+1)/2$-dimensional orthogonal vector space E_N whose scalar product is $(q', q'') = \operatorname{tr} q'q''$. The positive quadratic forms form

[13] The concept of strata is not explicitly mentioned in ITC.

a convex cone that we denote by $\mathscr{C}_+(\mathscr{Q}_d)$. From (2) we can define the action of $GL(d,Z)$ on $\mathscr{Q}_d$:

$$m \in GL(d,Z), \quad q \in \mathscr{Q}_d, \quad q \overset{m}{\to} mqm^\top . \tag{8}$$

This action transforms $\mathscr{C}_+(\mathscr{Q}_d)$ into itself.[14] So the definitions of intrinsic lattices and Bravais classes can be reformulated as orbit and stratum spaces

$$\mathscr{L}_d^i = \mathscr{C}_+(\mathscr{Q}_d) \,|\, GL(d,Z), \quad \{BC\}_d = \mathscr{C}_+(\mathscr{Q}_d) \,||\, GL(d,Z) . \tag{9}$$

As we have seen, the Bravais groups are finite. Since they are the stabilizers of the action of $GL(d,Z)$ on $\mathscr{C}_+(\mathscr{Q}_d)$, the theorem of Palais[15] (1961) proves the "good" stratification of this action: so there is a unique minimal symmetry stratum (the group $Z_2(-I_d)$), it is open dense and its boundary is the set of strata with larger symmetry.

A lattice is an *integral lattice* when its quadratic form has integer coefficients and they are relatively prime; as Eq. (8) shows, this property is basis independent. When the basis $\{\boldsymbol{b}_i\}$ generates L, for any positive real number λ we denote by λL the lattice generated by the basis of vectors $\{\lambda \boldsymbol{b}_i\}$; it is enough to consider $\lambda > 0$ since $-I \in P$. All lattices λL have the same symmetry.

Definition. The *dual lattice* L^* of L is the set of vectors whose scalar product with every vector of L is an integer. To prove that this set of vectors is a lattice, let $\{\boldsymbol{b}_j\}$ a basis generating L; we define the dual basis $\{\boldsymbol{b}_i^*\}$ by

$$(\boldsymbol{b}_i^*, \boldsymbol{b}_j) = \delta_{ij}; \quad \boldsymbol{x} = \sum_i \xi \boldsymbol{b}_i^*, \quad \boldsymbol{y} = \sum_j \eta_j \boldsymbol{b}_j, \quad \text{then } (\boldsymbol{x},\boldsymbol{y}) = \sum_i \xi_i \eta_i \tag{10}$$

with this simple form of the scalar product one verifies that the dual basis generates the dual lattice. It is also straightforward to verify that if the Bravais group of L is represented by the matrices g's, in the dual basis, $P_{L^*}^z$ is represented by the matrices

$$g \in P_L^z \leftrightarrow \tilde{g} \overset{\text{def}}{=} (g^\top)^{-1} = (g^{-1})^\top \in P_{L^*}^z . \tag{11}$$

These two representations of the holohedry P are equivalent on the real, but they may be inequivalent on Z.

The definition of dual basis in Eq. (10) shows that $(L^*)^* = L$. Note that an integral lattice is a sublattice of its dual.

3.2. Euclidean geometry and Euclidean lattices

The Euclidean group is the automorphism group of the Euclidean space $\mathscr{E}_d$; it is the semi-direct product $Eu_d = R^d \rtimes O_d$ where R^d is the invariant subgroup of translations. Instead of $y = \boldsymbol{t} \cdot x$, we denote by $y = \boldsymbol{t} + x$ the transformed one of the point $x \in E_d$ by the translation $\boldsymbol{t}$. This formalism has been established in the last quarter of the XIXth century: for instance we can also write

[14] Beware that this action (8) preserves $\det q$ but not the scalar product $\operatorname{tr} q'q''$.

[15] Also explained in Chapter I at the end of Section 4, before Section 4.1.

$\boldsymbol{t} = \boldsymbol{xy} = y - x$. For the mid-point o of the segment ab in $\mathscr{E}_d$ we can write $o = a + \frac{1}{2}\boldsymbol{ab} = \frac{1}{2}(a + b)$; we denote by σ_o the symmetry through the point o, so

$$b = \sigma_o a = a - 2\boldsymbol{oa} = 2o - a \Leftrightarrow o = \tfrac{1}{2}(a + b) \ . \tag{12}$$

More generally a point of $\mathscr{E}_d$ can be written as a linear combination of points with the sum of coefficients $= 1$. Let x_μ be a set of n points indexed by the values of μ, $1 \leq \mu \leq n$; with real coefficients λ_μ:

$\sum_\mu \lambda_\mu x_\mu$ with $\sum_\mu \lambda_\mu = 1$ is the linear manifold defined by the x_μ's,

$\sum_\mu \lambda_\mu x_\mu$ with $\lambda_\mu \geq 0$, $\sum_\mu \lambda_\mu = 1$ is the convex hull of the x_μ's,

$(1/n)\sum_\mu x_\mu$ is the barycenter of the x_μ's.

To write explicitly the group law of the Euclidean group Eu_d we choose an origin o on the Euclidean space $\mathscr{E}_d$. Then every element of Eu_d can be written as the product of first, an orthogonal transformation $A \in O_d$ and second, of a translation $\boldsymbol{t} \in R^d$. We write[16] such an element $\{\boldsymbol{t}, A\}$. Its action on the point $x \in \mathscr{E}_d$ and its group law are

$$\{\boldsymbol{t}, A\} \cdot x = Ax + \boldsymbol{t}; \quad \{\boldsymbol{s}, A\}\{\boldsymbol{t}, B\} = \{\boldsymbol{s} + A\boldsymbol{t}, AB\} \ ,$$
$$\{\boldsymbol{s}, A\}^{-1} = \{ -A^{-1}\boldsymbol{s}, A^{-1}\} \ . \tag{13}$$

Since a lattice L is a subgroup of the translation group R^d,

Definition. An *Euclidean lattice* $\bar{L} \subset \mathscr{E}_d$ is an orbit $L + x$ of a d-dimensional lattice of translations.[17] As is well known, by choosing a point $o \in \mathscr{E}_d$ we have an identification $x \leftrightarrow \boldsymbol{ox}$ of this Euclidean space with a vector space of origin o. Given an Euclidean lattice $\bar{L}$, by choosing any point $o \in \bar{L}$, we obtain its lattice (of translations). The symmetry group G_L of $\bar{L}$ is the stabilizer of $\bar{L}$ in Eu_d:

$$G_L = L \rtimes P^z \subset Eu_d, \quad \text{elements: } \{\ell, A\},\ \ell \in L,\ A \in P^z \ . \tag{14}$$

It is easy to verify that it is the Bravais group of L which enters the semi-direct product (indeed to build it one must know the action of P on L); hence we obtain a new definition of the Bravais class from the structure of the stabilizer $(Eu_d)_L$ of L in the Euclidean group

$$P^z_L = (Eu_d)_L / L \ . \tag{15}$$

Let $\ell, \ell', \ell'' \in L$; We know that $-I_d \in P$ and from Eqs. (14) and (13) we obtain

$$\{\ell' + \ell'', -I\} \cdot \ell = \ell' + \ell'' - \ell \ . \tag{16}$$

The comparison with Eq. (12) shows that the element of G_L in Eq. (16) is the symmetry through the middle of the segment $\ell'\ell''$; if we consider also the case $\ell' = \ell''$ we have proven:

[16] In the solid-state literature, as here, the usual convention for product of operators or group elements is adopted: $g_1 g_2$ means first g_2 then g_1. However, it seems to be a tradition to write the elements of the Euclidean group $\{A, \boldsymbol{t}\}$, with the operation A performed before the translation t. Here we cannot adopt this incoherence.

[17] The original paper of Bravais (1850) on Euclidean lattices is very interesting to read.

Proposition 3a. *An Euclidean lattice $\bar{L}$ has an infinity of symmetry centers: they are its points and the middle of the segments formed by any pair of its points.*

With the notation introduced between Eqs. (9) and (10).

Corollary 3a. *The symmetry centers of $\bar{L}$ form an Euclidean lattice that we denote $\frac{1}{2}\bar{L}$.*

We are interested by *intrinsic Euclidean lattices*: they are defined modulo their position in $\mathscr{E}_d$; so the set of intrinsic lattices can be identified with the set $\{Eu_d \cdot \bar{L}\}$ of Euclidean lattice orbits.

With the choice of a basis one easily defines a *fundamental domain* of $\bar{L}$, that is a domain in $\mathscr{E}_d$ which contains one, and one only, point of each orbit of the translation lattice L. Let us give examples of fundamental domains, defining them by the coordinates x_i of their points x:

$$\mathscr{P}_b = \{x; 0 \le x_i < 1\}, \quad \mathscr{P}_b^o = \mathscr{P}_b - \boldsymbol{w};\ \boldsymbol{w} = ([\tfrac{1}{2}]^d)\ , \tag{17}$$

the last expression means that every coordinate of $\boldsymbol{w}$ is $\frac{1}{2}$, so $\mathscr{P}_b^o$ is the same parallelepiped as $\mathscr{P}_b$, but it is centered at the origin. Remark that the closure of $\mathscr{P}_b$ (replace < 1 by ≤ 1 in the definition) contains 2^d points of the Euclidean lattice containing o.

We denote by L_a the set of lattice vectors of norm a. For the shortest vectors of L we also write $S = L_s$. The minimum distance for two points of the Euclidean lattice $\bar{L}$ is $d = \sqrt{s}$. As we have seen for Delone sets, the number of points of $\bar{L}$ in any bounded domain is finite (otherwise there would exist an accumulation point). So all L_a's are finite sets. The set $\mathscr{N}$ of values of the norm of the vectors of L is countable and discrete; it contains 0, the other values are positive and unbounded and s is the smallest positive value of $\mathscr{N}$. Then $L = \bigcup_{a\in\mathscr{N}} L_a$.

3.3. Two-dimensional crystallographic systems and Bravais classes

From Eq. (7) we know that the point group is a subgroup of O_d and is conjugate to the Bravais group P^z, a subgroup of $GL(n, Z)$. This implies the necessary condition that the trace of its matrices must be integers; this condition is sufficient for $d = 2$. As we saw in Chapter I, Section 3, Eqs. (7)–(8), the matrices of O_2 represent either rotations or reflections and their respective traces are $2\cos\theta$ and 0. So the rotations must be of order $1, 2, 3, 4, 6$. That gives

ten geometric classes: $1 = c_1$, $2 = c_2$, $3 = c_3$, $4 = c_4$, $6 = c_6$,

$m = c_s$, $2mm = c_{2v}$, $3m = c_{3v}$, $4mm = c_{4v}$, $6mm = c_{6v}$.

As we remark after Eq. (7), $-I_2$ is an element of every holohedry P. For $d = 2$ this matrix represents also the rotation by π. The groups of six geometric classes contain it. It is easy to show that $4 = c_4$ and $6 = c_6$ cannot be the full symmetry group of a lattice. Let us prove it for $4 = c_4$. Let S be the set of short vectors. They form one orbit of four vectors $\pm \boldsymbol{s}_i$, $(\boldsymbol{s}_i, \boldsymbol{s}_j) = s\delta_{ij}$, $i = 1, 2$; indeed if there were another c_4 orbit (of the same norm) we can verify that these two orbits of vectors would generate a dense subgroup of R^2. We prove that S generates the full lattice. Assume that it is not correct, i.e. S generates only a sublattice L' whose vectors are those with integer coordinates in the basis $\{\boldsymbol{s}_i\}$; so there should be in L, a vector $\boldsymbol{v} = \sum_i \lambda_i \boldsymbol{s}_i \notin L'$ whose coordinates λ_i are not both integers. By translation in L' we transform it to a vector $\boldsymbol{w}$ of coordinates v_i satisfying $0 \le v_i \le 1$;

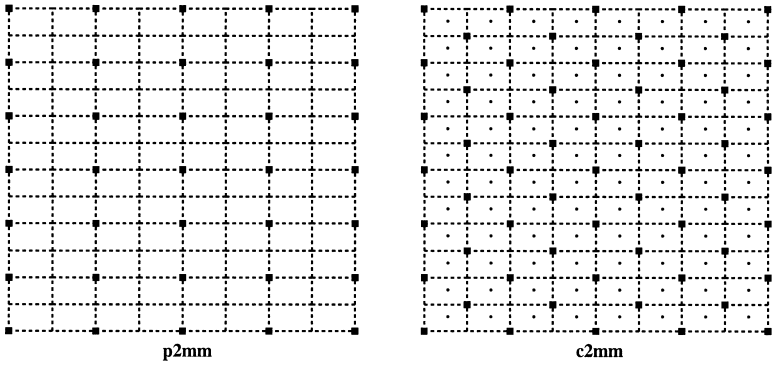

Fig. 1. Euclidean lattices illustrating the two orthorhombic Bravais classes. They have exactly the same symmetry reflection axes; the intersections of these symmetry axes are symmetry centers for both lattices. *c2mm* is obtained from *p2mm* by adding as lattice points the symmetry centers of the rectangles (= body centring). Then new symmetry centers appear for *c2mm*: they are the small dots. The Bravais groups of these two lattices are conjugated in O_2 but not in $GL(2,Z)$. Their space groups, also denoted by *p2mm*, *c2mm*, are not isomorphic.

then the norm of at least two of the four vectors $\boldsymbol{w}$, $\boldsymbol{w}-\boldsymbol{s}_i$, $\boldsymbol{w}-\boldsymbol{s}_1-\boldsymbol{s}_2$ is smaller than the norm of the $\boldsymbol{s}_i$: that is absurd. Since S has the symmetry group $4mm = c_{4v}$, that is also the holohedry of the lattice it generates. By a similar proof we obtain that $6 = c_6$ is not a holohedry.

So there exists four crystallographic systems in dimension 2; we list their names and their symmetry group

$$\{CS\}_2 = \text{diclinic: } 2 = c_2, \quad \text{orthorhombic: } 2mm = c_{2v}\ ,$$

$$\text{quadratic: } 4mm = c_{4v}, \quad \text{hexagonal: } 6mm = c_{6v}.$$

The group $2 = c_2$ is the center of $GL(2,Z)$ so the diclinic system has a unique Bravais class. We prove that the orthorhombic system has two Bravais classes. Fig. 1 shows two Euclidean lattices which have the same holohedry but belong to two different Bravais classes *p2mm*, *c2mm* (*p* is for principal and *c* for centered).

These two Euclidean lattices have exactly the same symmetry reflection axes *m* forming two families of parallel axes in orthogonal directions and whose intersections are symmetry centers. Following the definition of $\mathscr{P}_b$ in Eq. (17), *p2mm* has rectangles as fundamental domains and its points are the vertices of the rectangles. *c2mm* is obtained from *p2mm* by adding the rectangle centers as lattice points; crystallographers say "*c2mm* is obtained by *centering* p2mm". So *p2mm* is a sublattice of *c2mm* and, as Abelian groups, their quotient is Z_2. From Corollary 3a, *c2mm* has also a family of isolated symmetry centers obtained by centring the lattice $\frac{1}{2}L$ of the symmetry centers of $L = p2mm$. So the symmetry groups (= stabilizers in Eu_2) of the two lattices are different; their quotient is also Z_2. The Bravais groups that we obtain from Eq. (15) are different as we will show. The fundamental domain $\mathscr{P}_b$ of *c2mm* is a rhomb. Let $\{\boldsymbol{b}_i\}$, $(\boldsymbol{b}_i,\boldsymbol{b}_i) = b^2$, $(\boldsymbol{b}_1,\boldsymbol{b}_2) \neq 0$ be the corresponding basis of *c2mm*; then $\boldsymbol{a}_\pm = \boldsymbol{b}_1 \pm \boldsymbol{b}_2$ is an (orthogonal) basis of *p2mm*. The two

different representations of the holohedry are generated by the matrices

$$p2mm\colon \pm\sigma_3 = \pm\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad c2mm\colon \pm\sigma_1 = \pm\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \tag{18}$$

where σ_1, σ_3 are Pauli matrices given previously in Eqs. (16) of Chapter III. These two representations are equivalent on the complex, on the real and even on the rational numbers; but they are inequivalent on Z, the ring of integers. That means that the two (isomorphic) groups $p2mm$ and $c2mm$ are non-conjugate subgroups of $GL(2,Z)$. The proof is very simple: matrices conjugated in $GL(d,Z)$ have the same g.c.d.(= greatest common divisor) of their elements; the g.c.d. of the elements of the matrices $I_2 + \sigma_3$ and $I_2 + \sigma_1$ are, respectively, 2 and 1. Note that this difference comes from the existence of two inequivalent integral representations pm and cm of the reflections for $d = 2$. We leave to the reader to show that there are only two such representations[18] and to verify that the general integral matrix representing a reflection is

$$\begin{pmatrix}a & b\\ c & -a\end{pmatrix},\ a^2 + bc = 1,\quad a + b + c \text{ odd for } pm, \text{ even for } cm\ , \tag{19}$$

(hint: verify that $(a + b + c) \bmod 2$ is invariant by a conjugation in $GL(2,Z)$; by such a conjugation one can transform an element of this group into an upper triangular matrix, so $c = 0$, and for a reflection $a = \pm 1$ and $b \in Z$; then try to conjugate in $GL(2,Z)$ the matrices of this form). Note that the lattice $c2mm$ can be defined, in an orthogonal basis $\{\boldsymbol{a}_i\}$ as

$$(\boldsymbol{a}_i, \boldsymbol{a}_j) = a_i^2\delta_{ij},\ a_1^2 \neq a_2^2,\quad cmm = \left\{\sum_i \alpha_i \boldsymbol{a}_i\right\}$$

$$\text{with } \alpha_i \text{ both } \in Z \text{ or both } \in Z + \tfrac{1}{2}\ . \tag{20}$$

The dual basis $\{\boldsymbol{a}_i^*\}$ is also orthogonal. In this basis, the dual lattice is defined by

$$(cmm)^* = \left\{\sum_i \alpha_i' \boldsymbol{a}_i^*\right\}, \tag{21}$$

$$\text{with } \alpha_1' \in Z,\ \alpha_1' + \alpha_2' \in 2Z \Rightarrow (cmm)^* \sim 2(cmm)\ .$$

Indeed, although these two lattices are different, their fundamental domains are rhombs and their Bravais groups are Z-equivalent. Remark that if the centring of $p2mm$ is done by atoms Y different from the atoms X of this lattice, the symmetry is not changed and the space group of the new crystal is again $p2mm$. There is the same density of the two kinds of atoms, so the crystal has XY for its chemical formula; it is a pure convention to say that Y is a centring of the rectangles of X, the other convention exchanging $X \leftrightarrow Y$ is just as good.

We leave to the reader to check that when the rectangles of $p2mm$ become squares (the Bravais group is $p4mm$), the rhombs which define the fundamental domains of $c2mm$, also become squares; that is why there exists a unique Bravais class in the square crystallographic system. When it is

[18] It is also true in any dimension $d > 1$.

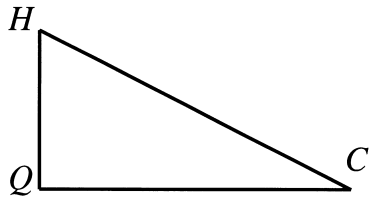

Fig. 2. A fundamental domain of the action of $GL(2,Z)$ on $\mathscr{C}_+(\mathscr{Q}_2)$, the cone of positive quadratic forms q. With the parametrization $\mathrm{tr}\, q = q_{11} + q_{22} > 0$, $\xi = (q_{11} - q_{22})(\mathrm{tr}\, q)^{-1}$, $\eta = 2q_{12}(\mathrm{tr}\, q)^{-1}$, $q = \frac{1}{2}(\mathrm{tr}\, q)(I_2 + \xi\sigma_3 + \eta\sigma_1)$ and the positivity implies $\xi^2 + \eta^2 < 1$, the fundamental domain is the triangle HQC minus the vertex $C(1,0)$ on the surface of the cone. $H(0,\frac{1}{2})$ represents the *p6mm* lattices, $Q(0,0)$ the *p4mm* lattices, the side QC the *p2mm* lattices, the two sides QH and HC the *cmm* lattices with, respectively, four and two shortest vectors; the interior of the triangle represents the diclinic lattices (generic case).

Table 1
The seven Bravais crystallographic systems and the geometrical class of their holohedry in the Schoenflies and the ITC notations

Bravais CS	Triclinic	Monoclinic	Orthorhombic	Tetragonal	Rhombohedral	Hexagonal	Cubic
Schoenflies	C_i	C_{2h}	D_{2h}	D_{4h}	D_{3d}	D_{6h}	O_h
ITC	$\bar{1}$	$2/m$	mmm	$4/mmm$	$\bar{3}m$	$6/mmm$	$m\bar{3}m$

possible, ITC prefer to use orthogonal bases (as we have done in the last two equations) although they are *not* generating bases of the lattice.[19]

It is very important to remark that when $a_1^2 = a_2^2$ (square lattice), the centring yields an equivalent lattice. So the quadratic system has only one Bravais class.

It is interesting to define a fundamental domain for the action of $GL(2,Z)$ on the cone $\mathscr{C}_+(\mathscr{Q}_2)$. That was first done by Lagrange (1773) under the heading "reduction of quadratic form". Following Michel (1995), we present the same result differently, in the basis of $\mathscr{C}_+(\mathscr{Q}_2)$ which is obtained by $\mathrm{tr}\, q = 1$. The result is given by triangle HQC of Fig. 2.

3.4. Three-dimensional Bravais crystallographic systems and classes

In Chapter I, Table 1 (in Section 3) we introduced the 32 geometric classes (conjugacy classes of point groups in O_3), essential for the classification of the symmetry of the macroscopic physics of crystalline states, and gave their Schoenflies and ITC notations. Eleven classes of point groups contain $-I_3$, the symmetry through the origin. By a proof similar to that we have done for $4 = c_4$,

[19] Note for reading the literature: as we have done in the last two equations, the orthogonal bases used in the ITC are not normalized (i.e. the basis vectors do not have unit length). On the contrary, solid state physicists prefer, in general, to use orthornormal bases. Here, in all chapters, we follow the ITC tradition.

we can show that four of them are not holohedry: they are $4/m = C_{4h}$, $\bar{3} = C_{3i}$, $6/m = C_{6h}$, $m\bar{3} = T_h$. The seven others are the holohedries defining the seven Bravais crystallographic[20] systems:

We now established that these seven crystallographic systems contain, respectively: 1, 2, 4, 2, 1, 1, 3 Bravais classes. We shall essentially follow[21] Bravais (1850); it is the standard approach in crystallography (Table 1).[22]

Group $\bar{1}$ has only the representation $\pm I_3$; its Bravais group is denoted by $P\bar{1}$. Group $2/m$ contains a reflection; so it has two inequivalent integral representations $P2/m$, $C2/m$ obtained by an obvious extension of Eq. (18). Similarly to the two-dimensional case, for the orthorhombic group lattices we denote by *Pmmm* the Bravais group of the lattice with a rectangular parallelepiped domain. The other possible Bravais classes are obtained by

(i) centring this domain with the vector $\boldsymbol{w}_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, which gives the Bravais class *Immm* (the I comes from "inner" centring),

(ii) centring the three faces with the vectors $\boldsymbol{f}_1 = (0, \frac{1}{2}, \frac{1}{2})$, $\boldsymbol{f}_2 = (\frac{1}{2}, 0, \frac{1}{2})$, $\boldsymbol{f}_3 = (\frac{1}{2}, \frac{1}{2}, 0)$ which gives the Bravais class *Fmmm* (the *F* comes from faces),

(iii) centring one face only: that is very similar to $d = 2$; which gives the Bravais class *Cmmm*.

The lattices *Fmmm* and *Immm* are dual of each other. When the symmetry becomes tetragonal, as for the two-dimensional case, the *P* and *C* lattices becomes equivalent; it can be shown that the same occurs for the *F* and *I* lattices. So the tetragonal system has two Bravais classes $P4/mmm$ and $I4/mmm$; the last choice is a convention.[23] However, for the cubic system, the equivalence between the tetragonal *I* and *F* centring no longer holds because the equivalence of representations does not extend from the group $4/mmm = D_{4h}$ to the larger group $m\bar{3}m = O_h$. So the cubic system has three Bravais classes: $Pm\bar{3}m$, $Fm\bar{3}m$, $Im\bar{3}m$. Finally the rhombohedral and hexagonal systems have only one Bravais class. The corresponding Bravais groups are, respectively, denoted by $R\bar{3}m$ and $P6/mmm$. Fig. 3 gives the partially ordered set of conjugacy classes of Bravais groups as subgroups of $GL(3, Z)$ and the map ϕ' on the partially ordered set of holohedries (conjugacy classes in O_3); this map is order preserving.

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[20] Their definition is given on p. 722 of ITC and they are called Bravais systems; while ITC calls crystal systems (p. 721) those introduced earlier by Weiss (1816); there are also seven of them with five which coincide with five of the Bravais systems. The union of the Bravais (rhombohedral$\cup$hexagonal) systems coincide with the union of the Weiss (trigonal$\cup$hexagonal) systems and it is called "hexagonal family" in the international tables. Strangely, these tables refuse to make a choice between the two partitions of the "family". The Weiss classification was remarkable but empirical; trigonal is for the crystals which have a 3 or $\bar{3}$ symmetry and hexagonal is for the crystals with a 6 or $\bar{6}$ symmetry. The latter belong also to the Bravais hexagonal system. The international tables distinguish among the space groups of the trigonal crystal systems by their first letter *R*, *P* those who belong, respectively, to the rhombohedral and hexagonal Bravais systems. More generally, in ITC, the "international symbols" for space groups follow the Bravais classification. Here we use the Bravais classification as the natural and fruitful one for the study of crystal symmetry.

[21] The first classification was made by Frankenheim (1842): he found 15 classes. Bravais (1850) not only corrected the error, but made a deep mathematical analysis of the two- and three-dimensional lattices (e.g. he introduced the concept of dual lattices) extending the work of Gauss (1805) that he quotes several times.

[22] The determination of the set of strata: $\mathscr{C}_+(\mathscr{Q}_3)\|GL(3, Z)$ has been made by Schwarzenberger (1980).

[23] Indeed the ITC could have chosen $F4/mmm$ (they do it for listing some subgroups of space groups); probably the inner centring was considered simpler than the 3-face centring.

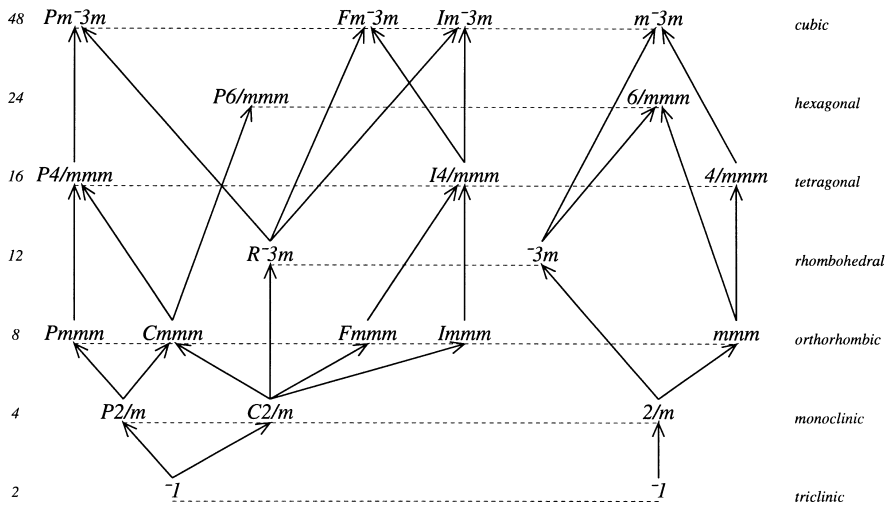

Fig. 3. For three dimensional crystallography, the left diagram shows the partial order on $\{BC\}_3$, the set of the 14 Bravais classes and the right one shows the partial order on $\{CS\}_3$, the set of the 7 Bravais crystallographic systems. The dotted horizontal lines give the order preserving map ϕ' defined after Eq. (7).

4. Geometric and arithmetic classes. Brillouin zone. Time reversal

4.1. Two maps on the set $\{AC\}_d$ of arithmetic classes

As we recall in the introduction, crystals have a translation lattice of symmetry L and the crystal structure is defined by the positions of the atoms in a fundamental domain of L. In the next section we will show the existence of a fundamental domain $\mathscr{D}_L$ invariant by the Bravais group[24] P_L^z of L. In $\mathscr{D}_L$, if the atom positions, for each kind of atom, are not a union of orbits of P^z, the point symmetry of the crystal is smaller and it corresponds to an *arithmetic class*, i.e. the conjugacy class of a finite group of $GL(d,Z)$ that we also denote by P^z (Bravais groups are particular examples of arithmetic classes). Since $GL(d,Z) < GL(d,R)$, the conjugacy class $[P^z]_{GL(d,Z)}$ defines the conjugacy class $[P^z]_{GL(d,R)}$, i.e. a real linear representation of P^z up to an equivalence. Since P^z is finite, it is well known that such a representation is equivalent to an orthogonal one, which defines the geometric class $P = [P^z]_{O_d}$ of P^z, i.e. its conjugacy class in O_d. In other words, we have constructed the natural map

$$\{AC\}_d \xrightarrow{\phi} \{GC\}_d \tag{22}$$

between the set of arithmetic and geometric classes in d-dimension. As we already explained, in general the symmetry of the macroscopic physical properties of the crystal depends only on its geometric class.

[24] This invariant domain is called the Wigner–Seitz domain by the physicists. It was known much before: see the beginning of Section 5.

The Bravais groups form a subset of the arithmetic classes. There is also a natural surjective map from the arithmetic classes to the Bravais classes (see e.g., Michel and Mozrzymas, 1989)

$$\{AC\}_d \xrightarrow{\alpha} \{BC\}_d \ . \tag{23}$$

This map is not obvious. Notice that, as all other symmetries, the crystal symmetry must be defined up to conjugacy class of the space group. Which one? It is more than the conjugacy class in Eu_d, the Euclidean group, but less that the conjugacy class in Aff_d, the affine group. It is only part of the latter: it is $Eu_d \cap [G]_{Aff_d}$, the intersection of the Euclidean group and of the conjugacy class of G in the affine group. Indeed, as long as no phase transition occurs, the variation of external parameters (e.g. temperature, pressure) does not change the symmetry of the crystal, but only conjugate the space group in Aff_d but with the condition that it remains a subgroup of Eu_d. The lattice of translations is modified and, when its symmetry is not that of a maximal Bravais class, it may increase and belong to every larger Bravais class (think, as an example, to the space group $P1$ for which the whole class $[G]_{Aff_d}$ is inside Eu_d). That larger symmetry of L, the translation lattice, has to be considered as accidental. We can make a mathematical description of this phenomenon by using the theorem of Palais (1961) of good stratification when all the stabilizers (here for the action on $GL(3,Z)$ on $\mathscr{C}_+(\mathscr{Q}_3)$) are finite. Indeed given a group K belonging to an arithmetic class P^z, we consider $\mathscr{C}_+(\mathscr{Q}_3)^K$, the set of positive quadratic form invariant by K. It is the intersection of the cone $\mathscr{C}_+(\mathscr{Q}_3)$ with the vector subspace in E_N (the vector space of quadratic forms) which carries the trivial representation of K. The stratification in Bravais classes on $\mathscr{C}_+(\mathscr{Q})_3$(= strata of the action of $GL(d,Z)$) induces by restriction on $\mathscr{C}_+(\mathscr{Q})_3^K$ a stratification with an open dense stratum; the corresponding Bravais class defines the value of the map α of Eq. (23) for the arithmetic class of K.

As a preliminary study of arithmetic and geometric classes, one can study the conjugacy classes of finite-order elements in $GL(3,Z)$ and $GL(3,R)$. We call these classes *arithmetic elements* and *geometric elements*.[25] As we know, for $d = 2, 3$ their order is $1, 2, 3, 4, 6$. To label the arithmetic and geometric elements we use the notation of ITC for the cyclic group they generate. These elements are the building bricks of the arithmetic and geometric classes. Their numbers are, respectively, 7 and 6 for $d = 2$, and, respectively, 16 and 10 for $d = 3$.

4.2. Geometric and arithmetic elements and classes in dimension 2

We have already listed in Section 3.3 the 10 geometric classes for $d = 2$. As we have seen, they are formed from six geometric elements: five rotations $1, 2, 3, 4, 6$ in SO_2 and m, the conjugacy class of the reflections through an axis; it contains all the elements of determinant -1 of O_2. It requires some arguments of number theory to prove that each of the geometric classes corresponding to the rotation groups 3, 4, 6 has a unique arithmetic class. We have shown in Eq. (19) that there are two arithmetic classes corresponding to m and given their notation pm, cm. To summarize:

[25] The ITC define the geometric elements and give their list in p. 6. The definition of the arithmetic elements is only implicit.

For $d = 2$, the arithmetic elements are: $p1$, $p2$, $p3$, $p4$, $p6$, pm, cm. A choice of matrices representing them is: $(p1) = I_2 = -(p2)$,

$$(pm) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (cm) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (p4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

$$(p3) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad (p6) = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}. \tag{24}$$

((pm) and (cm) were given in Eq. (18)). This simple choice of matrices in Eq. (24) requires the following restrictions on the vectors of the basis: their angle is $\pi/2$ for (pm) and $(p4)$, arbitrary for (cm) and $2\pi/3$ for $(p3)$, $(p6)$; except for (pm), the two vectors have the same norm.

The maximal geometric classes are $4mm = c_{4v}$, $6mm = c_{6v}$. From the fact that the arithmetic classes of 4 and 6 are unique it is easy to show that each one of these two maximal geometric classes have unique arithmetic classes $p4mm$, $p6mm$. The conjugacy classes of their subgroups are given in Chapter I, Fig. 1. For these two finite groups, when the same geometric class appears for different conjugacy classes, one has to check if those become conjugate in $GL(2, Z)$; if the answer is negative, these conjugacy classes are distinct arithmetic classes and we need some notations for distinguishing them. For $4mm = c_{4v}$ that is the case for c_s which yields pm, cm and c_{2v} which yields $p2mm, c2mm$. For $6mm = c_{6v}$, it is the case for c_{3v}; ITC denote the two corresponding arithmetic classes $p3m1$ and $p31m$ and distinguish them in a given coordinate system. Let us follow this pedestrian argument before giving one which is coordinate independent. In the system of coordinates corresponding to Eq. (24) the representations of $p3m1$ and $p31m$ are, respectively, generated by the pairs of matrices $(p3)$, (cm) and $(p3)$, $-(cm)$; the two $\pm(cm)$ correspond to the orthogonal duality between the sets of three symmetry axes in the two groups. These two representations are conjugated in $GL(2, R)$; the matrices x which conjugate them must satisfy the linear homogeneous system of equations

$$x(p3) = (p3)x, \quad x(cm) = -(cm)x\,,$$

$$\text{solutions } x = \lambda \begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix}, \quad \det x = 3\lambda^2\,. \tag{25}$$

The value of the determinant shows that if $\lambda \in Z$ the corresponding matrix cannot be in $GL(2, Z)$; for $\lambda = (\sqrt{3})^{-1}$, $x \in SO_2$. It is a rotation by $\pi/2$ since $x^2 = -I_2$; indeed Eq. (25) requires that x commutes with the rotations (so it is one of them) and transforms a symmetry axis into an orthogonal one. We could have made the same proof without a choice of coordinate: $(12)mm = c_{1\,2v} \in O_2$ is the normalizer of $6mm = c_{6v}$ in O_2 and is a realization of the automorphism group Aut $6mm$. The outer automorphisms exchange the two conjugacy classes of the subgroups $3m = c_{3v}$; but we know that $(12)mm$ has no two-dimensional integral representations.

The arithmetic classes $p3m1$ and $p31m$ are distinct and the space groups (semi-direct products with the hexagonal lattice of translation) that they define are non-isomorphic. Let S be the set of the six shortest vectors of this lattice: the 3 symmetry axes of $p3m1$ contain the S vectors while the 3 symmetry axes of $p31m$ are bisectors of the $\pi/3$ angles formed by the S vectors. The six endpoints of the S vectors define with the origin 6 equilateral triangles which are Delone cells of the hexagonal

lattice.[26] For the group $p3m1$ the sides of the Delone cells are carried by the symmetry axes; therefore it is a group generated by reflection. Indeed it is the group defined by the triangular kaleidoscope;[27] this kaleidoscope is popular as a toy and we strongly advise the reader to play with it if he has not yet done it!

Fig. 4 shows the two diagrams representing the partial order, the left one on $\{AC\}_2$ the set of the 13 arithmetic classes, the right one on $\{GC\}_2$, the set of the 10 geometric classes. The dotted horizontal lines give the order preserving map ϕ defined in Eq. (22). We give in the next equation the correspondence α defined in Eq. (23), mapping the 13 arithmetic classes on the five Bravais classes; the value of α is the last element of each subset:

$$\alpha: \quad p1, p2, \quad pm, p2mm, \quad cm, c2mm, \quad p4, p4mm, \quad p3, p3m1, p31m, p6, p6mm\ . \tag{26}$$

The first eight listed arithmetic classes are orthogonal (i.e. $\leq p4mm = \mathrm{O}(2, Z)$) and therefore self-dual. The five arithmetic classes belonging to the hexagonal Bravais class cannot be represented by orthogonal integral matrices; among them, the two arithmetic classes $p3m1$, $p31m$ which correspond to the same geometric class, form (up to an equivalence on Z) a pair of dual arithmetic classes. Indeed, by conjugation by the matrix

$$-\mathrm{i}\sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

the representation (given before Eq. (25)) of each one is transformed into the other representation. So, among the 13 arithmetic classes in dimension 2, there is a unique pair of dual arithmetic classes

$$\text{duality} \qquad p3m1 \leftrightarrow p31m\ . \tag{27}$$

4.3. Geometric and arithmetic elements and classes in dimension 3

As we showed in Chapter I, Table 1 there are two maximal geometric classes: $m\bar{3}m = O_h$ and $6/mmm = D_{6h}$. From the previous section (see Fig. 3), we know that the second one has a unique Bravais class, $P6/mmm$ while the first one has three. One of them has been implicitly studied in Chapter I, Fig. 2; it corresponds to $\mathrm{O}(3, Z) = Pm\bar{3}m$. We now built the two others and verify their properties:

$$(\boldsymbol{e}_i, \boldsymbol{e}_j) = \delta_{ij}, \quad Pm\bar{3}m = \left\{ \sum_i \mu_i \boldsymbol{e}_i \right\}, \quad \mu_i \in Z\ . \tag{28}$$

[26] Delone cells have been defined in Section 1. By the translations we obtain the Delone cells of any points; they are triangles so the hexagonal lattice is primitive (this concept is also defined in Section 1).

[27] The other two-dimensional space groups generated by reflection are $p6mm$, $p4mm$, $p2mm$. The kaleidoscope is the smaller polygon formed by the infinite set of symmetry axes; it is, respectively, a triangle of angles $\pi/2,\pi/3,\pi/6$, an isocele triangle of angles $\pi/2,\pi/4,\pi/4$, a rectangle (see Fig. 1); only in the last case the kaleidoscope is also a Delone cell of the lattice. There exists a classification of the reflection space groups in any dimension d; they are labelled by an extended Dynkin diagram and they are the Weyl groups of some Kac-Moody algebras. This beautiful theory is outside the scope of this monography, but it is used in other fields of physics.

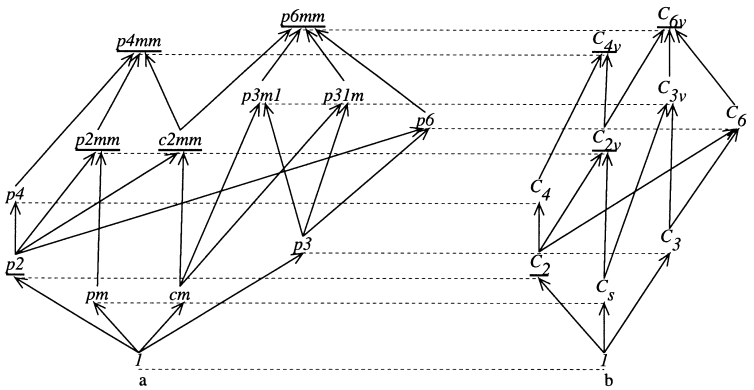

Fig. 4. For $d = 2$ the two diagrams show the partial order, the left one on $\{AC\}_2$, the set of the 13 arithmetic classes, the right one on $\{GC\}_2$, the set of the 10 geometric classes. The underlined classes in a, b are, respectively, the Bravais classes and the crystallograpic systems. The dotted horizontal lines give the order preserving map ϕ defined in Eq. (22).

Let us write the I-cubic lattice as the centering of the P-cubic one, with $\boldsymbol{w}_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$:

$$Im\bar{3}m = Pm\bar{3}m \cup (\boldsymbol{w}_3 + Pm\bar{3}m)$$

$$\Leftrightarrow Im\bar{3}m = \left\{ \sum_i \mu_i \boldsymbol{e}_i, \text{ either } \mu_i \in Z, \text{ or } \mu_i \in Z + \tfrac{1}{2} \right\}. \tag{29}$$

Let us define:

$$Fm\bar{3}m = (Im\bar{3}m)^* \Leftrightarrow Fm\bar{3}m = \left\{ \sum_i \mu_i \boldsymbol{e}_i \right\}, \quad \mu_i \in Z, \quad \sum_i \mu_i \in 2Z\ . \tag{30}$$

We may choose for the basis of the last two lattices, with the notation of Eq. (4):

$$\tilde{b}_F = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad \tilde{b}_I = \tfrac{1}{2} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \quad \Rightarrow \tilde{b}_F \tilde{b}_I^{\top} = I_3\ . \tag{31}$$

The basis $\tilde{b}_F$ shows explicitly that $Fm\bar{3}m$ is obtained from $Pm\bar{3}m$ by centering the three faces of the unit cube and the last relation of Eq. (31) proves the duality in Eq. (30).

The corresponding quadratic forms are

$$q_F \equiv q(Fm\bar{3}m) = I_3 + J_3, \quad q_I \equiv q(Im\bar{3}m) = I_3 - \tfrac{1}{4} J_3 \quad \text{with } (J_3)_{ij} = 1, \quad q_F q_I = I_3\ . \tag{32}$$

Instead of the cubic system we could have worked in the orthorhombic system. In Eq. (28) we start not from an orthonormal basis but from an orthogonal one: $(\boldsymbol{e}_i, \boldsymbol{e}_j) = a_i^2 \delta_{ij}$. Eqs. (28)–(31) are unchanged but in Eq. (31) the basis $\tilde{b}_I$ is expressed in the dual orthogonal basis $(\boldsymbol{e}_i, \boldsymbol{e}_j) = a_i^{-2} \delta_{ij}$. Then, from the matrices representing the reflection (Pm_i) (given in Chapter I, Eq. (16)) we can

compute those representing the reflections $(Fm_i) = \tilde{b}_F^{-1}(Pm_i)\tilde{b}_F$. We obtain

$$(Fm_1) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad (Fm_2) = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 1 & 1 \\ -1 & 0 & 0 \end{pmatrix},$$

$$(Fm_3) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 1 & 1 & 1. \end{pmatrix}. \tag{33}$$

We verify the relations:

$$(Fm_i)^2 = I, \quad i,j,k \text{ permutation of } 1,2,3,$$

$$(Fm_i)(Fm_j) = (Fm_j)(Fm_i) = -(Fm_k)\ . \tag{34}$$

So the (Fm_i)'s generate $Fmmm$, the $-(Fm_i)$'s generate $F222$ and $(Fm_i), (Fm_j)$ generate $(Fmm2)_k$. The reflections (Im_j) are represented by the dual matrices:

$$(Im_j) = (Fm_j)^{\top}\ . \tag{35}$$

The three F (respectively, I) reflections can be transformed into each other by conjugation by the matrices of the arithmetic class $R3$ which permute the coordinates circularly. To verify that these six matrices belong to the arithmetic class Cm [which we have represented, in Chapter I, Eq. (17) by $Z_2(Cm_3)$, where (Cm_3) is the permutation matrix permuting the coordinates 1, 2], it is sufficient to show it explicitly on one of them for each family:

$$(Fm_2) = X(Cm_3)X^{-1}, \quad (Im_2) = X^{-1\top}(Cm_3)X^{\top}\ ,$$

$$X = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \tag{36}$$

We will later need

$$(Fm_3) = X(Im_3)X^{-1}\ ,$$

$$(Fm_1) = -(Fm_2)(Fm_3) = -X(Cm_3)(Im_3)X^{-1}\ . \tag{37}$$

Notice that (Im_3) and (Cm_3) commute. To summarize we have introduced another (i.e. Z-equivalent) representative of the $Fmmm$ arithmetic class:

$$X^{-1}(Fm_i)X = (Fm_i)' = \{(-(Cm_3)(Im_3), (Cm_3), (Im_3)\}\ . \tag{38}$$

We now show that the two integral representations $Fmmm$ and $Immm$ of the geometric class mmm are inequivalent on Z. For that we consider the most general 3×3 real matrix S whose elements satisfy the system of linear equations: $(Im_1)S = S(Fm_1)$, $(Im_2)S = S(Fm_2)$; using Eq. (34) we verify

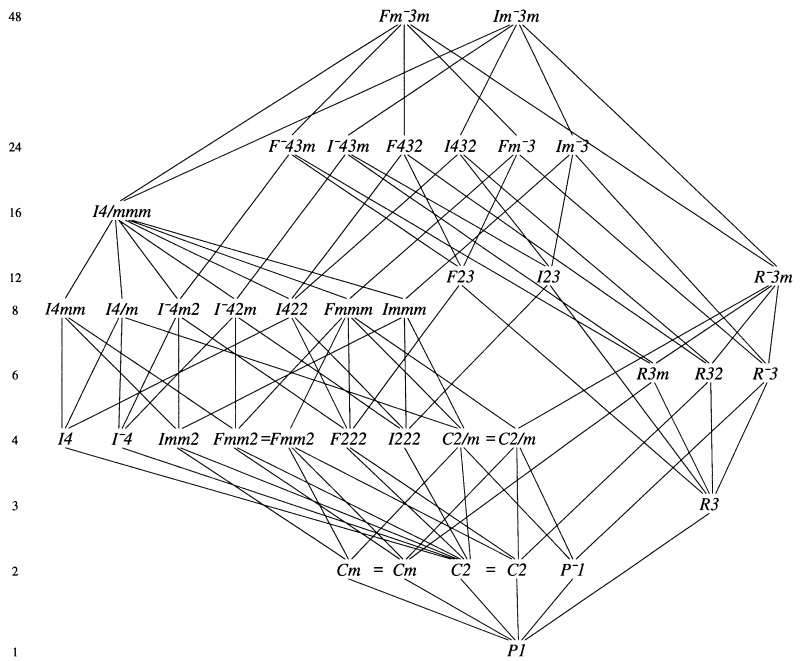

Fig. 5. Diagram of the partially ordered set of the conjugacy classes of subgroups of the maximal Bravais groups $Fm\bar{3}m$ and $Im\bar{3}m$; there are four pairs of classes whose elements belong to the same arithmetic classes: they have a = sign between them.

that this implies $(Im_3)S = S(Fm_3)$. The most general solution in integers is

$$S = \begin{pmatrix} \mu+\nu & \nu & \mu \\ \nu & \nu+\lambda & \lambda \\ \mu & \lambda & \lambda+\mu \end{pmatrix}, \quad \det S = 4\lambda\mu\nu,\ \lambda,\mu,\nu \in Z\ . \tag{39}$$

This shows that the two representations are equivalent on the real and the rational but are not equivalent on the integers: indeed the determinant of S cannot be ± 1 when λ, μ, ν are integers.

We verify in Chapter I, Fig. 2 that each of the five cubic group is generated by $222 = D_2$ and one of the five rhombohedral groups. So the inequivalence on Z of $F222$ and $I222$ can be extended to the representations $Fm\bar{3}m$ and $Im\bar{3}m$ or to any other pair of corresponding cubic arithmetic class. The partially ordered set of conjugacy classes of the subgroups of $Fm\bar{3}m$, $Im\bar{3}m$ are shown in Fig. 5 (We recall that those of $Pm\bar{3}m, P6/mmm$ are shown in Chapter I, Figs. 2 and 3).

We have seen in the previous section (after Eq. (21)) that for the square crystallographic system (= geometric class $4mmm$) there is a unique Bravais class whose Bravais group is $p4mm \sim \mathrm{O}(2, Z)$. The last expressions of Eqs. (29)–(30) define cubic lattices in any dimension d and it is not difficult to prove for $d > 4$ the existence of three maximal Bravais classes P, F, I for the geometric class (called also the Coxeter group B_d) of symmetry of the d-dimensional cube (one can use $\boldsymbol{w}_d$ with its d coordinates $= \frac{1}{2}$ in the orthonormal basis $(\boldsymbol{e}_i, \boldsymbol{e}_j) = \delta_{ij}$). For dimension $d = 4$, $(\boldsymbol{w}_4, \boldsymbol{w}_4) = 1 = (\boldsymbol{e}_i, \boldsymbol{e}_i)$; these vectors belong to the orbit of a larger Coxeter group F_4 (with $|F_4 : B_4| = 3$) which

has some deep relations with the quaternions and is the symmetry group of a regular self-dual polytope which exists only in $d = 4$. For this dimension the lattices F and I are equivalent and distinct from the P lattice of Bravais group $O(4, Z)$.

Another obvious generalization to any dimension is to extend the definition in Eq. (32) of the matrix J_3 to J_d (i.e. all its elements are 1); verify that $J_d^2 = dJ_d$. Then the quadratic forms

$$q_d^{\mathrm{r}} = I_d + J_d, \quad q_d^{\mathrm{w}} = I_d - (d+1)^{-1} J_d, \quad q_d^{\mathrm{r}} q_d^{\mathrm{w}} = I_d \ , \tag{40}$$

define two dual lattices denoted as A_d^{r} and A_d^{w} since they are the root and weight lattices of the simple Lie algebra $A_d \sim SU(d+1)$. We have already seen that for $d = 2$ they are in the same Bravais class: the hexagonal one. The lattice A_d^{w} has been studied in arbitrary dimensions, first by Voronoï (1908, 1909); it is studied here in Section 5.3.

We still have to study the tetragonal system. As we have done in Eq. (33) we compute

$$(F4) = \tilde{b}_F^{-1}(P4)\tilde{b}_F = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$$
$$= (Cm_3)(Fm_2) = (Fm_1)(Cm_3) \tag{41}$$

and find the equivalence with its dual arithmetic class:

$$(I4) = (\widetilde{F4}) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix} = X^{-1}(F4)X$$
$$= (Cm_3)(Im_2) = (Im_1)(Cm_3) \ , \tag{42}$$

where X has been defined in Eq. (36). So the tetragonal system has only two Bravais classes of lattices: P and $F \sim I$. In ITC, the notation I has been chosen;[28] naturally we follow the notations of ITC (e.g. in Fig. 5).

To see more explicitly the self-duality of the I-tetragonal Bravais class, we study the arithmetic class $I422$. First we notice that the square of the I-rotation by $\pi/2$ is $I(4)^2 = -(Im_3)$, the so-called "vertical" I-rotation by π. So $I422$ is generated by $(I4)$ and Im_1, Im_2, the two "horizontal" rotations (one is enough) by π. The two other "horizontal" rotations by π are (use the third equality in Eq. (41)): $-(I4)(Im_2) = -(Cm_3)$, $-(I4)(Im_1) = (Cm_3)(Im_3)$. From Eq. (38), we see that these rotations are $-(Fm_2)'$ and $-(Fm_1)'$ and moreover $-(Fm_3)' = -(Im_3)$. To summarize (and to be used in the future)

the three reflections of $F'mmm$ are: (Cm_3), (Im_3), $(Cm_3)(Im_3)$. (43)

We have also given a matrix realization of the arithmetic class $I422$; from it we find that

the maximal subgroups of $I422$ are $I4$, $I222$, $F'mmm$. (44)

[28] Although in several tables of tetragonal I space groups they use also F presentation in the subtables of maximal subgroups.

That can be read in Fig. 4, but only in terms of arithmetic class (hence independently of their realization). In this figure the duality corresponds to the exchange $F\leftrightarrow I$ in the cubic and orthorhombic system but not in the I tetragonal system except for the exchange of the two arithmetic classes $I\bar{4}m2\leftrightarrow I\bar{4}2m$ which belong to the same geometric class: we leave to the reader, with the use of Eq. (36), to check that the contragradient representation of one of them is Z-equivalent to the representation of the other.

To help the reader we list here the 15 pairs of dual arithmetic classes in 3D. By definition the orthogonal arithmetic classes are self-dual. We first recall the duality $F\leftrightarrow I$ between the elements of three pairs in the orthorhombic system and five pairs in the cubic system

$$\text{orthorhombic}\quad F222\leftrightarrow I222,\quad Fmm2\leftrightarrow Imm2,\quad Fmmm\leftrightarrow Immm\ . \tag{45}$$

$$\text{cubic}\quad F23\leftrightarrow I23,\quad Fm\bar{3}\leftrightarrow Im\bar{3},\quad F432\leftrightarrow I432,\quad F\bar{4}3m\leftrightarrow I\bar{4}3m,\quad Fm\bar{3}m\leftrightarrow Im\bar{3}m\ . \tag{46}$$

There are five other pairs of dual arithmetic classes belonging to the same geometric class and, by the map α of Eq. (23), to the same Bravais class. One verifies that the contragradient representation of one arithmetic group of such a pair is equivalent on Z to the representation of the other group of the pair; for the hexagonal system we use a generalization of the two-dimensional case (27)

$$I\bar{4}m2\leftrightarrow I\bar{4}2m,\quad P321\leftrightarrow P312,\quad P3m1\leftrightarrow P31m,$$

$$P\bar{3}m1\leftrightarrow P\bar{3}1m,\quad P\bar{6}m2\leftrightarrow P\bar{6}2m\ . \tag{47}$$

We have shown in Chapter I, Figs. 2, 3 that all 33 conjugacy classes of subgroups of $O(3,Z)=Pm\bar{3}m$ and the 16 conjugacy classes of subgroups of $P6/mmm$ which are not $\leq Cmmm$ are distinct arithmetic classes. The set of conjugacy classes of subgroups that $Fm\bar{3}m$ and $Im\bar{3}m$ have in common with $Pm\bar{3}m$ are the 10 arithmetic classes $\leq R\bar{3}m$. The set of other subgroup conjugacy classes among these two cubic groups only, defines 14 other arithmetic classes; their images by α of Eq. (23) are the $I4/mmm, Immm, Fmmm$ Bravais classes. Finally each of these two cubic Bravais groups have a specific set of five cubic arithmetic classes. That gives a total of 73 arithmetic classes.[29] The statistics according to the first letter is

$$P:37,\ R:5,\ C:6,\ A:1,\ F:8,\ I:16\ .$$

It is also interesting to look at the distribution of the arithmetic classes among the geometric classes

AC per GC:	1	2	3	4	5 ,	
GC:	8	12	8	3	1	total = 32 ,
AC:	8	24	24	12	5	total = 73 .

The cyclic point groups belong to 10 of the 32 geometric classes and define the 10 geometric elements. They are denoted in ITC: $1,2,3,4,6,\bar{1},m,\bar{3},\bar{4},\bar{6}$, ($m$ replaces $\bar{2}$); a matrix with a $^-$ is obtained by multiplying by $-I_3$ the corresponding rotation matrix.

[29] In his beautiful elementary book H. Weyl (1952) gives 70 for the number of arithmetic classes in three dimensions, reproducing an error which appeared and still appears in most mathematic books dealing with this topics.

For each geometric element there is an arithmetic element labelled P (= principal). There are six other arithmetic elements, and in total the labels for 16 arithmetic elements are

$$\begin{array}{ccccccccc} P1 & P2 & P3 & P4 & P6 & P\bar{1} & Pm & P\bar{3} & P\bar{4} & P\bar{6}\,, \\ & C2 & R3 & I4 & & & Cm & R\bar{3} & I\bar{4}\,. & \end{array}$$

We have shown that the reflections of *Fmmm* and *Immm* are all equivalent to *Cm* (see Eq. (39)): similarly the rotations of these two groups are equivalent to *C*2.

4.4. *Brillouin zone, its high symmetry points*

For periodic crystals, all functions describing their physical properties have the periods of the crystal. Most experiments measure the Fourier transforms of these functions, i.e. functions on the Brillouin zone. In this subsection we define the Brillouin zone and begin the study of the space group actions on it. In Section 3.1 we have defined L^*, the dual lattice of the lattice L, as the set of vectors whose scalar products with all $\ell \in L$ are integers. Physicists also consider the *reciprocal lattice* which is $2\pi L^*$. Indeed it is the one which is obtained in diffraction experiments (with X-rays, neutrons, electrons) by a crystal of translation lattice L. It corresponds to Fourier transform; the momentum variable is usually denoted by $\boldsymbol{k}$ and the vector space of the $\boldsymbol{k}$'s is called the momentum or the reciprocal space. A unitary irreducible representation of the translation group is given by $\boldsymbol{k}(\boldsymbol{x}) = \exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x})]$. Here we are interested in the subgroup of the translation group R^d defined by the lattice of translations L. By restriction to L, two unirreps $\boldsymbol{k}$ and $\boldsymbol{k}'$ of R^d such that $\boldsymbol{k}' - \boldsymbol{k} \in 2\pi L^*$, yield the same unirrep of L. So the set $\hat{L}$ of inequivalent unirreps is

$$L \ni \ell \mapsto \boldsymbol{k}(\ell) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\ell}, \quad \hat{L} = \{\boldsymbol{k} \bmod 2\pi L^*\}\,. \tag{48}$$

Equivalently, with a choice of dual bases (see Eq. (10))

$$\ell = \sum_j \mu_j \boldsymbol{b}_j, \quad \boldsymbol{k} = \sum_j \kappa_j \boldsymbol{b}_j^*, \quad \ell \mapsto \mathrm{e}^{\mathrm{i}\sum_j \kappa_j \mu_j}, \quad \mu_j \in Z,\ \kappa_j \bmod 2\pi\,. \tag{49}$$

The set $\hat{L}$ of the unirreps has the structure of a group, with the group law

$$\boldsymbol{k} \equiv \boldsymbol{k}^{(1)} + \boldsymbol{k}^{(2)} \bmod 2\pi L^* \Leftrightarrow \kappa_j \equiv \kappa_j^{(1)} + \kappa_j^{(2)} \bmod 2\pi\,. \tag{50}$$

This group is called the *dual group* of L by the mathematicians and the *Brillouin zone* (= BZ) by the physicists. It is isomorphic to the group

$$\hat{L} = BZ \sim U_1^d\,. \tag{51}$$

We denote by $\hat{k}$ the elements of BZ in order to distinguish clearly between $\boldsymbol{k}$ and $\hat{k} =: \boldsymbol{k} \bmod 2\pi L^*$. The Bravais group P_L^z of L acts on BZ through its contragradient representation $\tilde{P}_L^z =: (P_L^z)^{-1\top}$. More generally, since by definition of BZ the translation group acts trivially, a space group G acts through its quotient

$$G \xrightarrow{\theta} G/L = P^z\,. \tag{52}$$

So the space groups belonging to the same arithmetic class P^z have the same action. As usual, we denote by G_k the stabilizer in G of $\hat{k} \in BZ$ and $P^z_{\hat{k}}$ the stabilizer in P^z. The latter stabilizer depends only on the arithmetic class; beware that for a given $\hat{k}$ the stabilizers $G_k = \theta^{-1}(P^z_{\hat{k}})$ for[30] the different space groups of the arithmetic class P^z are, in general, non-isomorphic. Notice that the G_k's are also space groups.

The action of the space groups on BZ preserves its group structure, i.e.

$$\forall g \in G, \quad g \cdot \hat{k}^{(1)} + g \cdot \hat{k}^{(2)} = g \cdot (\hat{k}^{(1)} + \hat{k}^{(2)}) \,. \tag{53}$$

As a consequence we have the obvious proposition, that we write for any arithmetic class.

Proposition 4. *In the action of P^z on BZ, the fixed elements form a group, generally denoted by $(BZ)^{P^z}$; the elements of a coset of this group have the same stabilizer.*

We also remark that an orbit contains only elements of BZ of the same order v (we recall that v is the smallest integer such that[31] $v\hat{k} = 0$). A d-dimensional torus is the topological product of d circles; this is the topology of the group U_1^d. So there is a natural, global system of coordinates on it made of d angles ω_i, $1 \leq i \leq d$, with all $\omega_i = 0$ for the 0 element of this Abelian group; the group law is the addition modulo 2π of each coordinate ω_i. For instance the elements of order 2 have $0 \leq m < d$ coordinates 0 and $d - m$ coordinates π. So BZ has $2^d - 1$ elements of order 2.

In this section we only study for $d = 2,3$ the strata of dimension 0 which appear in the action on BZ of the 5, 14 Bravais groups (listed in Figs. 4 and 3, respectively). We point out that, even for this non-linear action, the stabilizers of these strata cannot belong to an axial or planar (i.e. leaving fixed an axis or a plane) geometrical class. The smallest Bravais group, in any dimension, is $Z_2(-I_d)$ (where $-I_d$ is the symmetry through the origin). Since $-\pi \equiv \pi \bmod 2$, this group has the 2^d fixed points: those who satisfy $2\hat{k} = 0$, i.e. the elements of order 2 and the origin. Since this group is a subgroup of any other Bravais group, for these groups the set of order 2 elements of BZ is partitioning into orbits belonging to strata of dimension 0.

For $d = 2$. The matrices generating the five Bravais groups are given in Eq. (24). The matrices of $p2$ and $p2mm$ are diagonal so the four points satisfying $2\hat{k} = 0$, i.e. $(0,0), (\pi,0), (0,\pi), (\pi,\pi)$, are fixed points. The reflection (cm) exchanges $(\pi,0)$ and $(0,\pi)$ and leaves (π,π) fixed; since the orthogonal Bravais group $p4mm$ is generated by $p2mm$ and $c2mm$ it has the same action on the $2\hat{k} = 0$ points as $c2mm$. To study the hexagonal Bravais group $p6mm$, let us compute the contragradient of $(p3)$ and study its action

$$\widetilde{(p3)} = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \quad \widetilde{(p3)} \begin{pmatrix} \kappa_1 \\ \kappa_2 \end{pmatrix} = \begin{pmatrix} -\kappa_1 - \kappa_2 \\ \kappa_1 \end{pmatrix}. \tag{54}$$

In the action of $p6mm$ on BZ, the element $(p3)$ transforms $(\pi,0)$ into (π,π) and this point into $(0,\pi)$. So the three elements of order 2 of BZ form a unique orbit. Eq. (54) tells us that the coordinates of

[30] The map θ is not invertible, so θ^{-1} alone has no meaning; but it is an accepted tradition to denote by $\theta^{-1}(P_k)$ the counter image of P_k by θ, i.e. the unique subgroup of G such that $\theta(G_k) = P^z_{\hat{k}}$.

[31] We use the additive notation for the group BZ.

Table 2
Strata of zero-dimension in the action of Bravais groups on BZ for $d = 2$. The points are grouped into orbits and the stabilizer is given

Points of BZ Their order	$\binom{0}{0}$ 1	$\binom{\pi}{0}$ 2	$\binom{0}{\pi}$ 2	$\binom{\pi}{\pi}$ 2	$\binom{2\pi/3}{2\pi/3}$, $\binom{4\pi/3}{4\pi/3}$ 3
Diclinic Orthorhombic	$p2$ $p2mm$	$p2$ $p2mm$	$p2$ $p2mm$	$p2$ $p2mm$	
Orthorhombic Square	$c2mm$ $p4mm$	$p2$ $p2mm$		$c2mm$ $p4mm$	
Hexagonal	$p6mm$	$p2mm$			$p3m1$

the fixed points of the group $p3$ satisfy:

$$2\kappa_1 + \kappa_2 \equiv 0 \bmod 2\pi, \quad \kappa_1 \equiv \kappa_2 \bmod 2\pi\ ,$$

$$\Rightarrow \text{solutions, } (0,0), \quad \hat{k}_C = \left(\frac{2\pi}{3}, \frac{2\pi}{3}\right), \quad \hat{k}'_C = \left(\frac{4\pi}{3}, \frac{4\pi}{3}\right), \quad 3\hat{k}_C = 3\hat{k}'_C = 0\ . \tag{55}$$

The points $\hat{k}_C, \hat{k}'_C$ are also invariant by (cm) and are exchanged by $(p2) = -I_2$; hence their stabilizer is $p3m1$ (whose representation was given just before Eq. (25)).

Table 2 gathers the information we have obtained on the strata of dimension zero in the action of the five two-dimensional Bravais groups on BZ.

For $d = 3$.

Triclinic, monoclinic systems and P-orthorhombic Bravais class: The extension of the results obtained for $d = 2$ is straightforward. The representations of the Bravais groups $P\bar{1}, P2/m, Pmmm$ can be made diagonal (on Z), so they produce on BZ a unique 0-dimensional stratum, that of the eight fixed points $2\hat{k} = 0$.

For the group $C2/m$, the zero-dimensional strata contain only the eight points $2\hat{k} = 0$; the seven elements of order 2 are partitioned into five orbits of $1, 1, 1, 2, 2$ elements; those of two elements are $(\pi, 0, 0), (0, \pi, 0)$ and $(\pi, 0, \pi), (0, \pi, \pi)$.

C-orthorhombic and P-tetragonal Bravais class: The same results are obtained for the groups $Cmmm, P4/mmm$ since these groups are generated by $C2/m$ and, respectively, by $P2/m$ and $Pmmm$.

Hexagonal Bravais class: For the Bravais group $P6/mmm$, $(0, 0, \pi)$ is a fixed point; the six other elements of order 2 are partitioned into two orbits: $(\pi, 0, 0), (0, \pi, 0), (\pi, \pi, 0)$ and $(\pi, 0, \pi), (0, \pi, \pi), (\pi, \pi, \pi)$ whose stabilizers are $P2/m$. Moreover, from Eq. (55), we obtain two orbits of two points: $(2\pi/3, 2\pi/3, 0), (4\pi/3, 4\pi/3, 0)$ and $(2\pi/3, 2\pi/3, \pi), (4\pi/3, 4\pi/3, \pi)$, whose common stabilizer is $P\bar{6}2m$ (do not forget the duality given in Eq. (47)). The elements of these two orbits satisfy, respectively: $3\hat{k} = 0$ and $6\hat{k} = 0$.

Rhombohedral Bravais class: The Bravais group $R\bar{3}m$ is generated by the groups $P\bar{1}$ and $R3m$ which is the permutation group of the three coordinates. So the zero-dimensional strata contains only 0 and the seven elements of order 2; those are partitioned into three orbits of $3, 3, 1$ elements which contain respectively $1, 2, 3$ coordinates π (and the others are 0).

P-cubic Bravais class: We obtain the same results as the rhombohedral one since $Pm\bar{3}m$ is generated by its subgroups $Pmmm$ and $R\bar{3}m$.

F-orthorhombic Bravais class: For the group $Fmmm$, we study first the action of the three rotations of $F222$ on BZ; their action is represented by the matrices $-(Im_j)$. One obtains, respectively, for $j = 1, 2, 3$:

$$\begin{pmatrix}\kappa_1\\ \kappa_2\\ \kappa_3\end{pmatrix}\mapsto\begin{pmatrix}-\kappa_1\\ -\kappa_1+\kappa_3\\ -\kappa_1+\kappa_2\end{pmatrix},\quad\begin{pmatrix}-\kappa_2+\kappa_3\\ -\kappa_2\\ -\kappa_2+\kappa_1\end{pmatrix},\quad\begin{pmatrix}-\kappa_3+\kappa_2\\ -\kappa_3+\kappa_1\\ -\kappa_3\end{pmatrix}. \tag{56}$$

We verify that among the seven elements of order 2 (which are the elements invariant by $-I_3$, the symmetry through the origin), three of them, $B_1 = (0, \pi, \pi)$, $B_2 = (\pi, 0, \pi)$, $B_3 = (\pi, \pi, 0)$ are fixed points and the four others form one orbit whose stabilizer is $P\bar{1}$. There are no other points in zero-dimensional strata. For the equivalent realization $F'mmm$ given in Eq. (43), one obtains for the three fixed points: $(0, 0, \pi)$,$(\pi, \pi, 0)$,(π, π, π) and the four other points of order 2 form one orbit (with stabilizer $P\bar{1}$).

It will also be useful later to know the one-dimensional stratum with $(Fmm2)_3$ as stabilizer. From Eq. (56) we find that the elements fixed by the rotation $-Im_3$ satisfy: $2\kappa_3 \equiv 0 \bmod 2\pi$, $\kappa_2 - \kappa_1 = \pm\kappa_3$. That defines three loops:

$$(\kappa_1, \kappa_1, 0),\ (\kappa_1, \kappa_1 + \pi, \pi),\ (\kappa_1, \kappa_1 - \pi, \pi)\ . \tag{57}$$

These three loops are the intersection of the two two-dimensional tori, submanifolds of BZ, $\kappa_2 - \kappa_1 = -\kappa_3, \kappa_2 - \kappa_1 = \kappa_3$ of fixed points by the matrices $-Im_1$ and $-Im_2$, respectively. So the stabilizer of the points of these three loops is $(Fmm2)_3$ except at the points B_i.

I-orthorhombic Bravais class: Similarly, for the group $Immm$, we study the action of the three rotations; their action is represented by the matrices $-(Fm_j)$. One obtains, respectively, for $j = 1, 2, 3$:

$$\begin{pmatrix}\kappa_1\\ \kappa_2\\ \kappa_3\end{pmatrix}\mapsto\begin{pmatrix}-\kappa_1-\kappa_2-\kappa_3\\ \kappa_3\\ \kappa_2\end{pmatrix},\quad\begin{pmatrix}\kappa_3\\ -\kappa_1-\kappa_2-\kappa_3\\ \kappa_1\end{pmatrix},\quad\begin{pmatrix}\kappa_2\\ \kappa_1\\ -\kappa_1-\kappa_2-\kappa_3\end{pmatrix}. \tag{58}$$

We verify that among the seven elements of order 2, there is a fixed point: (π, π, π) and the six others fall into three orbits of two points:

$$(\pi, 0, 0),\ (0, \pi, \pi), \qquad (0, \pi, 0),\ (\pi, 0, \pi); \qquad (0, 0, \pi),\ (\pi, \pi, 0)\ . \tag{59}$$

Their stabilizers are, respectively, the three $C2/m$ subgroups. Moreover there are two points invariant by the three rotations of Eq. (58):

$$\left(\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\right)\quad\text{and}\quad\left(\frac{3\pi}{2}, \frac{3\pi}{2}, \frac{3\pi}{2}\right);\quad\text{they satisfy } 4\hat{k} = 0\ . \tag{60}$$

The stabiliser is $I222$; obviously these two elements are exchanged by the space inversion.

I-tetragonal Bravais class: The group $I4/mmm$ is generated by its subgroups $Immm$ and $(I4)$ whose action on BZ is

$$\widetilde{(I4)}\cdot\begin{pmatrix}\kappa_1\\ \kappa_2\\ \kappa_3\end{pmatrix}=\begin{pmatrix}\kappa_1+\kappa_2+\kappa_3\\ -\kappa_3\\ -\kappa_1\end{pmatrix}. \tag{61}$$

This matrix leaves invariant the point (π,π,π) and exchanges the two points of the third orbit of Eq. (59); so the stabilizer is $I422$ (see Fig. 5). The matrix $\widetilde{(I\bar{4})}$ mixes the first two orbits, so the partition into $I4/mmm$-orbit of the set of points of order two is $1,2,4$ with $(C2/m)$ as stabilizers. This matrix exchanges the two points of Eq. (60); hence $I\bar{4}$ lets them fixed. So these two points of order 4 form an orbit of $I4/mmm$ with stabilizer $I\bar{4}2m$ (see e.g. Table 3).

I-cubic Bravais class: The group $Im\bar{3}m$ is generated by its subgroups $Immm$ and $R3m$, the permutation group of the three coordinates; so it leaves fixed (π,π,π) and it merges the three two-element orbits of Eq. (59) into a six-element orbit. So the stabilizers have eight elements and form a conjugacy class of $Im\bar{3}m$. Let us study the stabilizer of the orbit element: $B_3=(\pi,\pi,0)$; it is invariant by the matrices (Cm_3) (the permutation matrix of the coordinates $1,2$) and by $(Im_3)=(Fm_3)^{\top}$ (defined in Eq. (33)). We have shown in Eq. (38) that these two matrices generate the group $F'mmm$ of the arithmetic class $Fmmm$. $R3m$ leaves also fixed the two points of Eq. (60), so they form a two-element orbit of $Im\bar{3}m$ whose stabiliser is $I\bar{4}3m$ (see Table 3).

F-cubic Bravais class: The Bravais group $Fm\bar{3}m$ is generated by the two Bravais groups $Fmmm$ and $R\bar{3}m$. From the orbits of these two groups on the set of elements of order 2, we deduce that $Fm\bar{3}m$ has two orbits on this set: one has three elements, (defined as B_i when we studied $Fmmm$, see also Table 3), the other has four other elements (they form a unique orbit for $Fmmm$ and two orbits for $R\bar{3}m$). The stabilizers are, respectively, $F4/mmm\sim I4/mmm$ and $R\bar{3}m$ as the only $Fm\bar{3}m$ subgroups of index 3 and 4; for a direct verification, check that B_3 is fixed by both matrices $\widetilde{(F\bar{4})}$ (given in Eq. (42)) and $-\widetilde{(F\bar{4})}$ while $R\bar{3}m$ leaves fixed (π,π,π).

In general, when the group acting on BZ is enlarged some stratum of dimension 0 can appear if the stabilizer of strata of higher dimension is enlarged, at some isolated points, with an element whose fixed points are isolated. Let us start from the one-dimensional stratum of $Fmmm$ that we have studied (under the heading of this group) and whose stabilizer is $(Fmm2)_3$; Fig. 5 shows that it is a maximal subgroup of $I4mm$, $I\bar{4}2m$ and $Fmmm$ (irrelevant for our study). So we have to study the fixed points of the matrices $\pm\widetilde{(F\bar{4})}$ (defined in Eq. (42)) which generate the representation of $F4\sim I4$ and $F\bar{4}\sim I\bar{4}$ on the reciprocal space. The fixed points of $-\widetilde{(F\bar{4})}$ satisfy the equations

$$\kappa_1+\kappa_2=0,\quad 2\kappa_2=\kappa_3,\quad \kappa_1=\kappa_2+\kappa_3\ . \tag{62}$$

The coordinates of the fixed points of the group $I\bar{4}2m$ (generated by $I\bar{4}$ and $Fmm2$) satisfy Eqs. (62) and (57). They are: $(\pi/2,3\pi/2,\pi)$ and $(3\pi/2,\pi/2,\pi)$. The subgroup $R3m$ of $Fm\bar{3}m$ permutes the components of these BZ elements, making a six-element orbit with stabilizer $I\bar{4}2m$.

Table 3 presents the obtained results on the zero-dimensional strata in the action of the Bravais groups on BZ. For each Bravais group, the set Ω of the points in these orbits has a number of elements $6\leq|\Omega|\leq 14$. It is easy to decompose this set into orbits for any arithmetic class P^z: the set Ω is that of the Bravais group $\alpha(P^z)$ (this map is defined in Eq. (23)) and the stabilizers are the intersection with P^z of the stabilizers of the Table 3; in a few cases an orbit splits into two (with the

Table 3
Zero-dimensional strata in the action of Bravais groups on BZ. For each group, the table gives the corresponding orbits and their stabilizers. The number of elements in one orbit and the common order of the elements are (independently) 1, 2, 3, 4, 6. When the order of the orbit elements is > 2, only one element $\hat{k}$ is given for the orbit; the others are given in Eq. (63)

$\hat{k} \in BZ$	$\begin{pmatrix}0\\0\\0\end{pmatrix}$	$\begin{pmatrix}\pi\\\pi\\\pi\end{pmatrix}$	$\begin{pmatrix}\pi\\0\\0\end{pmatrix}$	$\begin{pmatrix}0\\\pi\\0\end{pmatrix}$	$\begin{pmatrix}0\\0\\\pi\end{pmatrix}$	$\begin{pmatrix}0\\\pi\\\pi\end{pmatrix}$	$\begin{pmatrix}\pi\\0\\\pi\end{pmatrix}$	$\begin{pmatrix}\pi\\\pi\\0\end{pmatrix}$
Their label	0	R	A_1	A_2	A_3	B_1	B_2	B_3
Their order	1	2	2	2	2	2	2	2
$P\bar{1}$	+	+	+	+	+	+	+	+
$P2/m$	+	+	+	+	+	+	+	+
$Pmmm$	+	+	+	+	+	+	+	+
$C2/m$	+	+	$P\bar{1}$		+	$P\bar{1}$		+
$Cmmm$	+	+	$P2/m$		+	$P2/m$		+
$P4/mmm$	+	+	$Pmmm$		+	$Pmmm$		+
$R\bar{3}m$	+	+	$C2/m_i$			$C2/m_i$		
$Pm\bar{3}m$	+	+	$P4/mmm$			$P4/mmm$		
$Fmmm$	+	$P\bar{1}$				+	+	+

No. orbit	1	Variable			2	6	2	2
$\hat{k}$	0	$R, A_1, A_2, A_3, B_1, B_2, B_3$			$\begin{pmatrix}\pi/2\\\pi/2\\\pi/2\end{pmatrix}$	$\begin{pmatrix}\pi/2\\3\pi/2\\\pi\end{pmatrix}$	$\begin{pmatrix}2\pi/3\\2\pi/3\\0\end{pmatrix}$	$\begin{pmatrix}2\pi/3\\2\pi/3\\\pi\end{pmatrix}$
Order	1	2			4	4	3	6
$P6/mmm$	0	A_3	$A_1A_2B_3,\ B_1B_2R$: $Cmmm$				$P\bar{6}2m$	$P\bar{6}2m$
$Immm$	0	R	$A_3B_3,\ A_1B_1,\ A_2B_2,$: C_2/m_i		$I222$			
$I4/mmm$	0	R	A_3B_3: $F'mmm$	$A_1A_2B_1B_2$: $C2/m$	$I\bar{4}2m$			
$Im\bar{3}m$	0	R	$A_1A_2A_3B_1B_2B_3$: $F'mmm$		$I\bar{4}3m$			
$Fm\bar{3}m$	0	$RA_1A_2A_3$: $R\bar{3}m$		$B_1B_2B_3$: $F4/mmm$		$I\bar{4}2m$		

same number of elements) when one passes from the Bravais group P_L^z to a subgroup P^z. When the order of the orbit elements is > 2, only one element $\hat{k}$ is given for the orbit in Table 3; we complete here the 2-element orbits:

$$4\hat{k} = 0, \qquad 3\hat{k} = 0, \qquad 6\hat{k} = 0,$$
$$\begin{pmatrix}\pi/2\\ \pi/2\\ \pi/2\end{pmatrix}, \quad \begin{pmatrix}3\pi/2\\ 3\pi/2\\ 3\pi/2\end{pmatrix}, \quad \begin{pmatrix}2\pi/3\\ 2\pi/3\\ 0\end{pmatrix}, \quad \begin{pmatrix}4\pi/3\\ 4\pi/3\\ 0\end{pmatrix}, \quad \begin{pmatrix}2\pi/3\\ 2\pi/3\\ \pi\end{pmatrix}, \quad \begin{pmatrix}4\pi/3\\ 4\pi/3\\ \pi\end{pmatrix}. \tag{63}$$

The six elements of the order 4 orbits of $Fm\bar{3}m$ are obtained by the permutations of the components: $(\pi/2, 3\pi/2, \pi)$.

4.5. Time reversal $\mathscr{T}$

In classical Hamiltonian mechanics if, at a given instant one reverses the momenta, the trajectories are unchanged but they are followed in the reverse direction. That symmetry has been called (a little abusively) *time reversal*; we denote it by $\mathscr{T}$. The fundamental paper on $\mathscr{T}$ in quantum mechanics is (Wigner, 1932); it has been extended to quantum field theory. In both frames, $\mathscr{T}$ is represented by an anti-unitary operator. In Section 8 we will study the merging of space group symmetry and time reversal.

Here we study only the modification of the space group action on BZ. The change of sign of momenta transforms a unirrep of the group L into its complex conjugate. This corresponds on BZ (= the set of inequivalent unirreps of L) to the transformation $\hat{k} \leftrightarrow -\hat{k}$. For simplicity, we study here $\mathscr{T}$ only when the spin coordinates do not intervene explicitly. Time reversal invariance is a symmetry of many equilibrium states; the real functions on BZ describing their physical properties, e.g. the energy function, must satisfy the relation $E(\hat{k}) = E(-\hat{k})$. The effect of this symmetry can be obtained by enlarging P^z, the group acting effectively on BZ, with $-I_d$, when P^z does not already contain the symmetry through the origin. We denote this enlarged group by $\check{P}^z$; this is simply P^z for the 7, 24 arithmetic classes (for $d = 2,3$) which contain the symmetry through the origin. Table 4 gives the list[32] of $P^z \neq \check{P}^z$'s which correspond to the same $\check{P}^z$.

5. Voronoï cells and Brillouin cells

The next two sections are based on some common work and many discussions with Peter Engel and Marjorie Senechal.

5.1. Voronoï cells, their faces and corona vectors

We have mentioned that one can built a fundamental domain of a lattice independently of the choice of a coordinate system. It was introduced for $d = 2$ by Dirichlet (1850) and also Hermite

[32] We give this table for the convenience of the reader because we have not seen it in textbooks.

Table 4
Arithmetic classes $\check{P}^z$ obtained by enlarging P^z with $-I_3$[a]

$\check{P}^z$	P^z	$\check{P}^z$	P^z
$(p2)$	$p1$;	$p4$	
$(p2mm)$	pm;	$(p4mm)$	
$(c2mm)$	cm;	$p6$	$p3$;
		$(p6mm)$	$p3m1, p31m$;
$(P\bar{1})$	$P1$;	$(R\bar{3}m)$	$R32, R3m$;
$(P2/m)$	$P2, Pm$;	$P\bar{3}$	$P3$;
$(C2/m)$	$C2, Cm$;	$P\bar{3}1m$	$P312, P31m$;
$(Pmmm)$	$P222, Pmm2$;	$P\bar{3}m1$	$P321, P3m1$;
$(Cmmm)$	$C222, Cmm2, Amm2$;	$P6/m$	$P6, P\bar{6}$;
$(Fmmm)$	$F222, Fmm2$;	$(P6/mmm)$	$P622, P6mm, P\bar{6}m2, P\bar{6}2m$;
$(Immm)$	$I222, Imm2$;	$Pm\bar{3}$	$P23$;
$P4/m$	$P4, P\bar{4}$;	$(Pm\bar{3}m)$	$P432, P\bar{4}3m$;
$(P4/mmm)$	$P422, P4mm, P\bar{4}2m, P\bar{4}m2$;	$Fm\bar{3}$	$F23$;
$I4/m$	$I4, I\bar{4}$;	$(Fm\bar{3}m)$	$F432, F\bar{4}3m$;
$(I4/mmm)$	$I422, I4mm, I\bar{4}m2, I\bar{4}2m$;	$Im\bar{3}$	$I23$;
$R\bar{3}$	$R3$;	$(Im\bar{3}m)$	$I432, I\bar{4}3m$;

[a]This enlargement includes the effect of time reversal on BZ. In dimension $d = 2, 3$, the 13, 73 arithmetic classes P^z and $\check{P}^z$ are mapped onto the 7, 24 ones containing $-I$ and denoted by $\check{P}^z$. The 5, 14 arithmetic classes of the Bravais groups are between ( ). For the labels of the arithmetic classes and for the order in their listing, we follow the "International Tables for Crystallography" [ITC].

(1850); these domains are hexagons or rectangles (with squares as a particular case). Fedorov (1885) wrote a book[33] on the $d = 3$ case; he found the five combinatorial types of polytopes realizing these domains. The first general study in arbitrary dimension d was done by[34] Voronoï (1908). He obtained remarkable results and these domains are called Voronoï cells in mathematics. The 3D-domains were introduced in physics much later: by Brillouin (1930) in the reciprocal space, by Wigner and Seitz (1933) in the direct space.[35]

We have already introduced Voronoï cells in Section 2, in the more general setting of Delone sets of points. We study them here; we begin to prove results in d-dimension because the proofs are exactly the same for $d = 3$. Let us first prove that Euclidean lattices are a particular case:

[33] E.S. Fedorov wrote this book between the age of 16 and 26, while serving in the army, or studying medicine, chemistry and physics. Then he became a mineralogist and six years later his book was accepted for publication in a crystallography series. No translation in a western language is known. A detailed analysis of it has been made in English by Senechal and Galiulin (1984).

[34] As we shall point out some results were first found by Minkowski (1897).

[35] These authors do not quote earlier references. Seitz told me that he learned Brillouin's use of the cells in the Brillouin (1931) book. The figures are in p.304 in the Chapter added to the original French edition.

Proposition 5a. *Euclidean lattices are Delone sets of points.*

There is a minimum distance between the points of a Euclidean lattice (see the end of Section 3.2). To complete the proof we have to give an upper limit of R, the largest radius of the holes. Let $2R_b$ the longest diagonal of the parallelepiped $\mathscr{P}_b$ (the fundamental domain defined in Eq. (17)) and S_b the sphere which has this diagonal as diameter; by construction this sphere has a radius $\geq$ that of any hole. When we consider the $GL(d,Z)$ orbit of bases, R_b (which has no upper bound) has a lower bound $R'_b \geq R$, the radius of the largest hole. The equality occurs when $\mathscr{P}_b$ is a hypercube, so $\tilde{b}\tilde{b}^{\top} = I_d$: it defines the simplest cubic lattice.

A fundamental domain of an Euclidean lattice $\bar{L}$ is its Voronoï cell defined in Eq. (1); it is a polyhedron, defined at each point $\ell \in \bar{L}$, independent of the choice of basis. We denote it by $\mathscr{D}_L(\ell)$; by the translations of L one obtains all of them from any chosen one. We now study $\mathscr{D}_L$ at the origin o; it can be defined directly from the translation lattice $L \subset E_d$, the vector space it spans. Eq. (1) becomes

$$\begin{aligned}\mathscr{D}_L &= \{\boldsymbol{x} \in R^d,\ \forall \ell \in L,\ N(\boldsymbol{x}) \leq N(\boldsymbol{x}-\ell)\} \\ &= \{\boldsymbol{x} \in R^d,\ \forall \ell \in L,\ (\boldsymbol{x},\ell) \leq \tfrac{1}{2}(\ell,\ell)\}\ . \end{aligned} \tag{64}$$

Since the lattice L is a subgroup of R^d, if we consider the coset $\boldsymbol{x} + L \equiv \boldsymbol{x} - L = \{\boldsymbol{x} - \ell,\ \ell \in L\}$, we can interpret Eq. (64) as

$$\boldsymbol{x} \in \mathscr{D}_L \Leftrightarrow \boldsymbol{x} \text{ is shortest in its coset } R^d/L\ . \tag{65}$$

$$\begin{aligned} &\boldsymbol{x} \text{ unique shortest vector} && \text{if } \boldsymbol{x} \in \text{ interior of } \mathscr{D}_L. \\ &\boldsymbol{x} \text{ not unique shortest vector} && \text{if } \boldsymbol{x} \in \partial\mathscr{D}_L \text{ the boundary}\ . \end{aligned} \tag{66}$$

So $\mathscr{D}$ is the fundamental domain of the translation group L. Since $\mathscr{D}_L$ has been defined in terms of norm or scalar product of vectors, the symmetry group P_L^z of the lattice is a symmetry group of the Voronoï cell $\mathscr{D}_L$.

We call corona the set of Voronoï cells which surround the one at the origin, i.e. they have with $\mathscr{D}_l(o)$ a non-empty intersection.

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

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

Denoting $\mathscr{D}_{2L}$ as $2\mathscr{D}_L$, we can give two equivalent definitions of C, the set of corona vectors of L:

$$C = \{\boldsymbol{c} \in L,\ \mathscr{D}_L(o) \cap \mathscr{D}_L(c) \neq \emptyset\} \Leftrightarrow C = L \cap \partial 2\mathscr{D}_L\ . \tag{67}$$

From Eq. (66) we deduce:

Proposition 5b. *The corona vectors are the shortest lattice vectors in their $L/2L$ cosets.*

Equivalently:

$$\boldsymbol{c}\in C\Leftrightarrow\forall 0\le\boldsymbol{\ell}\in L,\quad N(\boldsymbol{c}+2\boldsymbol{\ell})-N(\boldsymbol{c})\ge 0\Leftrightarrow\boldsymbol{c}\cdot\boldsymbol{\ell}+N(\boldsymbol{\ell})\ge 0\ . \tag{68}$$

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

$$2(2^d-1)\le|C|\ . \tag{69}$$

In Eq. (68), let us replace 2 by $m>2$:

$$\boldsymbol{c}\in C, m>2,\quad\forall 0\le\boldsymbol{\ell}\in L,$$

$$m^{-1}(N(\boldsymbol{c}+m\boldsymbol{\ell})-N(\boldsymbol{c}))=2(\boldsymbol{c}\cdot\boldsymbol{\ell}+N(\boldsymbol{\ell}))+(m-2)N(\boldsymbol{\ell})>0\ . \tag{70}$$

This shows that a corona vector is **the** shortest vector in its coset L/mL, $m>2$. So for $m=3$ and $\boldsymbol{c}\neq 0$, we obtain:[36]

$$|C|\le 3^d-1\ . \tag{71}$$

Definition (*Facet vectors*). When the bisector plane of the corona vector $\boldsymbol{c}$ supports a facet (= a face of dimension $d-1$) of $\mathscr{D}_L$, we say that $\boldsymbol{c}$ is a facet vector. We denote by F the set of facet vectors:

$$F=\{\boldsymbol{f}\in C,\ \dim(\mathscr{D}_L(o)\cap\mathscr{D}_L(f))=d-1\}\subset C\ . \tag{72}$$

In the Euclidean space the equation of the plane bisector of a lattice vector $\boldsymbol{f}$ is $(\boldsymbol{f},\boldsymbol{x})=\frac{1}{2}N(\boldsymbol{f})$; so, when F is known, $\mathscr{D}_L$ can be defined as

$$\mathscr{D}_L=\left\{\boldsymbol{x},\ \forall\boldsymbol{f}\in F,\ |\boldsymbol{f}\cdot\boldsymbol{x})|\le\frac{1}{2}N(\boldsymbol{f})\right\}\ . \tag{73}$$

Proposition 5c (Voronoï). *A lattice vector $\boldsymbol{f}$ is a face vector if and only if $\pm\boldsymbol{f}$ 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 $\pm\boldsymbol{c}$, $N(\boldsymbol{c})=N(\boldsymbol{f})$; so $\boldsymbol{\ell}=\frac{1}{2}(\boldsymbol{f}+\boldsymbol{c})\in L$. Then one computes $2(\boldsymbol{f},\boldsymbol{\ell})=N(\boldsymbol{f})+(\boldsymbol{f},\boldsymbol{c})=2N(\boldsymbol{\ell})$; comparing with Eq. (73) this means that $\frac{1}{2}\boldsymbol{f}$ is in the face of center $\frac{1}{2}c$. With $N(\boldsymbol{f})=N(\boldsymbol{c})$, that implies $\boldsymbol{f}=\boldsymbol{c}$.

Proof of "only if". Assume that $\pm c$ are strictly shorter in their $L/2L$ coset and that the corona vector is not a facet 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 vector 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 proposition proves that the number of faces [37] is $\le 2(2^d-1)$. A lower bound is $2d$; indeed, at least d pairs of parallel hyperplanes are necessary to envelop a bounded domain. Gathering these results and those of Eq. (69) and Eq. (71)

[36] This result was first obtained by Minkowski (1907) for the packing of a convex body on a lattice. For the Voronoï cells the proof is so much simpler!

[37] This inequality was proven first by Minkowski (1897).

we obtain

$$2d \leq |F| \leq 2(2^d - 1) \leq |C| \leq 3^d - 1 \ . \tag{74}$$

For the dimensions 2, 3, Eq. (74) reads

$$d = 2,\ 4 \leq |F| \leq 6 \leq |C| \leq 8, \qquad d = 3,\ 6 \leq |F| \leq 14 \leq |C| \leq 26 \ . \tag{75}$$

From the Proposition 5c, if $|F|$ is maximum, $F = C$ and conversely. If a d-dimensional Voronoï cell has $2d$ facets, one easily shows that 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 d orthogonal facet vectors; in that basis the quadratic form $q(L)$ is diagonal. If its diagonal elements are all different, the Bravais group $P_L^z \sim Z_2^d$ contains all diagonal matrices with elements ± 1; its Bravais class is usually called "orthorhombic P-lattice". When the multiplicities of equal elements in the diagonal $q(L)$ are d_i, the Bravais group is the direct product $\times_i O_{d_i}(Z)$. As we have seen, in the particular case where $q(L)$ is proportional to the unit matrix, the Bravais group is $O_d(Z)$ and the Voronoï cell is a d-dimensional cube. For all the cases in which $|F| = 2d$, all k-dimensional faces ($0 \leq k \leq d - 1$) have a symmetry center; it is the middle of a corona vector; so $|C| = 3^d - 1$.

We have also proven:

Proposition 5d. *The Voronoï cell has the symmetry of the Bravais group P_L^z. The cell, its facets and the smaller faces common with the Voronoï cells of the corona have a symmetry center.*

5.2. Delone cells. Primitive lattices

In Section 2 we have defined Delone cells and in Proposition 2a, we showed that they make a tessellation of the space; that was done in the broader frame of Delone sets with a complete symmetry between the two dual orthogonal tesselations by Delone (first treated) and by Voronoï cells. Here we are less general and we start from the results we have obtained on the Voronoï cells. This section is a presentation of a few results of Voronoï (1908) (the logical order is different).

A vertex of a Voronoï cell is at the intersection of at least d bisector hyperplanes corresponding to at least $d + 1$ points of L. The vertex v is equidistant from these points; in other words: these points are on a sphere Σ_v of center v and radius R_v and this set is the intersection $L \cap \Sigma_v$.

Definition. *The Delone cell*[38] $\Delta_L(v)$ *is the convex hull of* $L \cap \Sigma_v$. By definition it is a convex polytope inscribed in the sphere Σ_v of center v.

In the Euclidean space $\mathscr{E}_d$, a sphere is defined by $d + 1$ points in general position (i.e. they are vertices of a simplex). If more than $d + 1$ points are on a sphere they are not in general position.

[38] Voronoï (1908) had defined these cells and began to study them for arbitrary lattices. Later, they have been studied more thoroughly by Delone.

Definition. *A lattice L is primitive*[39] if, and only if, every vertex of its Voronoï tessellation belongs to exactly $d+1$ cells or, equivalently, if, and only if, every one of its Delone cells is a simplex.

Proposition 5e. *In the Voronoï tesselation of a primitive lattice, every m-dimensional facet F_d belongs to exactly $d+1-m$ adjacent Voronoï cells.*

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

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

Proposition 5f. *A d-dimensional primitive cell must have* $2(2^d-1)$ *faces* (*or, equivalently*, $F=C$).

If this condition is not satisfied there is a corona vector $\boldsymbol{c}$ which is not a facet vector. For instance if $\frac{1}{2}\boldsymbol{c}$ is the center of an m-face ($m<d-1$) which is the intersection $\mathscr{D}_L(c)\cap\mathscr{D}_L(o)$; it contains at least $m+1$ vertices. At any one of them, there is a cell whose intersection with $\mathscr{D}_L(o)$ has dimension $m<d-1$, so there must be more than d cells meeting $\mathscr{D}_L(o)$ at this vertex v. This proves that the cells are not primitive since more than $d+1$ cells meet at v. Beware that the converse is not true but there are no counter examples for $d=2,3$; there is one in dimension 4 (which was missed by Voronoï).

The set of m-faces, $0\leq m<d$, of a lattice Voronoï tesselation can be decomposed into orbits of the translations. Let us study the intersection of these orbits with a given Voronoï cell $\mathscr{D}_L(o)$. Let $\mathscr{F}_m$ be one of its m-faces; we have seen in the proof of Proposition 5e that it is the intersection of $d-m$ facets; let $\{\ell_\alpha\}$, $1\leq\alpha\leq d-m$ the set of their facet vectors; they give the centers $o+\ell_\alpha$ of the $d-m$ other Voronoï cells which share this m-face with $\mathscr{D}_L(o)$. Each translation $-\ell_\alpha$ transforms $\mathscr{D}_L(o+\ell_\alpha)$ into $\mathscr{D}_L(o)$ and therefore $\mathscr{F}_m$ into $\ell_\alpha+\mathscr{F}_m$, another m-face of the Voronoï cell $D_L(o)$. That proves

Proposition 5g. *A primitive Voronoï cell contains exactly* $(d+1-m)$ *m-faces which can be obtained form each other by a translation of L.*

The proof also implies, with Proposition 5f, that for $m<d-1$ this set of $(d+1-m)$ m-faces is transformed into a different similar set by the symmetry through the origin. We shall call "family" the disjoint union of these two sets; remark that the family is the intersection of the set of m-faces of $\mathscr{D}_L(o)$ with their orbit under the action of the space group $P\bar{1}$, minimal space group of symmetry for a Voronoï tessellation. We have thus obtained the simple

Corollary 5g. *In a primitive Voronoï cell the number of m-faces,* $0\leq m<d-1$, *is a multiple of* $2(d+1-m)$, *which is the number of k-faces in the same family of congruent faces* (*i.e. obtained from each other by Euclidean transformations: here translations and symmetry through a point*).

[39] One could have said generic, but Voronoï used the word primitive when he introduced this notion for lattices. Moreover, we have already defined the generic Euclidean lattices: those with the smallest possible symmetry, i.e. $P_L^z=Z_2(-I_d)$ (the space group is $P\bar{1}$). The primitive and the generic lattices form two open dense sets of $\mathscr{L}_d$ which do not coincide: as we will see there are primitive lattices whose Bravais group is maximal.

From the definition of primitive Voronoï cells, d facets meet at every vertex; the corresponding d facet vectors span the space E_d. They may not form a basis of L; they generate only a sublattice. This was discovered by Voronoï (1909, p. 84) for $d = 5$. We have suggested the following definition:

Definition. *A primitive lattice L and its Voronoï cell $\mathscr{D}_L$ are called principal* if at every vertex of $\mathscr{D}_L$ the d facet vectors form a basis of L. It has been proven[40] that all primitive lattices are principal for $d \leq 4$.

At each vertex v of a primitive principal Voronoï cell the d facet vectors $\boldsymbol{f}_\alpha$ of the facets meeting at v form a basis[41] of L; the Delone cell Δ_v is a simplex, convex hull of the $d+1$ points: $\{o, o+\boldsymbol{f}_\alpha\}$. We remind that the volume of a d-dimensional simplex is given by $\mathrm{vol}\Delta_v = |\det(\boldsymbol{f}_\alpha)|/d!$. The absolute values of the determinant of all bases of L are equal: it is the volume of any fundamental domain of L and we denote it by vol L. Let V be the set of vertices of $\mathscr{D}_L$ and $|V|$ is the number of vertices; Proposition 5g tells us that there are $|V|/(d+1)$ vertices in a fundamental domain. Gathering all results obtained in this paragraph we deduce:

for primitive principal $\mathscr{D}_L$:

$$|V| = (d+1)(\mathrm{vol}\ L)/(\mathrm{vol}\,\Delta_v) = (d+1)! \tag{76}$$

This proves the first part of

Proposition 5h. *In dimension d, a principal primitive Voronoï cell has $(d+1)!$ vertices and $(d+1)!\,d/2$ edges.*

In a primitive lattice, d edges meet at each vertex and each edge has two vertices. This proposition is a very particular case of Voronoï's remarkable results. Let $N_m(d)$ be the number of m-dimensional faces of an arbitrary d-dimensional Voronoï cell; Voronoï (1909, p. 78 − 83,136) established the upper bound of the $N_m(d)$'s. A simple closed form can be given to the Voronoï expression (Michel 1997a)

$$0 \leq m \leq d: \quad N_m(d) = (d+1-m)!\ S_{d+1}^{(d+1-m)}\,, \tag{77}$$

where the $S_d^{(\ell)}$ are the Stirling numbers of second kind, e.g. (Abramowitz and Stegun 1964, Graham et al., 1988). Remark that the values of $N_m(d)$ for $m = 0, 1$ are those of Proposition 5h and, for $m = d-1$, it verifies Eq. (74). Notice also that $N_d(d) = 1$; it corresponds to a very natural (and usual) convention; with it the relation imposed by the Euler–Poincaré characteristic is

$$\sum_{0 \leq m \leq d} (-1)^m N_m(d) = 1\,. \tag{78}$$

[40] We have given the references for $d = 2,3$ (unique combinatorial type of primitive Voronoï cell). Voronoï (1909) proved that for $d = 4$ there are three types of primitive cells, all principal. For $d = 5$ Baranovskii and Ryshkov (1973), completed by Engel (1986) classified the 222 types of primitive Voronoï cells; 21 of them are non-principal.

[41] A famous unsolved problem is to know if every lattice has a basis among its facet vectors.

With our knowledge of $N_m(d)$ for $m = 0, 1, d-1$ we have for primitive cells in dimension $d \leq 4$:

$$N_0(2) = N_1(2) = 6, \quad N_0(3) = 24, \quad N_1(3) = 36, \quad N_2(3) = 14\ ,$$
$$N_0(4) = 120, \quad N_1(4) = 240, \quad N_2(4) = 150, \quad N_3(4) = 30\ . \tag{79}$$

5.3. The primitive principal Voronoï cells of type I

Voronoï (1909, p. 137–147) defines and studies a combinatorial type of primitive cells; he called it type I. Consider the open set in $\mathscr{C}_+(\mathscr{Q}_d)$ made of the quadratic forms (= symmetric real matrices) satisfying:

$$1 \leq i,j \leq d, \quad i \neq j, \quad -q_{ij} =: \lambda_{ij} > 0, \quad q_{ii} - \sum_{j,j\neq i} \lambda_{ij} =: \lambda_{0i} > 0\ . \tag{80}$$

Notice that q is a positive matrix; indeed it defines the positive quadratic form

$$Q_\lambda(x_i) = \sum_i \lambda_{0i} x_i^2 + \sum_{i,j,i<j} 2\lambda_{ij}(x_i - x_j)^2\ . \tag{81}$$

Therefore there exist a basis $\{\boldsymbol{b}_i\}$ of E_d, defined up to orthogonal transformations, which satisfies $(\boldsymbol{b}_i \cdot \boldsymbol{b}_j) = q_{ij}$. This basis generates a lattice L. Using proposition 5c on a characterization of facet vectors and Eq. (81), we find that facet vectors of the lattice L_λ defined by the quadratic form of Eqs. (80)–(81) have for coordinates either 1's and 0's or -1's and 0's; explicitly

$$F(L_\lambda) = \Big\{ \pm \boldsymbol{b}_i, \pm(\boldsymbol{b}_i + \boldsymbol{b}_j),\ i \neq j, \pm(\boldsymbol{b}_i + \boldsymbol{b}_j + \boldsymbol{b}_k),$$
$$i \neq j \neq k \neq i, \ldots, \pm\Big(-\boldsymbol{b}_i + \sum_j \boldsymbol{b}_j\Big),\ \pm\sum_j \boldsymbol{b}_j \Big\}\ . \tag{82}$$

Let us give a more elegant writing of this set of vectors: let $\mathscr{N}_d^+$ be the set of the first d integers > 0 and X any non-empty subset. Then we define

$$\emptyset \neq X \subseteq \mathscr{N}_d^+, \quad \boldsymbol{f}_X = \sum_{i\in X} \boldsymbol{b}_i, \quad \text{then } F(L_\lambda) = \{\boldsymbol{f}_X\}\ . \tag{83}$$

The proof is straightforward: compute $Q(\boldsymbol{v})$ for arbitrary integer coordinates of $\boldsymbol{v}$ and transform $\boldsymbol{v} \mapsto \boldsymbol{f}$ replacing the even coordinates of $\boldsymbol{v}$ by 0 and the odd ones by 1; $\boldsymbol{v}$ and $\boldsymbol{f}$ are in the same $L/2L$ coset. One checks that $Q(\boldsymbol{v}) > Q(\boldsymbol{f})$. One finds that $|F(L_\lambda)| = 2(2^d - 1)$, the maximal possible value given in Eq. (74). That is a necessary condition for primitivity; it has been proven by Voronoï who showed that d facets meet at each vertex (see also, Michel, 1997a).

Generalizing the work of Selling (1874), written for $d = 2,3$ we introduce some notations and the definition of $\boldsymbol{b}_0$ from the $\boldsymbol{b}_i$'s; $\mu,\nu \in Z$, $0 \leq \mu,\nu \leq d$, $\mu \neq \nu$:

$$\lambda_{\mu\mu} = 0,\ \lambda_{\mu\nu} = \lambda_{\nu\mu} > 0, \quad \sum_\mu \boldsymbol{b}_\mu = 0 \ \Rightarrow\ (\boldsymbol{b}_\mu, \boldsymbol{b}_\mu) = \sum_\nu \lambda_{\mu\nu}, \quad (\boldsymbol{b}_\mu, \boldsymbol{b}_\nu) = -\lambda_{\mu\nu}\ . \tag{84}$$

This shows a syntactic symmetry of the domain of the quadratic forms Q_λ's; it is made by the group $\mathscr{S}_{d+1}$ of permutations of the values of the index μ. This permutes the values of the parameters $\lambda_{\mu\nu}$. If these $d(d+1)/2$ parameters are all equal, one obtains a lattice whose Bravais group contains the permutation group[42] $\mathscr{S}_{d+1}$ and its first study was made by Voronoï (1909, p. 137) If we put in Eq. (81)

$$\forall \mu,\nu: \lambda_{\mu\nu} = (d+1)^{-1} \quad \text{then } q = I_d - (d+1)^{-1} J_d \ . \tag{85}$$

We have already found this q in Eq. (40); it defines the weight lattice [43] of the simple Lie algebra A_d. Voronoï showed that the cell of this lattice is primitive principal. He showed that its $(d+1)!$ vertices form one orbit of the Bravais group and that for all positive values of the λ parameters, the Voronoï cells have the same combinatorial type. As shown in Coxeter and Moser (1972, end of Section 6.2), the Voronoï cell of A_d^w had already been defined in another problem of mathematics as the Cayley graph of $\mathscr{S}_{d+1}$.

In a d-dimensional Voronoï cell if a vertex v is common to exactly d facets, we have already noticed that their d facet vectors form a basis of the space. An edge from this vertex is the intersection of $d-1$ facets, so it is orthogonal to their facet vectors; this shows that the d edges from v are carried by the vectors of the dual basis. Let us assume now that at each vertex of the cell only d facets meet.[44] Since the set of facet vectors $F(L)$ generates the lattice,[45] the edges of such a cell must be parallel to vectors of the dual lattice. It is well known in the theory of semi-simple Lie algebras that the weight lattices (the irreducible representation of the algebra are labelled by its points) and the root lattice (= the lattice generated by the roots of the algebra) are dual of each other. Moreover we can choose as basis of the dual lattice the fundamental weight whose scalar product with any root is ± 1 or 0.

From these general facts it is easy to prove that the (oriented) edges of $\mathscr{D}_{A_d^w}$ are the $N = d(d+1)/2$ positive roots of the Lie algebra $A_d \sim SU(d+1)$ and that the combinatorial type of $\mathscr{D}_{A_d^w}$ (which is also the type of all the Voronoï cells corresponding to the Q_λ quadratic forms) is that of a (d,N) zonotope. We have to give its definition.

Definition (*Zonotope*). Given $N \geq d$ vectors $\boldsymbol{v}_\rho \in E_d$ which span this space and are contained in a half-space, a (d,N) *zonotope* is the convex hull (defined up to a translation in the associated Euclidean space) of the points: $o + \boldsymbol{v}_X$, $X \subseteq \mathscr{N}_N$, $\boldsymbol{v}_X = \sum_{\rho \in X} \boldsymbol{v}_\rho$. We use the notation similar to that of Eq. (83) with the difference that $\mathscr{N}_N$ is the set of non-negative integers $\leq N$ and X can also be the empty subset $\emptyset$. An equivalent definition is: a (d,N) zonotope is the projection of a N-cube on a d-space (when $N = d$ it is a parallelepiped). One calls a zone of a Voronoï cell, a set of parallel edges (= 1-face). For a zonotope, the edges of a zone are parallel to one of the $\boldsymbol{v}_\rho$. One proves (see e.g., Grünbaum, 1967) that a zonotope and all its m-faces have a symmetry center; indeed they are

[42] This d-dimensional representation of $\mathscr{S}_{d+1}$ is also the Weyl group of the simple Lie algebra $A_d \sim SU(d+1)$. It does not contains $-I_d$, so the Bravais group is $\bar{A}_d = A_d \times Z_2(-I_d)$.

[43] That was not known in the lifetime of Voronoï. He died at 40, just before the appearance of the second part of his memoir.

[44] This is the case of primitive cells but also many others.

[45] In the Voronoï tesselation one can pass from any lattice point (= center of a Voronoï cell) to any other by going along facet vectors.

themselves zonotopes. For $\mathscr{D}_{A_d^*}$ the $d(d+1)/2$ generating vectors are the positive roots of the Lie algebra $A_d \sim SU(d+1)$. Using this property Michel (1997a) gives, for each type Ω of m-dimensional zonotope which can be combinatorially equivalent to a m-dimensional Voronoï cell, the number $N_m(d,\Omega)$ of copies contained in $\mathscr{D}_{A_d^*}$ (these numbers are combinatorial invariants.)

As we show in Eq. (81) the forms Q_λ are expressed in a basis of facet vectors. Let us denote the vector generating the zonotope by $\boldsymbol{e}_\rho^*$ since they are in the space of the dual lattice. Then one shows that the quadratic forms can be written as

$$Q(\boldsymbol{x}) = \sum_\rho \lambda_\rho (\boldsymbol{e}_\rho^*, \boldsymbol{x}), \quad \lambda_\rho > 0 \,. \tag{86}$$

We can now answer the question: what happens at the boundary of the domain Q_λ, i.e. when λ becomes 0? Since Q_λ of Eq. (81) is of the form of Eq. (86), we know that the corresponding generating vector of the zonotope vanishes: this phenomena is called zone contraction: one shrinks simultaneously all edges of a zone and one obtains a new type of zonotope with one less zone. When $d > 2$, several contractions can be made successively; since the first contraction destroys the $\mathscr{S}_{d+1}$ syntactic geometry, there are often the choice of several inequivalent zone contractions for the successive ones to be made. We obtain a family of contractions with a genealogy until we find a non-contractible cell, i.e. any contraction would make it collapse into a smaller dimension. Starting from $\mathscr{D}_{A_d^*}$, there is a unique end for the family of contractions: the rectangular parallelepiped with d zones. Before going to the dimensions 2,3, let us emphasize that contractions can be made on every contractible Voronoï cell. But we have to distinguish between closed zones (all 2-faces contain 2 or 0 edges of the zone) and open zones (there is at least a 2-face containing only one edge of the zone). A Voronoï cell which has only open zones is non-contractible. In dimension 4 there are two families of contractions:

(i) the one of non-zonotopes has two maximal primitive principal cells with $30 = 2(2^4 - 1)$ faces and 10 closed zones; it has 37 members and the terminal non-contractible one is the regular polytope of symmetry F_4;

(ii) the one of the 17 zonotopes with two maximal cells, the primitive $\mathscr{D}_{A_d^*}$ and a non-primitive one with 30 faces and nine zones. These are the only maximal cells missed by Voronoï. There are 84 contraction families in dimension 5 (Engel, 1986). They have not been counted for $d = 6$; Engel (private communication) has studied some of them and he has found contraction families containing only one member!

5.4. *Voronoï cells for* $d = 2, 3$

$d = 2$. Any two variable quadratic form can be written as

$$Q(x) = q_{11}x_1^2 - 2q_{12}x_1x_2 + q_{22}x_2^2 \,. \tag{87}$$

If the coefficient of the x_1x_2 term were positive, this form would be obtained by changing the sign of one coordinate. We learned from Selling (1874) that an efficient way for studying this form is to introduce the parameters $\lambda_{\mu\nu} \geq 0$:

$$q = \begin{pmatrix} \lambda_{01} + \lambda_{12} & -\lambda_{12} \\ -\lambda_{12} & \lambda_{02} + \lambda_{12} \end{pmatrix}, \tag{88}$$

then

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

These two equations are the 2-D particular case of the Eqs. (80)–(81) for arbitrary dimension. When the three $\lambda_{\mu\nu}$ are > 0, with Proposition 5c (a Voronoï theorem), one can verify by the same method given for any d after Eq. (83), that the basis vectors $\boldsymbol{b}_i$ (defined up to a rotation by Eq. (87)) are facet vectors as well as $\boldsymbol{b}_1 + \boldsymbol{b}_2$ and the negative of these three vectors. So the Voronoï cell is a hexagon with a symmetry center. The six edges are orthogonal to the facet vectors and Eq. (88), a particular case of Eq. (86), gives their direction in the dual basis. Corollary 5g tells us that the six vertices of the hexagon form a unique family: so every two-dimensional Voronoï cell is inscribable in a circle.[46] From this property we immediately obtain that when the edges of a pair of facets symmetric through the center shrink to zero, one obtains a rectangle. That is the simplest example of zone contraction; analytically it is obtained of Eq. (88) by making one of the three λ coefficients $= 0$. The sides of the rectangle carry the coordinates axis when $\lambda_{12} = 0$. If a second λ is 0, then $\det q = 0$ which confirm the obvious fact that a contracted rectangle collapses to a one dimensional segment.

Let us apply what we know on the 2-D Voronoï cells to the structure of those in arbitrary dimension. Another important concept for Voronoï cells is that of a belt: consider a $(d-2)$-face $\mathscr{F}_0$; it belongs to a facet. Let $\mathscr{F}_1$ be the symmetric image of $\mathscr{F}_0$ through the center of this facet; it is at the intersection of two facets. Let $\mathscr{F}_2$ be the symmetric image of $\mathscr{F}_1$ through the center of the other facet. Repeating the same operation we obtain a chain $\mathscr{F}_\alpha$ which has to be periodic since the set of $(d-2)$-dimensional faces is finite; what is its period?

Definition. *A belt* of a Voronoï cell is the set of $(d-2)$-faces parallel to a given one. The $(d-2)$-faces of a belt are orthogonal to a 2-plane. One can show (Venkov 1959) that the orthogonal projection of $\mathscr{D}_L$ on this two-plane is a two-dimensional Voronoï cells. That proves:

Proposition 5i. *A belt of a Voronoï cell has six or four* $(d-2)$*-faces and therefore six or four facets. In the four facet belts the hyperplanes of adjacent facets are perpendicular.*

All the belts of a Voronoï cell which have the maximal number of faces ($|F| = 2(2^d - 1)$) have 6 facets. For $d = 3$ the belts and the zones are the same; this will help us for the study of this dimension.

$d = 3$. Any three-variable quadratic form can be written in the form of Eq. (80) with (see Eq. (84)) the $\lambda_{\mu\nu} \geq 0$. It is easy to choose a basis of three vectors $\boldsymbol{b}_i$ generating the lattice such that their three scalar products are ≤ 0; so the three λ_{ij} are ≥ 0. But to have that the 3 λ_{0i} are also ≥ 0 one may have to transform this basis. This has been done by Selling (1874) and Delaunay (1932a, b) The Delaunay ($=$ Delone) algorithm for transforming any generating basis of a lattice into a basis (80) is given in the old edition of international tables of crystallography (ITC, 1952, Vol. I, p. 530–535), but has been suppressed in the new one! This implies that all 3D Voronoï cells belong to the family of contractions of the primitive cell corresponding to the quadratic form of Eq. (80). This family

[46] It is obvious for a rectangle. For the general cell, I never found this statement and I would be grateful to be given a reference.

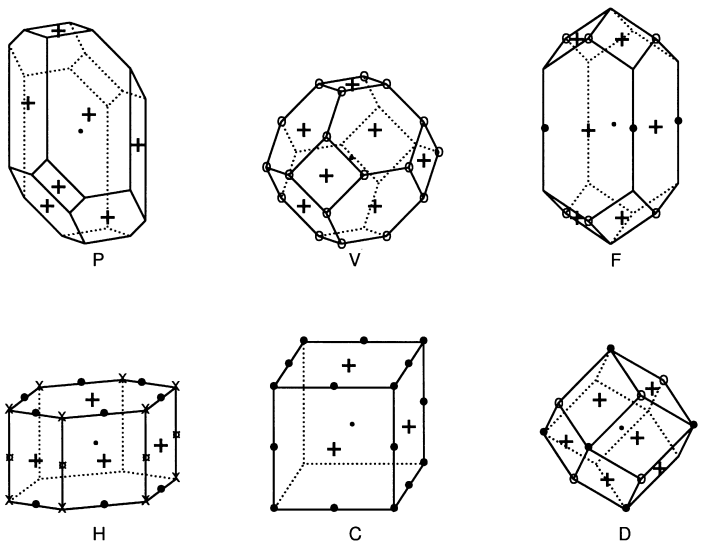

Fig. 6. The five types of Voronoï cells for $d = 3$. P is the primitive cell with minimal symmetry. V, F, H, D, C show the five cells with their maximal symmetry. The middle of the facets are marked by $+$. The middle of corona vectors are marked by a heavy dot $\bullet$; they are vertices or middle of edges common to the cell and its neighbors (which form the corona) in the Voronoï tessellation. $\circ$ or $\times$ marks the other high-symmetry points of the Brillouin cell for lattices with high symmetry (see the next subsection). They are in a direct relation with those of Table 3.

contains five types which are shown in Fig. 6; for V, F, D, H, C the cells are shown in the form of their highest symmetry while P is the primitive one in a low symmetry. The $+$ marks the symmetry centers of the facets ($=$ middle of facet vectors); the small $\bullet$ indicate the middle of the corona vectors. We call these two kinds of points *contact points*; indeed they are in the intersection of the cell with the neighboring ($=$ member of the corona) cells in the Voronoï tessellation. When they are not vertices, the intersection contains the facets or the edges which contain them as symmetry centers.

It is easier to study the primitive Voronoï cell in its highest symmetrical form corresponding to Eqs. (80) and(84) when all $\lambda_{\mu\nu}$ are equal and already found in Eq. (40): $q_3^{\mathrm{w}} = I_3 - (\frac{1}{4})J_3$. The cell is obtained by truncating the vertices of a cube (or a regular octahedron) by a plane orthogonal to the diagonals and such that some facets are regular hexagons (there are eight of them); what is left of the cube faces are six squares. We shall use also the notation $|F|(|V|)$ i.e. number of facets followed (in brackets) by the number of vertices for labelling the five types of cells.

14(24). V,P. The number of k-faces has been given in Eq. (79): $14, 36, 24$. In the case of higher symmetry (Fig. 6, V) its Bravais group is $Im\bar{3}m$. In the orthonormal coordinate system defined by the facet vectors of the truncated cube[47] the coordinates of the 14 facet vectors are: eight vectors with $(\varepsilon_1, \varepsilon_2, \varepsilon_3), \varepsilon_i^2 = 1$ (the corresponding facets are eight regular hexagons) and six vectors with $[2\varepsilon_i, 0, 0]$ (when the coordinates are between [ ], apply to them all permutations) whose corresponding facets are squares. The 24 vertices are trivalent i.e. each one is the intersection of three

[47] Beware that, although they are also facet vectors of the primitive cell 14(24), they are not generating the primitive lattice; indeed the lattice determinant is 4 while the basis determinant is 8.

Table 5
The five types of 3D Voronoï cells[a]

F-edg.		$\|F\|$	$\|E\|$	$\|V\|$	V-val.		$L/2L$	$\|C\|$	Zones belts	$z=b$	
6	4				4	3				6	4
8	6	14	36	24		24	2.2.2.2.2.2.2	14	6	6	
4	8	12	28	18	2	16	2.2.2.2.2.2.4	16	5	4	1
	12	12	24	14	6	8	2.2.2.2.2.2.6	18	4	4	
2	6	8	18	12		12	2.2.2.2.4.4.4	20	4	1	3
	6	6	12	8		8	2.2.2.4.4.4.8	26	3		3

[a]Listing of the columns: $|F|,|E|,|V|$ give the number of facets, edges, vertices (we recall that $|F|-|E|+|V|=2$); F-edges gives the number of facets (= polygons) with 6,4 edges, V-valence gives the number of vertices at the intersection of 4, 3 edges. $L/2L$ has 7 non-trivial cosets; the number of shortest vectors in each coset is given (they are corona vectors), the sum of 2's is $|F|$, the total is $|C|$, the number of corona vectors. In $3D$-case the zones and the belts are identical; their numbers are given, and the last column gives the numbers of them with 6, 4 elements.

edges (also three facets); their coordinates are: $[\varepsilon_1, \varepsilon_2/2, 0]$. It is a zonotope generated by the six vectors $[1, \varepsilon_i, 0]_c$ where $[\ ]_c$ tells us to use only the circular permutations. Any transformation of this set of six vectors by an element of $GL(d,R)$ generates a combinatorially equivalent zonotope (Fig. 6, P). It has six belts (= zones) containing four hexagons (with a symmetry center), two parallelograms and six parallel equal edges which form a family (Corollary 5g). In Fig. 6, the symmetry center of a facet (= middle of a facet vector) is marked by the sign $+$. The information on the five types of 3D Voronoï cells are recapitulated in Table 5.

12(18). F (We choose F for Fedorov). In the contraction of any zone of 14(24) the two parallelograms collapse (each one into an edge), the four hexagons are transformed into quadrilaterals, and the six edges become points. So the number of $2,1,0$-faces of the contracted polytope are 12,28,18; among these vertices two are tetravalent (they come from the collapse of the two zone edges which were between two hexagons) and the 16 others are trivalent. The facet vectors of the two collapsed parallelograms become corona vectors and at least two other corona vectors in the same $L/2L$ coset must appear in the contraction. Indeed the middle of each of the first two corona vectors are the middles of an edge between two hexagons; they belong to a four-element zone (= a four-hexagon belt) so the middle of its four edges are the middle of the four corona vectors (they are marked by a heavy dot in Fig. 6). Moreover, from proposition 5i, a section of this belt by a plane orthogonal to the four edges is a rectangle. For the maximal symmetry (it is tetragonal) this section is a square and the parallelograms are rhombs. The four other zones (= belts) are equivalent; each one contains two hexagons and four parallelograms. The two types of zone will lead to two different contractions.

12(14). D (for rhombohedral dodecagon). It is obtained from the contraction of the four-edge zone (= four-hexagon belt) of 12(18). The four hexagons become four parallelograms; the four edges (and their middle of corona vectors) become tetravalent and middle of corona vectors; that is also the case of the two tetravalent vertices of 12(18). The other eight trivalent vertices are preserved and no facet has disappeared in the contraction, so the number of $2,1,0$-faces are respectively $12,24,14$. All facets are parallelograms and there are four zones = belts of six edges and six parallelograms; they are equivalent. Beside the 12 facet vectors, the six four-valent vertices are

corona vectors in one $L/2L$ coset. There are four equivalent zones = belts of six edges, six parallelograms. The maximal symmetry is $Fm\bar{3}m$ and the cell is the convex hull of the centers of 14(24) faces (it is easy to see it in Fig. 6 D,V); the centers of the six squares, eight hexagons become the six 4-valence, eight 3-valence vertices, respectively. The 12 facet vectors have four coordinates in the orthonormal basis used for 14(24): $[\varepsilon_1, \varepsilon_2, 0]_c$. Notice that all faces are rhombs with a ratio of diagonal lengths $= \sqrt{2}$.

8(12). H (= hexagonal prism). This cell is obtained from the contraction of a zone of 12(18) which contains two hexagons and four parallelograms. So four facets disappear and two hexagons are transformed in quadrilaterals; the two other hexagons stay and have no common edges while the parallelograms have one common edge with each of the two hexagons. So combinatorially it is a hexagonal prism: the 2, 1, 0-faces numbers are, respectively, 8, 18, 12. The two hexagons belong to three four-belts. Proposition 5i tells us that in each belt the two pairs of parallel planes are orthogonal; this implies that the six quadrilaterals are rectangles. In Fig. 6 H we put the hexagons horizontally and the rectangles vertically. Obviously the hexagons are Voronoï cells of the 2D horizontal sub-lattice; we showed that they are inscribable in a circle, so all 8(12) cells are inscribable in a sphere. The centers of the facets which have disappeared in the contraction of 12(18) as well as the middle of the corona vectors of the later cell, form 12 corona vectors (four in each of the three $L/2L$ cosets they belong); their middles are the middles of the horizontal edges. It is easy to visualize from Fig. 6 H that these edges are common to the cells of the corona. The maximal symmetry of this hexagonal prism is obtained when the two bases are regular hexagons; this is the Voronoï cell of the lattices of the hexagonal Bravais class. It is visible in the figure that the prism collapses in the contraction along the vertical edges (which form one zone). The zone contraction along any of the three other zone = belts contracts the two hexagons into a rectangle (as we have seen it in $d = 2$), so the cells become a rectangle parallelepiped.

6(8). C. We have seen how the hexagonal prism contracts into a rectangle parallelepiped which, in its highest symmetry form is a cube. The numbers of 2, 1, 0-faces are 6, 12, 8. To the three cosets of four corona vectors of the prism 8(12) one has to add a new coset coming from the two disappearing rectangles: it gives one family of eight vectors whose middles are the vertices. The rectangular parallelepiped can also be obtained by the contraction of the rhombohedral dodecagon 12(14) along any of its four equivalent six-zones. To the six corona vectors of 12(14) forming one coset one has to add three cosets of corona vectors: the facet vectors of the three pairs of rhombs which collapse into one edge in the contraction. The middle of these three cosets of corona vectors are the middle of the edges of the three zones of the rectangular parallelepiped each one has four edges in the same orbit of the group of lattice translations. The contact point of 6(8) in the corona are well known and obvious in Fig. 6. This cell has three equivalent zones = belts; since they have four elements, the rectangular parallelepiped collapses in any zone contraction.

5.5. *High-symmetry points of the Brillouin cells*

We have introduced the reciprocal space and the Brillouin zone (= BZ) in Section 4.4. Here we call the Voronoï cell of the reciprocal lattice $2\pi L^*$, the *Brillouin cell* (indeed it was introduced by Brillouin, 1930). It is a geometrical representation of the Brillouin zone; the torus of BZ is obtained when one identifies in any pair of facets $\mathscr{F}_\pm$ with opposite facet vectors $\pm \boldsymbol{f}$ the points corresponding by lattice translations i.e. $\mathscr{F}_- \ni x \leftrightarrow x + \boldsymbol{f} \in \mathscr{F}_+$. So a point at the intersection of m facets is

identified with at least m other points of the Brillouin cell and they all represent the same element of BZ. For instance:

Proposition 5j. *In a Brillouin cell, the symmetry center (generally denoted by Γ in the physics literature) represent the 0 of the group BZ; the middles of the corona vectors belonging to a $L/2L$ non-trivial coset represent an element of order 2 of the group BZ (i.e. $0 \neq \hat{k}$, $2\hat{k} = 0$).*

We have shown that there are $2^d - 1$ such points. In Fig. 6 these points are marked by $+$ when they are the center of a facet and by $\bullet$ otherwise. In this section we want to identify on the Brillouin cell the other "high-symmetry" points of BZ, i.e. those of the zero-dimensional stratum in the actions of the Bravais groups on BZ; those elements are listed in Tables 2 and 3 for $d = 2, 3$. Let us begin with

$d = 2$.

The five Bravais groups are self-dual. Moreover to a Bravais class corresponds a unique type of Brillouin cell; the correspondence (type of Brillouin cell) $\leftarrow$ Bravais class (the Bravais group is added in ( )):

hexagon for the diclinic ($p2$), c-orthorhombic ($c2mm$), hexagonal ($p6mm$);

rectangle for the p-orthorhombic ($p2mm$), square ($p4mm$) (the rectangle is a square).

As we have seen the hexagon is the primitive cell of the quadratic form Eq. (88) with the three parameters $\lambda_{\mu\nu} > 0$. In the generating basis $\boldsymbol{b}_1, \boldsymbol{b}_2$ we can compute the coordinates of the vertices.[48] They are rational when the λ's are rational, so in that case there is an integer m such that for each vertex $\boldsymbol{v}$, $m\boldsymbol{v} \in L$. We have already seen that the vertices (for any symmetry) form one family which splits into two orbits for the translations so they represent two points in BZ of order m_1, m_2. That is irrelevant; what we want to know is "when do they belong to a stratum of dimension 0 for the action of the Bravais group?". That occurs for the largest symmetry only, $p6mm$; then, for the six vertices, $3\boldsymbol{v} \in L$. So they correspond to two points of order 3 in BZ; their coordinates in the dual basis are given in Table 2.

The rectangular cell has two pairs of facet vectors; they correspond to two points of index 2 in BZ. The third one represents the four vertices; they are the middles of four corona vectors in the same $L/2L$ coset.

$d = 3$.

It would be too long to study with the same details the three-dimensional case. Notice that there are no new concepts to introduce from what we have done for $d = 2$. But a new fact is that several types of Brillouin cells may correspond to a Bravais class. For instance, let us consider the open dense domain of generic lattices, i.e. those of minimal symmetry ($= P\bar{1}$) in $\mathscr{L}_3$ (the topological space made by the set of all 3D lattices); in a dense six-dimensional subdomain (that of $\lambda_{\mu\nu} > 0$), the Brillouin cells are primitive (14(24)), but there is a five-dimensional subdomain where they are 12(18) and even a four-dimensional boundary between those two domains where the Brillouin cells are 12(14): see Delaunay, (1932a, b) and Delone et al., (1974), (in Russian, but explained in Michel, 1995). We give the full correspondence between the 14 Bravais classes and the five types of Voronoï cells in Table 6. Most of the information — but not all of it — can be found in some classical books, e.g. Zak et al. (1969) and Bradley and Cracknell (1972).

[48] They are given in Michel (1995), Eq. 3(22); they are the quotient of two homogeneous polynomials of degree 2.

Table 6
The Brillouin cells corresponding to each Brillouin class in 3D. When there are two cells, oblate and prolate qualify the shape of the fundamental domain built on the generating basis. When there are three cells, the domain of 12(14) in $\mathscr{C}_+(\mathscr{Q}_3)$ or $\mathscr{L}_3$, is a boundary between the domain of the two other cells; so its dimension is smaller.

P-cubic ($Pm\bar{3}m$), *P*-tetra ($P4/mmm$), *P*-ortho ($Pmmm$),	6(8)
P-hexa ($P6/mmm$), *C*-ortho ($Cmmm$), *P*-mono ($P2/m$),	8(12)
I-cubic ($Im\bar{3}m$)	12(14)
F-cubic ($Fm\bar{3}m$), *I*-ortho ($Immm$)	14(24)
I-tetra ($I4/mmm$)	Oblate: 14(24), Prolate: 12(18)
R-rhombo ($R\bar{3}m$)	Oblate: 14(24), Prolate: 12(14)
F-ortho ($Fmmm$), *C*-mono ($C2/m$), *P*-tric($P\bar{1}$)	14(24), 12(18), 12(14)

With this information, and starting from the highest symmetry lattices, the reader easily identifies for each Bravais class the *BZ* points of order >2 in the zero-dimensional strata tabulated in Table 3 with the points marked by a $\circ$ or a $\times$ in Fig. 6. These *BZ* points have been computed explicitly for building Table 3 with the use of a very natural system of coordinates adapted to the property of *BZ* to be an Abelian group on a 3D torus. Let us review rapidly these points in Fig. 6.

6(8) There are none of them on the cube or the rectangular parallelepiped.

8(12) Let us first consider the two-dimensional sub-lattice $L' \subset L$ in the horizontal plane containing the center of the hexagonal prism; it cuts the prism along the hexagon = Voronoï cell of L'. If the Bravais class of L is *P*-hexagonal, that of L' is *p*-hexagonal and as we have seen for $d=2$, the vertices $\boldsymbol{v}'_\alpha$ of its cell (which are the middles of the vertical edges of the prism marked by $\circ$) correspond to the elements of order 3 of the Brillouin zones of L'; so they also correspond to the elements of order 3 of the *BZ* of L (see Table 3). The vertices of the prism have the same horizontal coordinates while their vertical coordinate is π (half of the period 2π); they correspond in the L Brillouin zone to the points of order 6 (the smallest common multiple of 2 and 3) and they are marked by $\times$.

12(14) For the lattice $Im\bar{3}m$, in the coordinate system of Section 5.4, the eight vertices of valence 3 of this cell can be identified with the middles of the eight hexagonal facets of 14(24); so their coordinates are $\boldsymbol{v}'_\alpha = \frac{1}{2}(\varepsilon_1, \varepsilon_2, \varepsilon_3)$. The six vertices of valence 4 can be identified with the middles of the square facets of 14(24); so their coordinates are $\boldsymbol{v}_\rho = [\varepsilon_i, 0, 0]_c$. The 12 facet vectors generate the lattice; their coordinates are $\boldsymbol{f}_\sigma = [\varepsilon_1, \varepsilon_2, 0]_c$. Since $2\boldsymbol{v}_\rho \in L$, the verticies of valence 4 are marked by a $\bullet$: indeed these six vertices represent one of the seven elements of order 2 in *BZ* while the six others are represented by the middles of opposite facets (we remind that they form one orbit of the Bravais group). Since $4\boldsymbol{v}'_\alpha \in L$, the vertices of valence 3 are marked by a $\circ$ and represent two elements of order 4 in *BZ*; this relation disappears when the lattice symmetry is smaller.

14(24) We have studied in detail the structure of this cell. The middle of the faces of the eight hexagons, six squares form the orbits of 4, three elements of order 2 in *BZ* (so no points are represented by $\bullet$). For the symmetry $Fm\bar{3}m$, the 24 vertices satisfy $4\boldsymbol{v}_\alpha \in L$ and represent the orbit of six elements of order 4 in *BZ*; that is why all vertices are marked by a $\circ$. For smaller Bravais groups ($I4/mmm, Immm$) that is no longer true, but a subset of them still represents an orbit of two elements of order 4 in *BZ*.

Remarks. Do not forget that the system of coordinates used in this section (and in ITC) for F and I-cubic system is not a basis generating the lattice[49] that we use generally elsewhere, and in particular in Table 3. But the geometric results (for instance in terms of $L/2L$ coset in the direct or reciprocal lattice) are independent of the choice of coordinate system. This has also to be true of any physical property of a crystal! The Voronoï cell, which is the Brillouin cell for the reciprocal lattice, has the great quality to be coordinate independent; however, the group structure U_1^d that carries the Brillouin cell[50] is not directly apparent. Not only several points of the surface of the Brillouin cell describe a unique element $\hat{k} \in BZ$ but it is not easy to find where is $2\hat{k}$ in the Brillouin cell, except in the special case of middle of facet vectors (marked $+$) or corona vectors (marked $\bullet$) for which $2\hat{k}$ is represented by the symmetry center of the cell (the 0 of the group). If $\bar{k}$ is of order 4, then $2\hat{k}$ is of order 2: which element among the seven ones existing on BZ? Let us consider for 12(14) the eight vertices of valence 3 $\boldsymbol{v}'_\alpha$; from their coordinates given above for the maximal symmetry $Im\bar{3}m$ we see that $2\boldsymbol{v}'_\alpha - \boldsymbol{v}_\rho \in F(L)$ and that shows that it is the element of BZ represented by the vertices of valence 4. Similarly, for the maximal symmetry $Fm\bar{3}m$, the 24 vertices of 14(24) represent an orbit of six elements $\hat{k}_\alpha$ of order 4 in BZ. Which centers of faces represent the $2\hat{k}_\alpha$? They must form an orbit whose number of elements is a divisor of 6; it is the three-element orbit represented by the centers of the square facets and Table 3 tells immediately which square center correspond to $2\hat{k}$ for a given vertex. For 8(12), the hexagonal prism, the 12 vertices (marked by $\times$) represent an orbit of two elements of order 6 of BZ whose double is represented by the middles (marked by $\circ$) of the six vertical edges; those represent two elements of order 3 which constitute with 0 a group $\sim Z_3$.

The geometry of the Brillouin cell is interesting; many monocrystals have their shape or the shapes obtained by translating some facets. Simple physical assumptions explain these facts. But for the quantum theory of solids it is the group law of BZ which is fundamental while the geometry of the Brillouin cell is secondary.[51] So we stop here the unnecessary lengthy study for the cases of the last three lines of Table 6, for the five Bravais classes whose BZ is represented by two or three types of Brillouin cells.

6. The positions and nature of extrema of invariant functions on the Brillouin zone

This section is an application of Section 4.4, mainly the Tables 2,3 and several theorems and methods explained in Chapter I. Physical functions defined and measured on the Brillouin zone of

[49] The bases generating a lattice are called primitive in ITC.

[50] For symmorphic space groups (they are defined in Section 7.2) only, the Voronoï cell of their translation lattice has also a natural structure of a group, that of U_1^d.

[51] Brillouin introduced Brillouin cells in papers or books written in French and German. The fundamental paper (Bouckaert, Smoluchowski, Wigner 1936) for the theory of bands introduced the cubic Brillouin cells and studied their strata (the letters they used to label them have been generally kept up to now); however the authors say in conclusion, near the end of the introduction: "Thus a certain topology for the representations must exist and it will be shown that part of this topology is independent of the special B-Z.". See also, for instance the beginning of their Section IV which inspired the treatment presented here for BZ. Contrary to a popular belief, this paper does not mention Born and von Karman (1912) method which replaces the space group by a finite quotient G/mL. This was a remarkable trick when it was invented, but it kills the topological structure of BZ.

an isolated crystal are invariant by the space group symmetry. We have explained in Section 4.4 that the effective action of the space groups on BZ depends only on its arithmetic class; so we have only 13, 73 cases (for $d = 2, 3$) to study when spin effects are irrelevant. We restrict furthermore the scope of this section to time reversal invariant phenomena (e.g. energy of bound electrons, Fermi surface, vibration spectrum, etc.); in Section 4.5 we showed that with this assumption, we have only 7, 24 cases to study. Among them there are the actions on BZ of the 5, 14 Bravais groups P_L^z; as we will see, the results are very similar for the 2, 10 other arithmetic classes containing the symmetry $-I_d$. Then for differentiable functions, Theorem 4b in Chapter I tells us that all these functions have an extremum at *each high symmetry point* of BZ, i.e. the points of the strata of 0-dimension in the action of P^z on BZ. Such type of arguments were already used in particular cases by Wigner and Seitz (1933) (in direct space), and by Bouckaert et al. (1936, Section IV).

Morse theory, explained in Chapter I, Section 6 makes predictions on the nature of these extrema for "Morse functions", i.e. the functions whose extrema are isolated. It was first used by Van Hove (1953) for this problem, using only the invariance under the lattice translations; he proved that the number of extrema on BZ is ≥ 8. In the same paper Van Hove (1953) studied the singularities[52] which are now called by his name; he proved, as an example, that density of vibration states may have a logarithmic singularities for $d = 2$ and singularities in the derivatives of a continuous function for $d = 3$. Morse himself extended his theory to such functions; the topology of their level lines determines the nature of the extrema and tells if they are isolated. Those assumptions are satisfied for most physical applications of the present chapter.[53]

Phillips (1956) and Phillips and Rosenstock (1958) extended the translational invariance to that of the full space group on some cubic examples. But a systematic treatment of this problem had never been done before 1996. To study the consequences of the symmetry under P^z, we have also to use Theorem 4c and Corollary 4c from Chapter I for BZ and apply them to the closure of each stratum. For the $d = 2$ the results are given in Section 4, Table 2. We give in Table 7 the results for dimension 3 (this allows me to correct one error — for the I-cubic system — in the previous publication (Michel, 1996)). This table gives for each of the 24 cases the minimum number of extrema for the invariant functions. Most of these extrema belong to critical orbits; when it is not the case we give the conditions which can be established for their location. In Chapter I we have called the *simplest Morse functions* those which have the minimum number of extrema.

To help reading Table 7 we recall that the Hessian $H_p(f)$ is the symmetric 3×3 matrix (= quadratic form) of the value at the point p of the second derivatives of the function f so its eigenvalues are real. At an extremum, by definition of a Morse function, $H(f)$ has no vanishing eigenvalue ($= \det H \neq 0$) and the number of its negative eigenvalues is called the Morse index of

[52] Singularities can also be added artificially. The decomposition of band systems into "distinct bands" is often done in text books by the following procedure: the first band is defined by the lowest-energy value at each $\hat{k} \in BZ$; then remove this band from the graph and define each next band in turn by the same procedure. For instance, at each crossing point between the branches of an analytic function on a multi covering of BZ one obtains a maximum with discontinuity in the derivatives. Van Hove already alluded to this procedure and had doubts on its interest.

[53] In the Appendix B to Chapter I we sketch an extension of Morse theory to functions with degenerate Hessians at the extrema, which can be very necessary in the case of symmetry under a compact group (not finite!). That is not the case here; however we apply (in the very easy case of dimension 1) another extension of Morse theory justified in Goresky and MacPhersons (1980).

Table 7
Minimum number of extrema and their positions for the functions on the three-dimensional Brillouin zone, invariant by the crystallographic group and time reversal[a]

arithm. class	0	$2\hat{k}=0$	$4\hat{k}=0$	$3\hat{k}=0$	$6\hat{k}=0$	nb	0,3	1,2	2,1	3,0	$Q(t)$
$P\bar{1}$	1	1,1,1,1,1,1,1				8	1	1+1+1	1+1+1	1	0
$P2/m$	1	1,1,1,1,1,1,1				8	1	1+1+1	1+1+1	1	0
$C2/m$	1	1,1,1,2,2				8	1	1+2	1+2	1	0
$Pmmm$	1	1,1,1,1,1,1,1				8	1	1+1+1	1+1+1	1	0
$Cmmm$	1	1,1,1,2,2				8	1	1+2	1+2	1	0
$Fmmm$	1	1,1,1,4				8+(2)	1 1+1	4 4	1+1+(2) 1+(2)	1 1	t $1,t^2$
$Immm$	1	1,2,2,2	2			10	1 2	2+2 2+2	2+2 1+2	1 1	t $1,t^2$
$P4/m$ $P4/mmm$	1	1,1,1,2,2				8	1	1+2	1+2	1	0
$I4/m$ $I4/mmm$	1	1,2,4	2			10	1 2	4 4	2+2 1+2	1 1	t $1,t^2$
$R\bar{3}$ $R\bar{3}m$	1	1,3,3				8	1	3	3	1	0
$P\bar{3}$ $P\bar{3}1m$	1	1,3,3		{2}c	{2}c	8+{4}	1 {2} {2}	{2}+3 {2}+3 1+3	{2}+3 1+3 1+3	1 1 {2}	$2t$ $1+t,t(1+t)$ $1+t^2$
$P\bar{3}m1$ $P6/m$ $P6/mmm$	1	1,3,3		2	2	12	1 2 2	2+3 2+3 1+3	2+3 1+3 1+3	1 1 2	$2t$ $1+t,t(1+t)$ $1+t^2$
$Pm\bar{3}$ $Pm\bar{3}m$	[1]	[1],3,3				8	[1]	3	3	[1]	0
$Fm\bar{3}$	[1]	3,4	{6}c			8+{6}	[1] [1]	3 4	{6} {6}	4 3	$3t^2,3$ $t+2t^2,2t+t^2$
$Fm\bar{3}m$	[1]	3,4	6			14	[1] [1]	3 4	6 6	4 3	$3t^2,3$ $t+2t^2,2t+t^2$
$I\bar{3}m$ $Im\bar{3}m$	[1]	[1],6	[2]			10+(6)	[2] [2]	(6) 6	6 (6)	[1]+[1] [1]+[1]	$1+2t+t^2$

[a]Column 1 lists the 24 arithmetic classes obtained from Table 4. Columns 2 and 3 give the critical orbits $\hat{k}=0$ and the seven elements $2\hat{k}=0$ in BZ; they are listed by their number of points. With the same notation, columns 4–6 (depending on the order of $\hat{k}$) give the number of points of other critical orbits when they exists; [ ] are orbits of maxima or minima. Column 7 gives the minimum number "nb" of extrema for any invariant function as a sum of the number of critical and non-critical points. When Morse theory requires that it *must* have extrema outside the critical orbits, the smallest orbit of those extrema is given between parentheses ( ), { } or {}. Columns 8–11 give the orbits of extrema with a given Morse index. The last column gives the corresponding polynomial $Q(t)$.

the extremum (it is 0 for a minimum and d (= the dimension of the manifold) for a maximum. At a point $p \in BZ$, we denote as usual P^z_p the stabilizer of P^z and R its (real) representation. If f is a P^z-invariant function, its Hessian at $p \in BZ$ must satisfy $g \in P^z_p$, $H_p(f) = R(g)H_p(f)R(g)^\top$. If the representation R is irreducible (on the real), the (non-degenerate) $H_p(f)$ has to be a multiple of the identity operator; this implies that the extremum is either a maximum or a minimum. Orbits which satisfy this condition are given between [ ] in Table 7.

In this table we see that for eight Bravais groups[54] (and two others: $R\bar{3}, Pm\bar{3}$) the number of critical points is 8. Every invariant function has extrema at these critical points. There exist functions, the *perfect Morse functions*, with no other extrema; indeed, the corresponding Q polynomial (introduced in Chapter I, Eq. (132)) vanishes. In the rhombohedral system, these functions have a maximum and a minimum on the orbits of one point. In the P-cubic system, that is true for *all* invariant functions (in the Brillouin cell the two points correspond to the center of the cube and to the set of eight vertices).

For the action of *Fmmm* there are also only eight critical points; they belong to five orbits; but, because there exists an orbit of four points among them, the polynomial Q cannot vanish. So there are no perfect Morse functions and any invariant function must have extrema somewhere. The closures of the one-, two-dimensional strata have, respectively, two and four critical points which are the fixed points of the groups (use Eq. (56) and Table 3); that imposes no condition on the other extrema. The smallest non-critical orbits have two elements (they are on a rotation axis with stabiliser *Fmm*2); so the functions with the minimal number of extrema have 10 of them. They are the simplest Morse functions; this situation is explained by 8 + (2) in the column "nb" of Table 7.

For four Bravais groups (and three others $I4/m$, $P\bar{3}m1$, $P6/m$) the number of critical points are 10, 12, 14. There exist simplest Morse functions with their extrema at these points. Morover for $Fm\bar{3}m$, all invariant functions must have a maximum or a minimum at $\hat{k} = 0$.

In the case of the (last studied) Bravais group, $Im\bar{3}m$, the minimum number of maxima and minima for the invariant functions is 4; they are located at the center and the quadrivalent vertices of the Brillouin cell (they represent the two fixed points of BZ) and at the trivalent vertices (they represent the critical orbit whose two elements satisfy $4\hat{k} = 0$ and $2\hat{k}$ is the fixed point $\neq 0$). With the critical orbit of six points, it is impossible to find a Morse function which has extrema only on the 10 critical points. The situation is similar to that of *Fmmm*. We verify that no new conditions for the location of extrema appear from the study of the closure of strata of positive dimension. The largest stabilizers for the non-critical points are those of the conjugacy class of $I4mm$; the corresponding orbits have six points (they are generic points of the three rotation axes of order 4). This explains the 10 (6) in the column of "nb". So for the I-cubic Bravais class, the simplest Morse functions have 16 extrema.

There are five arithmetic classes in the hexagonal system which contain $-I_3$. For two of them the two two-element orbits in the columns $3\hat{k} = 0$ and $6\hat{k} = 0$ are not critical; indeed the respective stabilizers (obtained from Table 3 and Fig. 3 from Chapter I) $P31m = P\bar{6}2m \cap P\bar{3}1m$ and $P3 = P\bar{6}2m \cap P\bar{3}$ are those of a one-dimensional closed stratum (made of two circles in BZ and represented by the vertical edges of the Brillouin cell). From Corollary 4c of Chapter I, every invariant function must have at least two extrema on each of the two connected components of the

[54] Van Hove and his successors knew it for the P-cubic.

stratum. It is possible to have only two extrema, a maximum and a minimum, on each one-dimensional component; the two maxima and the two minima form two two-element orbits for the symmetry group. Hence the notations $\{\}_c$ for the non-critical orbits, $8+\{4\}$ for eight critical extrema (common to all invariant functions) and four confined on the two components of a closed stratum.

The last case to study is $Fm\bar{3}$. The stabilizer of the orbit of six elements of order 4 is $Fmm2 = Fm\bar{3}\cap I\bar{4}2m$ (from Table 3 and Fig. 5). Since $mm2$ is an axial group, it is the stabilizer of a one-dimensional stratum and the orbit is no longer critical. Then the arithmetic class $Fm\bar{3}$ has only three critical orbits; Morse theory requires more extrema. We have to study the closure of strata of positive dimension. One of them gives a new condition; it is the stratum with the stabilizer $Fmm2$. To close this stratum in BZ we must add $\hat{k}=0$ and this closure $\bar{S}$ is made of six circles with one common point ($\hat{k}=0$); so $\bar{S}$ is not a manifold! However it is obvious that on each circle one must have (at least) another extremum. It is possible to add only one extremum if on the six circles they are on the same orbit $Fm\bar{3}$:$Fmm2$. This orbit is indicated in the column $4\hat{k}=0$ by $\{6\}$. Similarly, in the column "nb" there is $8+\{6\}$.

As a conclusion, we obtain:

Theorem 6. *The number of extrema for the simplest Morse functions on BZ, invariant by the space group and time reversal, depends only on the Bravais class. It is* 16 *for I-cubic*, 14 *for F-cubic*, 12 *for P-hexagonal*, 10 *for I-tetragonal, I- and F-orthorhombic and eight for the eight other Bravais classes.*

7. Classification of space groups from their non-symmorphic elements

7.1. Action of the Euclidean group on its space

The crystallographic space groups are the subgroups of the Euclidean group Eu_d which contains a d-dimensional lattice of translations. We first introduce notations for the Euclidean group and recall simple properties of its law and its action on the Euclidean space $\mathscr{E}_d$.

The Euclidean group $Eu_d = R^d \rtimes O_d$ is the semi-direct product of the orthogonal group by the translations; moreover one can prove that all subgroups $O_d < Eu_d$ are conjugate in Eu_d. Let us choose an origin o on the Euclidean space $\mathscr{E}_d$; then every point $x\in\mathscr{E}_d$ can be labelled by the vector $\boldsymbol{x}$ which translates o to x. Every element of Eu_d can be written as the product of first, an orthogonal transformation A and second, of a translation $\boldsymbol{s}$. We write such an element $\{\boldsymbol{s}, A\}$. Its action on the point $x\in\mathscr{E}_d$ is

$$\{\boldsymbol{s}, A\}\cdot\boldsymbol{x} = \boldsymbol{s} + A\boldsymbol{x}\ . \tag{89}$$

As a semi-direct product, the Euclidean group law is

$$\{\boldsymbol{s}, A\}\{\boldsymbol{t}, B\} = \{\boldsymbol{s} + A\boldsymbol{t}, AB\},\quad \{\boldsymbol{s}, A\}^{-1} = \{-A^{-1}\boldsymbol{s}, A^{-1}\}\ . \tag{90}$$

To obtain the form of the elements of Eu_d with the origin o' of the coordinate system we conjugate the elements by the translation $\boldsymbol{o'o}$. Explicitly the conjugation by the translation $\boldsymbol{t}$ gives

$$\{\boldsymbol{t}, I\}\{\boldsymbol{s}, A\}\{-\boldsymbol{t}, I\} = \{D_A\boldsymbol{t} + \boldsymbol{s}, A\}\quad \text{with } D_A = I - A\ . \tag{91}$$

From Eq. (89) we obtain the condition for the existence of fixed points of $\{\boldsymbol{s}, A\}$; let x be such a fixed point

$$\{\boldsymbol{s}, A\}\boldsymbol{x} = \boldsymbol{x} \Leftrightarrow \boldsymbol{s} = (I - A)\boldsymbol{x} \quad \text{i.e. } \boldsymbol{s} \in \operatorname{Im} D_A \ . \tag{92}$$

For instance, if D_A is invertible, i.e. A leaves no vector fixed ($= A$ has no eigenvalue 1), for every translation $\boldsymbol{s}$, the Euclidean transformation $\{\boldsymbol{s}, A\}$ has the unique fixed point $\boldsymbol{x} = D_A^{-1}\boldsymbol{s}$. This is the case of the connected Euclidean group in the plane, Eu_2^+. A non-trivial A is a rotation and any element of Eu_2^+ which is not a translation, is conjugated (by the translations) to a rotation.

In the general case D_A has a kernel $\operatorname{Ker} D_A$: it is the subspace of vectors $\boldsymbol{w}$ satisfying $D_A\boldsymbol{w} = 0$. Since A is orthogonal, one proves that E_d is the direct sum of the two orthogonal spaces $\operatorname{Im} D_A$ and $\operatorname{Ker} D_A$:

$$E_d = \operatorname{Im} D_A \overset{\perp}{\oplus} \operatorname{Ker} D_A \ . \tag{93}$$

Indeed let $\boldsymbol{s} = D_A\boldsymbol{t}$ and $\boldsymbol{w} \in \operatorname{Ker} D_A$, i.e. $A\boldsymbol{w} = \boldsymbol{w}$. Then $(\boldsymbol{s}, \boldsymbol{w}) = (\boldsymbol{t} - A\boldsymbol{t}, \boldsymbol{w}) = (\boldsymbol{t}, \boldsymbol{w}) - (A\boldsymbol{t}, A\boldsymbol{w}) = 0$ since A is orthogonal. If the Euclidean transformation $\{\boldsymbol{s}, A\}$ has a fixed point $o + \boldsymbol{t}$, the set of fixed points is of the form $o + \boldsymbol{t} + \operatorname{Ker} D_A$. We can summarize the obtained results in the

Proposition 7a. *The Euclidean transformation* $\{\boldsymbol{s}, A\}$ *has a fixed point* $\Leftrightarrow \boldsymbol{s} \in \operatorname{Im} D_A$, *i.e.* $\exists \boldsymbol{t}$, $\boldsymbol{s} = D_A\boldsymbol{t}$ $\Leftrightarrow$ *the component of* $\boldsymbol{s}$ *in* $\operatorname{Ker} D_A$ *is trivial. The set of fixed points is* $\boldsymbol{t} + \operatorname{Ker} D_A$.

When $\{\boldsymbol{s}, A\}$ has a fixed point, Eq. (91) shows that by taking this point as origin one transforms $\{\boldsymbol{s}, A\}$ into $\{0, A\}$. It is a trivial remark to say that any non-trivial coset of translations in Eu_d contains elements with fixed points (subtract to $\boldsymbol{s}$ its component in $\operatorname{Ker} D_A$); that is no longer trivial for a space group because its subgroup of translations, L, contains not a continuous set of elements, but only a countable one since it is a discrete subgroup of R^d. Hence, unlike the full Euclidean group, a space group may not be a semi-direct product.

Let us consider first the case of space groups which are semi-direct products. Given a finite subgroup P^z of $GL(d, Z)$, it acts naturally on a lattice L and we can define the semi-direct product $L \rtimes P^z$ by the law (90). One obtains the same space group by taking another group mP^zm^{-1}, $m \in GL(d, Z)$, of the same arithmetic class in the m transformed lattice basis. So for $d = 2,3$ there exists, respectively, 13, 73 space groups which are semi-direct products. The crystallographers call them *symmorphic*. In this section we want to characterize the $17 - 13 = 4$, $230 - 73 = 157$ *non-symmorphic* space groups. They will be characterized by their action on the Euclidean space. We first give general features of this action for all space groups.

7.2. *Space group stabilizers and their strata* (= *Wyckoff positions*)

Given a space group G, we recall the group homomorphism $G \overset{\theta}{\to} P = G/L$. Translations have no fixed points, so a stabilizer G_x does not contain translations and $G_x \sim \theta(G_x) \leq P$; in plain words the stabilizers are finite subgroups isomorphic to subgroups of the point group. We recall that two points x and y are in the same stratum when their stabilizers G_x and G_y are conjugate in G. Then their image by θ are conjugated in P. The converse is not true but one can prove that the number of

conjugacy classes of finite subgroups of G mapped by θ on a conjugacy class of P is at most 2^d and this implies that in the action of G on the Euclidean space the number of strata is finite. For each space group in $\dim d = 2, 3$ ITC give the list of strata and their structure under the heading *Wyckoff positions*. We recall that the set of strata has a natural partial order (induced from the partial order of the conjugacy classes of finite subgroups of the space group G).

Proposition 7b. *Every finite group stabilizes points of space. If it is a maximal finite subgroup of G, it is a maximal stabilizer of G.*

Given any finite subgroup H of the Euclidean group, for any point x of space the barycenter of the orbit $H \cdot x$ is invariant by H. If H is maximal among the finite subgroups of G, it is a stabilizer of G.

Proposition 7c. *If G_x is a stabilizer of the space group G, then $L \rtimes G_x$ is an equitranslational subgroup of G.*

Proof. Let us choose x as the origin of coordinates; by Eq. (90), the Euclidean group law of $L \rtimes G_x$ is written as a semi-direct product. Conversely, if G is a semi-direct product, its law can be written with Eq. (90) and P is the stabilizer of the origin of coordinates. That proves:

Corollary 7c. *The space group G is symmorphic $\Leftrightarrow$ it has at least one stabilizer $G_x \sim P$ in its action on the space.*

Proposition 7d. *$L \rtimes H$ is a maximal equitranslational subgroup of $G \Leftrightarrow H$ is a maximal stabilizer of G.*

The proof of $\Rightarrow$ is obvious. Proof of $\Leftarrow$: admit that H is not a maximal finite subgroup of G; then it is a strict subgroup of K, a maximal finite subgroup of G. From Proposition 7b, it is a stabilizer of G and from Proposition 7c, $L \rtimes K$ is an equitranslational subgroup of G; it is strictly larger than $L \rtimes H$ and that is absurd.

Proposition 7e. *In the action of a space group G on the Euclidean space, the intersection of stabilizers is a stabilizer.*

Hint: It is sufficient to prove it for any pair of stabilizers. Let G_x and G_y be the stabilizers of the two points x, y; there is a dense subset of the straight line containing x and y whose points have $G_x \cap G_y$ as stabilizer.

Since all stabilizers are finite, the Palais theorem (Palais, 1961) mentioned in Chapter I Section 2 applies and Theorem 2a (Chapter I) is valid. More precisely: there exists a stratum with trivial symmetry; it is open dense in $\mathscr{E}_d$. The closure of a stratum is the union of the strata with a higher symmetry; in particular the strata with maximal symmetry are closed. The number of parameters (among x, y, z) which define a Wyckoff position in ITC is the dimension of the strata.[55]

[55] Table 8 gives a statistics on the dimension of the maximal symmetry strata.

7.3. Non-symmorphic elements of space groups. Their classification

We need some criterion for discussing the structure of the non-symmorphic space groups in dimension $d = 2, 3$. It is natural to introduce:

Definition. Let G be a space group and $G \ni g \notin L$; if no elements of its translation coset $gL = Lg$ leaves a fix point of space, the coset elements are called *non-symmorphic*.

One can also say that no element of this coset can belong to the stabilizer of a point of space, so the stabilizers of G are isomorphic only to strict subgroups of the point group P. Hence, if a space group G has a non-symmorphic element, from Corollary 7c, it has to be a non-symmorphic space group. As we shall see later the converse is not true! In dimension 3 there exist two non-symmorphic space groups which have no non-symmorphic elements.

Since the linear components A of the elements of a space group G have a finite order v (it is the smallest positive integer such that $A^v = I$) it is useful to introduce the operator N_A (acting on the real vector space E_d):

$$\text{order}(A) = v, \quad N_A = I + A + A^2 + \cdots + A^{v-1} = \sum_{j=0}^{v-1} A^j ,$$

$$AN_A = N_A = N_A A . \tag{94}$$

With D_A defined in Eq. (91) we have the relations

$$N_A D_A = 0 = D_A N_A \Leftrightarrow \operatorname{Im} D_A \subseteq \operatorname{Ker} N_A, \quad \operatorname{Im} N_A \subseteq \operatorname{Ker} D_A . \tag{95}$$

It is easy to prove that the equality holds in the last two relations for these operators on E_d. Let $\boldsymbol{v} \in \operatorname{Ker} D_A$, i.e. $A\boldsymbol{v} = \boldsymbol{v}$; then $\boldsymbol{v} = N_A v(A)^{-1}\boldsymbol{v}$ which proves $\operatorname{Ker} D_A \subseteq \operatorname{Im} N_A$ and therefore the last equality. By a similar proof to that for D_A, Eq. (93) is also true for N_A; then we deduce the first equality in Eq. (95) from the second one. So we can sharpen Eq. (95) by

$$\operatorname{Ker} D_A = \operatorname{Im} N_A, \qquad \operatorname{Im} D_A = \operatorname{Ker} N_A . \tag{96}$$

Beware, that is not true if we restrict the action of these two operators to a lattice L.

Let $\{\boldsymbol{v}(A), A\}$ be an element of the space group G written as an element of the Euclidean group for a choice of origin. Then

$$\text{order}(A) = v, \quad G \ni \{\boldsymbol{v}(A), A\}^v = \{N_A \boldsymbol{v}(A), I\} \Leftrightarrow N_A \boldsymbol{v}(A) \in L . \tag{97}$$

Proposition 7f. *The element $\{\boldsymbol{v}(A), A\} \in G$ has a fix point for its action on the Euclidean space if, and only if $N_A \boldsymbol{v}(A) = 0$.*

Indeed if $\{\boldsymbol{v}(A), A\}$ has a fixed point its vth power $\{\boldsymbol{v}(A), A\}^v = \{N_A \boldsymbol{v}(A), I\}$ has the same fixed point; this implies $N_A \boldsymbol{v}(A) = 0$. Conversely, the second equality of (96) shows that $\boldsymbol{v}(A) \in \operatorname{Ker} N_A$ implies the condition of Proposition 7a.

We can now give a test for determining the non-symmorphic elements of a space group.

Corollary 7f. *The element* $\{\boldsymbol{v}(A), A\} \in G$ *is non-symmorphic if, and only if,* $N_A \boldsymbol{v}(A) \notin N_A L$.

Indeed this requires $N_A \boldsymbol{v}(A) \neq 0$. Assume the contrary of what is to be proven, i.e. there exists $\ell \in L$ such that $N_A \boldsymbol{v}(A) = N_A \ell$; that is equivalent to say, from Proposition 7f that $\{\boldsymbol{v}(A) - \ell, A\}$ has a fixed point and therefore $\{\boldsymbol{v}(A), A\}$ which is in the same L coset, is not non-symmorphic.

As we have shown after Eq. (92), if D_A is invertible (i.e. A has no eigenvalue $= 1$) $\operatorname{Im} D_A$ is the whole space. From Eq. (96) this is also true for $\operatorname{Ker} N_A$ so Corollary 7c is not satisfied. We conclude that non-symmorphic elements cannot have a linear part A without eigenvalues $= 1$, so, when $d = 2, 3$, *there are no non-symmorphic elements whose orthogonal part A belongs to the following arithmetic elements* (we have to add the two trivial arithmetic classes $p1, P1$ since the corresponding space groups contain only translations):

$$p1, p2, p3, p4, p6, \quad \text{and} \quad P1, P\bar{1}, P\bar{3}, P\bar{4}, P\bar{6}, R\bar{3}, I\bar{4}\ . \tag{98}$$

We now show that Corollary 7d eliminates also $cm, C2, R3$.

For

$$cm = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\colon\ N_{cm} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

then the vectors $N_{cm}\boldsymbol{v}(cm)$ are of the form $\binom{m}{m}$ with m integer. But these vectors are in $N_{cm}L$; indeed $N_{cm}\binom{0}{m} = \binom{m}{m}$.

For $C2$:

$$C2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad L \cap \operatorname{Im} N_{C2} = \left\{ \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}, m \in Z \right\}, \tag{99}$$

$$N_{C2}\begin{pmatrix} m \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}.$$

For $R3$:

$$R3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad L \cap \operatorname{Im} N_{R3} = \left\{ \begin{pmatrix} m \\ m \\ m \end{pmatrix}, m \in Z \right\}, \tag{100}$$

$$N_{R3}\begin{pmatrix} m \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m \\ m \\ m \end{pmatrix}.$$

Hence we can add cm, $C2$, $R3$ to the list of the 12 arithmetic elements given in Eq. (98).

We are left to study the 8 arithmetic elements (out of $7 + 16 = 23$) which can produce non-symmorphic elements

$$pm, P2, P3, P4, P6, I4, Pm, Cm\ . \tag{101}$$

We now establish the list of non-symmorphic elements they produce.

Let us begin by the first five of them. They have a one-dimensional eigenspace with the eigenvalue 1, i.e.; $\operatorname{Im} N_A = \operatorname{Ker} D_A$ is an axis. It contains a one-dimensional sublattice generated by the lattice vector $\boldsymbol{b}$ (we choose arbitrarily its sign) and $N_A \boldsymbol{v}(A) = \mu \boldsymbol{b}$. For these (p, P)-lattices, this axis of fixed points is orthogonal to $\operatorname{Ker} N_A = \operatorname{Im} D_A$; by a choice of origin of coordinates we can bring to zero the component of $\boldsymbol{v}(A)$ in $\operatorname{Im} D_A$, so it becomes $\boldsymbol{v}(A) = v^{-1}\mu \boldsymbol{b}$. On the other hand $N_A L = \{vm\boldsymbol{b}, m \in Z\}$. So we obtain the complete solutions for these five cases:

$$A = pm, P2, P3, P4, P6, \quad v = \text{ order of } A\ ,$$

$$\boldsymbol{v}(A) = \frac{\mu}{v}\boldsymbol{b},\ 0 < \mu < v\ . \tag{102}$$

Explicitly this gives the following 13 non-symmorphic elements in the notation of ITC:

$$pg,\ Pc,\ P2_1,\ P3_1 \sim P3_2,\ P4_1 \sim P4_3\ ,$$

$$P4_2,\ P6_1 \sim P6_5,\ P6_2 \sim P6_4,\ P6_3\ . \tag{103}$$

With the translations, these 13 non-symmorphic elements generate 13 space groups which are denoted by the same labels as in ITC. The sign $\sim$ indicates an isomorphism: it is obtained by conjugation with a reflection through a plane containing the invariant axis. ITC list them as two different orientations which can be distinguished by physical phenomena (e.g. with circularly polarized light); in nature they appear together as domains in crystalline structures or as a result of some phase transitions. The four $\sim$ of Eq. (103) indicate four of the 11 enantiomorphic pairs [they are listed below in Eq. (109)].

The case of the arithmetic element Pm is similar: $(\operatorname{Im} N_{Pm} = \operatorname{Ker} D_{Pm}) \perp (\operatorname{Ker} N_{Pm} = \operatorname{Im} D_{Pm})$ but $\dim \operatorname{Im} N_{Pm} = 2$. Hence $L \cap \operatorname{Im} N_{Pm}$ is a two-dimensional lattice. We say that a vector ℓ of this lattice is *visible* if no vector $m^{-1}\ell$, $1 < m \in Z$ is a lattice vector; in other words ℓ belongs to the $GL(2, Z)$ orbit of vectors which can be basis vectors. This non-symmorphic element is denoted by Pc with $\boldsymbol{v}(Pc) = \frac{1}{2}\ell$. When the point group contains the non-symmorphic element Pc and has more than two elements, the direction of the glide vector $\boldsymbol{v}(Pm)$ is constrained by the preferred directions of the other point group elements. To distinguish between the different possibilities one of the following symbols are used: Pa, Pb, Pc, Pd, Pn; we refer to ITC for their definition.

Case Cm:

$$Cm = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad L \cap \operatorname{Im} N_{Cm} = \left\{ \begin{pmatrix} m \\ m \\ n \end{pmatrix},\ m, n \in Z \right\},$$

$$N_{Cm} \begin{pmatrix} m \\ 0 \\ n \end{pmatrix} = \begin{pmatrix} m \\ m \\ 2n \end{pmatrix} \quad \Rightarrow \boldsymbol{v}(Cc) = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}. \tag{104}$$

This non-symmorphic element, as well as the space group it generates with the translations, is labelled *Cc* in ITC. Since its glide reflection vector is uniquely defined, no other label is necessary; however, in ITC, *Ca* is also used for giving the direction of the plane. Below we list the different notations used when the first (= lattice) letter is A, I, F.

The last case to be considered is the arithmetic element $I4$:

$$I4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix}, \quad L \cap \mathrm{Im}\, N_{I4} = \left\{ \begin{pmatrix} m \\ m \\ 0 \end{pmatrix}, m \in Z \right\},$$

$$N_{I4} L = \left\{ \begin{pmatrix} 2m \\ 2m \\ 0 \end{pmatrix}, m \in Z \right\} \quad \Rightarrow \quad \boldsymbol{v}(I4_1) = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}. \tag{105}$$

This non-symmorphic element is denoted by $I4_1$ in ITC; its square is symmorphic:[56] it is C2 up to a lattice translation. The square of $P4_1$ is the non-symmorphic element $P2_1$. The symbol 4_1 is completely ambiguous; its meaning is defined only when one knows the first letter P on one hand, I or F on the other hand.

The non-symmorphic space group $I4_1$ is a sub-space group with the same translations, of six space groups in the I-tetragonal Bravais class and of $F4_132, I4_132$ in the cubic crystallographic system.

The arithmetic class $P2$ has one non-symmorphic group $P2_1$. Similarly the non-symmorphic groups of the arithmetic class $P222$ are $P2_122$, $P2_12_12$ and $P2_12_12_1$.

The arithmetic class $C2$ has no non-symmorphic space groups. The groups of the arithmetic class $C222$, contain three rotations by π around three orthogonal axes; by convention in ITC, the first two are of C type and the last one is of the P type. So the only non-symmorphic space group of the arithmetic class $C222$ is $C222_1$. The rotations by π in the space groups of Bravais classes F, I are of type $C2$; however, the labels of two space groups of the 24 F, I arithmetic classes contain 2_1, i.e. $I2_12_12_1$ and $I2_13$. These two groups are the only non-symmorphic space groups *without* non-symmorphic elements; these labels are a (non-explicitly explained) way for the Hermann–Maughin notation of ITC to signal that these two exceptional groups have no stabilizers $G_q \sim P$ for the points of space, i.e. there is no origin for which all $\boldsymbol{v}(A)$ can be simultaneously removed (note that $I2_13$ is the automorphism group of its subgroup $I2_12_12_1$ when the three fundamental periods of translations become equal). On the other hand $F222$ is the only space group of its arithmetical class and this is also the case of its automorphism group $F23$ since it is generated by $F222$ and the element $(R3)$.

A group of the arithmetic class $R32$ contains only the arithmetic elements $P1$, $R3$, $C2$; so there are no non-symmorphic space groups in the arithmetic class $R32$. In dimension 2, the only arithmetic element from which one can obtain a non-symmorphic element is *pm*; from Fig. 1 we see that the only arithmetic classes which contain it are *pm*, *p2mm*, *p4mm*. To summarize, for $d = 2,3$ there are 10, 12 arithmetic classes containing only one space group: the semi-direct product

[56] It seems to me that it would have been better to denote it by $I4_2$.

(= symmorphic one)

$$p1, p2, cm, p4, c2mm, p3, p3m1, p31m, p6, p6mm\ ,$$

$$P1, P\bar{1}, C2, P\bar{4}, I\bar{4}, R3, R\bar{3}, R32, P\bar{3}, P\bar{6}, F222, F23. \tag{106}$$

By a convention similar to that for $C222$, in the arithmetic class $Cmm2$, the two reflections belong to the Cm class while the rotation belongs to the $P2$ class. So the non-symmorphic space groups of the arithmetic class $Cmm2$ are $Ccc2$ and $Cmc2_1$. There is another arithmetic class (of the same geometric class[57] $mm2$), denoted by $Amm2$; its rotation is of the $C2$ class and the two reflections belong, respectively, to the two different classes Pm, Cm. The three non-symmorphic space groups are $Abm2, Ama2, Aba2$. The reflections Cm occur also in the I classes (where they are denoted by Ia, Ib, Ic, Id) and the F class (where they are denoted by Fd, Fc).

7.4. Some statistics on space groups

In this section we limit ourselves to $d = 3$. We first give a statistics of SpG/AC, the number of space groups per arithmetic class

SpG/AC	1	2	3	4	6	8	10	16		
AC	12	32	6	15	3	2	1	2	73	
SpG	12	64	18	60	18	16	10	32	230	(107)

The list of arithmetic classes containing only one space group (this symmorphic space group has the same label) is given in Eq. (106). For the 32 arithmetic classes which contain two space groups we list the corresponding 32 non-symmorphic space groups (grouping them by Bravais classes)

$P2_1$	Pc	Cc	$C2/c$	$C222_1$	$I2_12_12_1$	$Fdd2$	$Fddd$
$I4_1$	$I4_1/a$	$I4_122$	$I\bar{4}c2$	$I\bar{4}2d$	$R3c$	$R\bar{3}c$	$P3c1$
$P31c$	$P\bar{3}1c$	$P\bar{3}c1$	$P6_3/m$	$P\bar{6}c2$	$P\bar{6}2c$	$P2_13$	$P\bar{4}3n$
$Fd\bar{3}$	$F4_13d$	$F\bar{4}3c$	$I2_13$	$Ia\bar{3}$	$I4_132$	$I\bar{4}3d$	$Ia\bar{3}d$

(108)

To find the arithmetic class (and the symmorphic space group in it), one suppresses the indices in the labels and replaces the lower case letters a, c, d, n by m.

After Eq. (103) we pointed out the existence of enantiomorphic pairs of isomorphic space groups. For the convenience of the reader we give here the list of the 11 enantiomorphic pairs

$P4_1 \sim P4_3$	$P3_1 \sim P3_2$	$P6_1 \sim P6_5$	$P6_222 \sim P6_422$
$P4_122 \sim P4_322$	$P3_112 \sim P3_212$	$P6_2 \sim P6_4$	$P4_132 \sim P4_332$
$P4_12_12 \sim P4_32_12$	$P3_121 \sim P3_221$	$P6_122 \sim P6_522$	

(109)

[57] This geometric class $mm2$ is the one which has the biggest number of corresponding arithmetic classes: five of them. They are denoted by: $Pmm2$, $Cmm2$, $Amm2$, $Fmm2$, $Imm2$.

Table 8
Number of space groups with given dimension of closed strata

230	104	63	5	13	38	2	4	1
dim 0	x				x	x		x
dim 1		x			x		x	x
dim 2			x			x	x	x
dim 3				x				

If all non-trivial elements of a space group are either translations or non-symmorphic elements the stabilizers on the Euclidean space are all 1, i.e. there is the unique stratum: the whole space; mathematicians call this action *free*. This is the case of nine of the space groups of Eq. (103). The first of them, *pg* is the only free acting non-trivial space group for $d = 2$. In dimension 3 there are 13 space groups with free action on the space

$$P1, P2_1, Pc, Cc, P2_12_12_1, Pca2_1, Pna2_1 \ ,$$
$$P4_1 \sim P4_3, P3_1 \sim P3_2, P6_1 \sim P6_5 \ . \tag{110}$$

It is interesting to give a statistics of the dimension of the maximal symmetry (= closed) strata of space groups. We reproduce in Table 8 the statistics given in Bacry et al. (1988) for dimension 3.

By X-rays, neutron diffraction, etc. one can obtain the reciprocal lattice and in principle the crystal lattice; it has to belong to one of the 14 Bravais classes. The crystal may belong to a smaller symmetry; that is not a generic situation: with a change of temperature, pressure, etc. the lattice Bravais class is likely to go to that of the crystal. One also knows the volume of the fundamental cell.

When the chemical composition and the weight density are also known, this determines the number n_i of the different kinds A_i of atoms per fundamental cell. We define:

$$n_i = \text{number of atoms } A_i \text{ per fundamental cell} \quad n_m = \min n_i \ . \tag{111}$$

Let us explain how this knowledge already excludes some space groups.

Definition. The index of symmorphy (= *IS*) of a space group G is the minimum value of $|P|/|G_x|$ for all stabilizers of G.

Then we must have the inequality

$$IS \leq n_m \ . \tag{112}$$

Note that $IS = 1$ for a symmorphic space group; so if $n_m = 1$, i.e. there is a unique atom of a kind in the fundamental cell, then the space group has to be symmorphic. From Proposition 7d, if we know that G has an equitranslational symmorphic subgroup of index i then $IS(G) \leq i$. Let us give some arguments based on the list in Eq. (106) of the arithmetic classes containing only the symmorphic groups. The presence in this list of $F23$ implies that for the cubic-F groups, $IS \leq 4$ for those of the arithmetic class $Fm\bar{3}m$ and $IS \leq 2$ for the others. The presence of $R3, R\bar{3}, R32$ implies

that for the other cubic groups $IS \leq 8$ and for the rhombohedral subgroup $IS \leq 2$. The presence of $I\bar{4}$, $P\bar{4}$ implies for the cubic groups of the arithmetic classes $I\bar{4}3m$, $P\bar{4}3m$ their $IS \leq 6$.

In the hexagonal system, the symbols $3_1, 3_2, 6_2, 6_4$ in the label of a space group can disappear only for subgroups of index 3, so $IS \geq 3$.

Similarly the symbols $6_1, 6_5$ in the label of a space group can disappear only for subgroups of index 6, so $IS \geq 6$.

In the tetragonal system, the symbols 4_1,4_3 in the label of a space group can disappear only for subgroups of index 4, so $IS \geq 4$.

So we know here to look in ITC for space groups with $IS \geq 3$. Here is their list:

$IS = 3$: $P3_1, P3_2, P3_112 \sim P3_212, P3_121, P3_221, P6_2, P6_4, P6_222, P6_422$.
$IS = 4$: $P2_12_12_1, Pca2_1, Pna2_1, Pcca, Pccn, Pbcm, Pbca, Pnma, Ibam, Ibca$.
$P4_1 \sim P4_3, P4_122 \sim P4_322, P4_12_12 \sim P4_32_12, P4_2bc, I4_1cd, P/ncc, P4_2/nbc$,
$P4_2/ncm, I4_1/ncd, P2_13, I2_13, Pa\bar{3}, Ia\bar{3}, P4_132 \sim P4_332, I4_132, Fd\bar{3}c$.
$IS = 6$: $P6_1 \sim P6_3, P6_122 \sim P6_322, I\bar{4}3d$.
$IS = 8$: $Ia\bar{3}d$.

To summarize, the number of space groups with the different possible values of IS are

1	2	3	4	6	8
73	110	10	31	5	1

For the space group which satisfies Eq. (112) one has also to find for each kind of atoms the values of $v_x = |P|/|G_x|$ which satisfy $n_i = \sum v_x$ without using more than once the strata of dimension zero. The dynamics of interatomic forces favors generally the high-symmetry strata for the atom positions; it might be a strict symmetry requirement when the n_i are small.

For instance a little more than half of the chemical elements have the space group symmetries $Fm\bar{3}m$ and $Im\bar{3}m$ with a small preference for the former which is also the most frequent space group (more than 8%) for all inorganic compounds. As shown in Section 4.4 the strata (= Wyckoff positions) of dimension 0 of $Fm\bar{3}m$ contain two fixed points (origin and quadrivalent vertices of the Voronoï cell), one orbit of two elements (the trivalent vertices) and one orbit of six elements (the center of faces). Many of the inorganic chemical compounds which crystallize with this symmetry have the stoichiometries XY, XZ_2, XYZ_2, XW_6, XYW_6, XYZ_2W_6.

In frequency of occurrence the $Fm\bar{3}m$ is followed by the space groups $Pnma$, $Fd\bar{3}m$, $P6_3mm$, $P2_1/c$, $Pm\bar{3}m$, etc. These six groups represent more than the third of the inorganic compounds.

$Fd\bar{3}m$ is the space group of the chemical elements C (diamond) and Si, Ge, Se, Sn (gray tin) and the dense packing hexagonal group $P6_3/mmc$ is that of C (graphite), As, Sb, Bi, Cr, Ti, etc. (more than 20). $P2_1/c$ represents 5% of the inorganic compounds and 30% (the most abundant) of the organic ones (see below). The symmorphic group $Pm\bar{3}m$ has four strata of dimension 0; two orbits of one element (center and vertices of the cube) and two orbits of three elements (center of faces and middle of edges). It represents W, O_2, F_2 and many compounds of the types XY (as NaCl, ionic crystal), XZ_3, XZ_6, XYZ_3 and more complicated ones.

For organic crystals, which are essentially molecular, the situation is quite different. These molecules can form crystals with larger symmetry point groups than their own symmetry group;

indeed there are most often several molecules per fundamental cell and their positions in the cell have the symmetry of the crystal point group (see e.g., Kitaigorodsky, 1973). Half of the organic compounds have the crystal symmetries $P2_1/c$, $P2_12_12_1$ and $P2_1$.

8. The unirreps of G_k and G and their corepresentations with $\mathscr{T}$

8.1. The unitary irreducible representations of G_k

In the previous section we have recalled in Eq. (90) the group law of Eu_d, the Euclidean group, and in Eq. (91) the effect of a change of origin in $\mathscr{E}_d$, the Euclidean space. Since a space group G is a discrete subgroup of Eu_d, we can use for the element of G the notation $\boldsymbol{t}\in L$ for the translations and take for each coset of L an element that is traditionally denoted (as in Eq. (97)) $\{\boldsymbol{v}(A), A\}$ with A an element of the point group P and $\boldsymbol{v}(A)$ a translation often called "imprimitive" to tell that it is not in L. The product of two elements of G is

$$\boldsymbol{s},\boldsymbol{t}\in L,\quad A,B\in P\ ,$$
$$\{\boldsymbol{s}+\boldsymbol{v}(A),A\}\{\boldsymbol{t}+\boldsymbol{v}(B),B\}=\{\boldsymbol{s}+\boldsymbol{v}(A)+A(\boldsymbol{t}+\boldsymbol{v}(B)),AB\}\ . \tag{113}$$

Assuming that the imprimitive translations are known for every point group element, we want $\boldsymbol{v}(AB)$ to appear in the right-hand side; so the group law of G can be written as

$$\boldsymbol{s},\boldsymbol{t}\in L,\quad A,B\in P\ ,$$
$$\{\boldsymbol{s}+\boldsymbol{v}(A),A\}\{\boldsymbol{t}+\boldsymbol{v}(B),B\}=\{\boldsymbol{s}+A\boldsymbol{t}+\boldsymbol{v}(AB)+\boldsymbol{z}(A,B),AB\} \tag{114}$$

with the definition

$$\boldsymbol{z}(A,B):=\boldsymbol{v}(A)-\boldsymbol{v}(AB)+A\boldsymbol{v}(B)\in L\ , \tag{115}$$

indeed $\boldsymbol{z}(A,B)$ can be at most a translation. We will always make the convention

$$\boldsymbol{v}(I)=0,\quad \text{so } \boldsymbol{z}(I,A)=0=\boldsymbol{z}(A,I)\ . \tag{116}$$

The function $\boldsymbol{v}(A)$ depends on the choice of origin in the Euclidean space. From Eq. (91) we know that if we translate the origin o by the translation $\boldsymbol{x}=o'-o$, we make a conjugation in Eu_d by the element $\{\boldsymbol{x},I\}$; then $\boldsymbol{v}'(A)$, the new imprimitive translation function is related to $\boldsymbol{v}(A)$ by

$$\boldsymbol{v}'(A)=\boldsymbol{v}(A)+D_A\boldsymbol{x}\quad \text{with } D_A=I-A\ . \tag{117}$$

It is straightforward to verify that $\boldsymbol{z}(A,B)$ is invariant by change of the origin[58] in $\mathscr{E}_d$.

Corollary 7c tells that for any stabilizer G_x in the action of G on the Euclidean space, the semi-direct product $L\rtimes G_x$ is a subgroup of G. If a stabilizer G_x is isomorphic to the point group, then the space group is a semi-direct product $G=L\rtimes P$ (crystallographers say G is symmorphic). By taking the origin at such point x the space group law has the same form as that of the Euclidean group in Eq. (90), i.e. all $\boldsymbol{v}(A)=0$ and therefore all $\boldsymbol{z}(A,B)=0$.

[58] That does not mean that $\boldsymbol{z}(A,B)$ is completely fixed for a given space group G. We leave the discussion of this point to Section 8.3.

We use the shorthand *unirrep* for "unitary irreducible representation". As we saw in Section 4.4 before Eq. (53), we recall that G_k (the stabilizer of $\boldsymbol{k}$ in the action of G on BZ) is a space group with P_k as point group. Moreover $G_k = G$ for $\hat{k} = 0$ and other points of BZ (listed in Table 3) except for the space groups of the Bravais class cubic-F.

As we explained in Section 4.4, the subgroup of translations is represented by the one-dimensional unirreps labelled by $\hat{k} \in BZ$

$$L \ni \boldsymbol{t} \mapsto \hat{k}(\boldsymbol{t}) := \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}}, \quad \hat{k} = \text{class } \boldsymbol{k} \bmod 2\pi L^* \,, \tag{118}$$

since for all $\boldsymbol{k} \in 2\pi L^*$, i.e. all vectors of the reciprocal lattice, the representation (118) is trivial. It is important to consider the kernel and the image of the unirrep $\hat{k}$ of the translation group L. We recall the definitions:[59]

$$\begin{aligned} &\mathrm{Ker}\,\hat{k} := \{\boldsymbol{t} \in L;\ \hat{k}(\boldsymbol{t}) = 1\} \leq L \,, \\ &\mathrm{Im}\,\hat{k} := \hat{k}(L) \sim (L/\mathrm{Ker}\,\hat{k}) < U_1 \,. \end{aligned} \tag{119}$$

We recall the nearly obvious proposition:

Proposition 8a. *$\hat{k}$ is of finite order m in BZ $\Leftrightarrow$ the coordinates of $\boldsymbol{k}$ in the reciprocal lattice $2\pi L^*$ are rational. Moreover* $\mathrm{Im}\,\hat{k} \sim Z_m$.

Remember that in Section 4.4 and everywhere else we use the coordinates κ_i of $\boldsymbol{k}$ in the dual lattice L^*; so the coordinates of $\boldsymbol{k}$ in the reciprocal lattice are $\kappa_i/2\pi$.

As we saw in Section 4.4, the translations act trivially on BZ, so the space group G acts on BZ through the point group P^z; this action (and therefore the decomposition of BZ into strata and orbits) is the same for all space groups of an arithmetic class. We denote by $P^z_{\hat{k}}$ the P^z-stabilizer of $\hat{k} \in BZ$. The G-stabilizer G_k contains all translations (so it is a space group with the same translations as G) and for two space groups of the same arithmetic class, the two sets of G_k's, $\hat{k} \in BZ$ are distinct. Indeed at least some corresponding G_k are not isomorphic.

Since G_k is the stabilizer of $\boldsymbol{k}$, it is easy to verify that $\mathrm{Ker}\,\hat{k}$ is an invariant subgroup of G_k. It is natural to consider the corresponding quotient group; this has been done by Herring (1942), so we call this group the Herring group and we denote it by $P^z(\boldsymbol{k})$. To see the structure of this very interesting group we use the theorem of group theory on the simplification of fractions. Let us "simplify" the fraction G_k/L by $\mathrm{Ker}\,\boldsymbol{k}$ which is an invariant subgroup of both numerator and denominator (see Eq. (119)). We obtain

$$G_k \xrightarrow{\theta_k} P^z(\boldsymbol{k}) := G_k/\mathrm{Ker}\,\boldsymbol{k}, \quad P^z(\boldsymbol{k})/\mathrm{Im}\,\hat{k} = P^z_{\hat{k}}, \quad \mathrm{Im}\,\hat{k} \lhd C(P^z(\boldsymbol{k})) \,, \tag{120}$$

the center of $P^z(\boldsymbol{k})$ (use again that G_k stabilizes $\boldsymbol{k}$); we recall (see Section 4) that $P^z_{\hat{k}}$ is the stabilizer of $\hat{k}$ in its action on BZ. From the definition of $P^z(\boldsymbol{k})$ we verify that the unirreps of G_k are unirreps of $P^z(\boldsymbol{k})$. The converse is not true; indeed we have to consider only a subset of $P^z(\boldsymbol{k})$ unirreps.

[59] We recall that here the relation $<$ between groups means "subgroup"; U_1, the one-dimensional unitary group, is the group of phases in the complex plane.

Definition. *The allowed unirreps of $P^z(\boldsymbol{k})$ are those which represent faithfully the subgroup* $\mathrm{Im}\,\boldsymbol{k}$ by the matrices $\exp(i\boldsymbol{k}\cdot\boldsymbol{t})I_d$ where n is the dimension of the unirrep of $P^z(\boldsymbol{k})$. This definition is tailored for the following:

Proposition 8b. *There is a bijective correspondence between the unirreps of G_k and the allowed unirreps of $P^z(\boldsymbol{k})$; the corresponding unirreps have the same image.*

As is well known, in the trivial case of $\boldsymbol{k}=0$, $G_0=G$, $P^z(\boldsymbol{0})=P_0^z=P^z$: the unirreps of the point group P are those of G for $\boldsymbol{k}=0$.

We recall that crystallographers call symmorphic space groups, those G's which are semi-direct products of P^z by L; i.e. P^z is a subgroup of G. That implies that P_k^z is a subgroup of $P^z(\boldsymbol{k})$; since $\mathrm{Im}\,\hat{k}$ is in the center of $P^z(\boldsymbol{k})$, this group is a direct product. To summarize:

$$G=L\rtimes P^z\Rightarrow P^z(\boldsymbol{k})=\mathrm{Im}\,\hat{k}\times P_k^z\ . \tag{121}$$

Beware that the converse is not true! We will see counter examples below.

Proposition 8c. *When P_k^z is cyclic, $P^z(\boldsymbol{k})$ is Abelian. Then their allowed unirreps are one-dimensional and their image is a subgroup of U_1.*

Eq. (121) proves it for symmorphic groups. For the non-symmorphic groups we have studied in the previous section their "non-symmorphic elements"; for them, the proof is based on the fact that their nth powers, for $n\geq v$, are translations. We study in detail the representation of the non-symmorphic space groups when $G=G_k$ is generated by L and the arithmetic elements listed in Eq. (101) (i.e. the list of those which can produce non-symmorphic elements). Let us begin by those of Eq. (102):

$$A=pm,P2,P3,P4,P6,\quad v=\text{order of } A,\quad \boldsymbol{v}(A)=\frac{\mu}{v}\boldsymbol{b},\ 0<\mu<v\ . \tag{122}$$

With the different possible values of μ we saw that we can form 13 non-symmorphic groups generated by $\{\boldsymbol{v}(A),A\}$ and the translations

$$pg,Pc,P2_1,P3_1\sim P3_2,P4_1\sim P4_3,P4_2,P6_1\sim P6_5,P6_2\sim P6_4,P6_3\ , \tag{123}$$

when A is a rotation, the index is μ and for reflections $\mu=1$. We can take the visible vector $\boldsymbol{b}$ as a basis vector. The points $\boldsymbol{k}\in BZ$ such that $G_k=G$ are those of the form $\boldsymbol{k}=\kappa\boldsymbol{b}^*$. In the corresponding representation, the translations are represented by $\boldsymbol{t}\mapsto\exp(i\boldsymbol{t}\cdot\boldsymbol{b}^*\kappa)$. So $\mathrm{Im}\,\boldsymbol{k}=\{\exp(in\kappa),\ n\in Z\}$ where n is the component of $\boldsymbol{t}$ on the basis vector $\boldsymbol{b}$; it is a finite or infinite cyclic group depending whether κ/π is rational or irrational.[60] From Eqs. (97) and (102) $\{\boldsymbol{v}(A),A\}^v$ is represented by $\exp(i\mu\kappa)$; so $\{\boldsymbol{v}(A),A\}$ is represented by a vth root of this expression. There are v such roots; they are obtained by multiplication of a fixed one by the v roots of 1, i.e. $\exp(i2\pi\rho/v)$, $0\leq\rho<v$. We summarize in the next equation what we established for the v unirreps of the G_k's of

[60] That mathematical fact might be abhorred by physicists. It is irrelevant when m (defined in the statement of Proposition 8a) is very large; but it is very important when m is small.

Eq. (103) labelled by ρ:

$$0 \le \rho < \nu \text{ labels unirreps } \boldsymbol{k} = \kappa \boldsymbol{b}^* ,$$

$$\{\boldsymbol{t}, I\} \mapsto \mathrm{e}^{\mathrm{i}\kappa \boldsymbol{b}^* \cdot \boldsymbol{t}}, \quad \{\boldsymbol{v}(A), A\} \mapsto \mathrm{e}^{\mathrm{i}(\mu\kappa + 2\pi\rho)/\nu} . \tag{124}$$

Because of the division by ν in the exponent the equation does not seem to satisfy the periodicity $\kappa \mapsto \kappa + 2\pi$ which corresponds to the definition of $\boldsymbol{k} \bmod 2\pi L^*$ of BZ; indeed

$$\kappa \mapsto \kappa + 2\pi, \quad \mathrm{e}^{\mathrm{i}(\mu\kappa + 2\pi\rho)/\nu} \mapsto \mathrm{e}^{\mathrm{i}(\mu(\kappa + 2\pi) + 2\pi\rho)/\nu} = \mathrm{e}^{\mathrm{i}(\mu\kappa + 2\pi(\rho + \mu))/\nu} . \tag{125}$$

So the set of ν unirreps respects the periodicity $\boldsymbol{k} \bmod 2\pi L^*$ but when one completes a circle on BZ along the direction $\boldsymbol{b}^*$ one obtains a permutation of the ν unirreps. If the greatest commun divisor $\lceil \mu, \nu \rfloor$ of μ, ν is 1, the permutation is circular and the ν unirreps form a unique orbit of the generated permutation group. More generally the number of orbits is $\nu/\lceil \mu, \nu \rfloor$. This phenomenon is called *monodromy* in mathematics:[61] for the unirreps of space groups, it was first observed in the first detailed study of them on two examples ($Fd\bar{3}m$ and $P6_3/mmc$)[62] by Herring (1937a, pp. 538, 543).

To complete this study of non-symmorphic elements, the extension to the last three arithmetic elements of Eq. (101) is straightforward. $\{\boldsymbol{v}(A), A\}$ is a non-symmorphic element which generates, with the translations, one of the three space groups $I4_1, Cc, Pc$; we have given the corresponding $\boldsymbol{v}(A)$ in Eqs. (104)–(105) as half of the visible vector ℓ which defines the rotation axis for $I4_1$ or the "glide vector" for Cc and Pc (for the latter case the glide vector can be any visible vector of the reflection plane). The vectors $\boldsymbol{k} = \kappa \ell^*$ are fixed by these non-symmorphic elements and the corresponding $P^z(\boldsymbol{k})$ has two unirreps which are exchanged by $\kappa \mapsto \kappa + 2\pi$.

This monodromy phenomenon is ignored in the tables of space group unirreps and by nearly all solid state physicists. To my knowledge it has never been applied to physical properties up to the very recent paper: (Michel and Zak, 1999). This physical application is explained in Chapter VI. Depending whether the order of $\hat{k}$ in BZ is infinite or of order m, the corresponding Herring groups are isomorphic to Z or to $Z_{m\nu}$.

Note that when P_k^z is Abelian but not cyclic, the Herring group $P^z(\boldsymbol{k})$ may be non-Abelian. Let us study the simple example: $P_k = D_2$ (or C_{2v}) with $\hat{k}$ of order 2. Then $\mathrm{Im}\,\hat{k} = Z_2$. So $P^z(\boldsymbol{k})$ is a eight-element Herring group H such that $Z_2 < C(H)$ and $H/Z_2 \sim Z_2^2$. It is easy to find the four groups which satisfy these conditions;[63] there are four of them and for the non-Abelian group we give the faithful two-dimensional unirreps in terms of Pauli matrices:

$$G: \quad Z_2^3, \quad Z_2 \times Z_4 ,$$

$$c_{4v} = \{ \pm I_2, \pm \sigma_3, \pm \sigma_1, \pm \mathrm{i}\sigma_2 \}, \quad q_2 = \{ \pm I_2, \pm \mathrm{i}\sigma_1, \pm \mathrm{i}\sigma_2, \pm \mathrm{i}\sigma_3 \} . \tag{126}$$

The first group is the direct product; the second is Abelian. The last group, q_2, is called the quaternionic group. The center of the two non-Abelian groups has two elements; they are denoted

[61] It corresponds to an action on the set of unirreps, by the homotopy group π_1 of the BZ torus.

[62] These two groups are also often mentioned, respectively, as "diamond structure" and "hexagonal close packing". They are third and fourth rank in the space group frequency of inorganic crystals, each group representing more than 5% of them (see (Mighell et al., 1977)).

[63] The list and structure of non-Abelian groups of the order $|G| \le 24$ are given in the very good book by Coxeter and Moser (1972).

by ± 1. Remark that in these two groups (c_{4v}, q_2), if the product of two elements is not in the center, these two elements anticommute. Remark also that the square of any element is in the center; the number of elements of square -1 is two for c_{4v} and six for q_2. For these two non-Abelian groups, their allowed representations must represent faithfully the center; so each non-Abelian Herring group has a unique allowed representation which is the one given in Eq. (126). For the first Abelian group, $Z_2(\mathrm{Im}\,\boldsymbol{k})$ has to be represented faithfully, so there are four allowed representations obtained by making the tensor product of this representation with those of $P_k \sim Z_2^2$; their images are z_2. For $Z_4 \times Z_2$, the allowedness condition requires Z_4 to be represented faithfully (two such unirreps) and the tensor product with the two unirreps of Z_2 yields four allowed representations of image z_4.

The point $\hat{k} = 0$ and the seven other points which satisfy $2\hat{k} = 0$ are the fixed points on BZ for the 40 space groups of the Bravais classes *triclinic*, *P-monoclinic*, *P-orthorhombic*, (see Table 3 and ITC). It is easy to determine the eight corresponding $P^z(\boldsymbol{k})$ for these space groups.

The group $P2_12_12_1$ illustrates the four examples of Eq. (126). Let us study this space group,[64] its eight $G_k = G$ and their unirreps. The three generators of the translation lattice L along the rotation axes of the point group $P = D_2$ satisfy $\boldsymbol{b}_i \cdot \boldsymbol{b}_j = \lambda_i^2 \delta_{ij}$. In this basis the three matrices representing the non-trivial elements of P are diagonal matrices that we define by their action on the basis

$$R_i \boldsymbol{b}_i = \boldsymbol{b}_i, \quad i \neq j, \quad R_i \boldsymbol{b}_j = -\boldsymbol{b}_j \ . \tag{127}$$

Let i, j, k be a circular permutation of $1, 2, 3$. The three generators of $P2_12_12_1$ are

$$r_i = \{\tfrac{1}{2}(\boldsymbol{b}_i + \boldsymbol{b}_j), R_i\} \ ,$$

then

$$r_i^2 = \{\boldsymbol{b}_i, I\}, \quad r_i r_j = \{\boldsymbol{v}_{ij}, I\} r_j r_i, \quad \boldsymbol{v}_{ij} = \boldsymbol{b}_i - \boldsymbol{b}_j - \boldsymbol{b}_k \ . \tag{128}$$

In BZ, the eight elements $2\hat{k} = 0$ have coordinates 0 or π in the dual basis (see Table 3). The three elements $\hat{k}_F^{(m)}$ (π at the coordinate m and 0 for the two other coordinates) are represented by the center of the six faces of the BZ-cell (a rectangle parallelepiped); the three elements $\hat{k}_E^{(m')}$ (0 at m' and π for the two other coordinates) are represented by the middle of the 12 edges and the element $\hat{k}_V$, with its three coordinates $= \pi$, is represented by the eight vertices. From

$$\mathrm{e}^{\mathrm{i}\boldsymbol{k}_X^{(m)} \cdot \boldsymbol{v}_{ij}} = \begin{cases} 1 & \text{for } X = E \ , \\ -1 & \text{for } X = F, V \ , \end{cases} \tag{129}$$

we know that the Herring groups $P(\hat{k}_E^{(m')})$ are Abelian and the others are not. To know the nature of the non-Abelian ones we have to compute their number of elements whose square are -1. From the second equality in Eq. (128) we count

$$\text{number of } \mathrm{e}^{\mathrm{i}\boldsymbol{k}_X \cdot \boldsymbol{b}_i} = -1 \text{ is } 1, 2, 3 \quad \text{for } X = F, E, V \ . \tag{130}$$

[64] The most abundant space groups for the crystals of organic compounds are, according to (Mighell et al., 1977), $P2_1/c$ (about 30%), $P2_12_12_1$ (more than 12%), $P2_1$ (less than 8%). So these three space groups represent half of the organic crystals. Their energy band structure will be studied in Chapter VI.

So we can deduce the nature of the eight Herring groups of

$$P2_12_12_1\colon P(\hat{k}_0)\sim Z_2^2,\quad P(\hat{k}_E^{(m')})\sim Z_4\times Z_2\ ,$$
$$P(\hat{k}_F^{(m)})\sim c_{4v},\quad P(\hat{k}_V)\sim q_2\ . \tag{131}$$

8.2. The irreducible corepresentations of $\check{G}_k$

As we saw in Section 4.5, time reversal $\mathscr{T}$ acts on the Brillouin zone according to $\mathscr{T}\cdot\hat{k}=-\hat{k}\bmod 2\pi L^*$. So the points $2\hat{k}=0$ are $\mathscr{T}$ invariant. Adding $\mathscr{T}$ to G we obtain the[65] *cogroup* $\check{G}$ and we can define the stabilizer $\check{G}_k$. Wigner (1932) showed that in quantum mechanics, the action of $\mathscr{T}$ on the Hilbert space of vector states must be represented by an antiunitary operator $V(\mathscr{T})$ which, in absence of spin, satisfies $V(\mathscr{T})^2=I$ (the identity operator).[66] The elements of $\check{G}$, $\check{G}_k$ which contain time reversal must be represented by antiunitary operators. The simplest antiunitary operator acts as complex conjugation on the complex field of the Hilbert space; this semilinear[67] operation is denoted by $\mathscr{K}$ and $\mathscr{K}^2=I$. So we can write an antiunitary operator as the product $V=U\mathscr{K}$ where $U=V\mathscr{K}$ is a unitary operator. It is easy to compute

$$UU^*=U^*U=I,\quad V=U\mathscr{K}\ \Rightarrow\ V^{-1}=\mathscr{K}U^*=(\mathscr{K}U^*\mathscr{K})\mathscr{K}\ . \tag{132}$$

In the absence of spin effects, since time reversal $\mathscr{T}$ changes the sign of momenta, it is represented on the reciprocal space and on the functions on this space, by the operators:

$$V(\mathscr{T})=(-I)\mathscr{K},\quad \mathscr{T}\cdot f(\boldsymbol{k})=\hat{f}(-\boldsymbol{k})\ , \tag{133}$$

where $\hat{}$ denotes the complex conjugation. To study the (non-linear) group action on BZ we replace $\boldsymbol{k}$ by $\hat{k}$ which represents the class of equivalence: $\boldsymbol{k}\bmod 2\pi L^*$. Hence we have two cases to consider:

$2\hat{k}=0$: Then G_k is a subgroup of index 2 of $\check{G}_k$. Given an irreducible representation $\rho(G_k)$, to build the corepresentation of $\check{G}_k$ we have again to distinguish two cases:

$\rho(G_k)$ is (equivalent to) a real representation; then $V(\mathscr{T})$ commutes with it and the corepresentation has the same dimension;

$\rho(G_k)$ is not equivalent to a real representation. Then the direct sum $\rho\oplus\bar{\rho}$ of ρ and its complex conjugate is equivalent to a *real irreducible* representation of G_k; we are back to the previous case, but notice that the dimension of the irreducible corepresentation is $2\dim\rho(G_k)$.

$2\hat{k}\neq 0$: G_k and $\mathscr{T}$ generate a cogroup which contains both G_k and G_{-k} and the cosubgroup $\check{G}_k$ is not necessarily trivial. This has already been studied by Herring in his thesis, summarized in (Herring, 1937a, b). The simplest case occurs for the space groups $P2$ or $P2_1$. We assume that the rotation by π is around the axis defined by the basis vector $\boldsymbol{b}_3$; note that the two other vectors in a basis generating L have to be orthogonal to $\boldsymbol{b}_3$. In the reciprocal space the tip of the vectors $\boldsymbol{k}$ of

[65] That is the name usually given in the physics literature; of course it is a group.

[66] A state of half-integer angular momentum is an eigenstate of $V(\mathscr{T})^2$ with eigenvalue -1. In the first English edition (Wigner, 1959) of his book on group theory and quantum mechanics, Wigner added a chapter on time reversal. From this time, this topic is dealt with in many text books; so we introduce in this section the minimal content which explains the use of time reversal in Chapter VI.

[67] In mathematics, the product of the two operations on a vector space: that of a linear operator and that of an automorphism of the vector space field, is called *semilinear*.

coordinates $\boldsymbol{k} = (\kappa_1, \kappa_2, \pi)$ are in the face of the Brillouin cell orthogonal to the dual basis vector $\boldsymbol{b}_3^*$ (since the space groups belong to the P-monoclinic Bravais class and from Fig. 6 and Table 6 we know that it is the horizontal face of the hexagonal prism Brillouin cell). The rotation R (by π around the third axis) of $P2$, the skew rotation $r = \{\frac{1}{2}\boldsymbol{b}_3, R\}$ and $\mathscr{T}$ have the same effect on these vectors $\boldsymbol{k}$; they change the sign of κ_i, $i = 1, 2$. So the products $R\mathscr{T}$ for $P2$ and $r\mathscr{T}$ for $P2_1$ belong to the respective $\check{G}_k$'s. In the one-dimensional unirreps of the Abelian groups G_k, the elements R, r are represented, respectively, by ± 1, $\pm i$ (apply Eq. (124) with $\nu = 2$, $\mu = 1$ and $\kappa = \pi$). The result is that these co-unirreps are of dimension 1 for $P2$ and 2 for $P2_1$. Herring (1937a) extended it to the space groups containing $P2_1$: the dimension is doubled when one passes from the representation to the co-representation with $\mathscr{T}$ for $\hat{k} \in BZ$ represented by the points of the face of the Brillouin cell orthogonal to the skew rotation axis.

We have considered some allowed unirreps of Herring groups. One can establish a systematic method for constructing the Herring groups and their allowed unirreps. By a decomposition of the Herring groups similar to what Table 1 from Chapter I is doing for the 32 (geometric) point groups, Michel and Mozrzymas (unpublished) have written the finite Herring groups in the form $P(\boldsymbol{k}) = A(\boldsymbol{k}) \times P'(\boldsymbol{k})$ where $A(\boldsymbol{k})$ is a finite Abelian group and $P'(\boldsymbol{k})$ is a member of a much smaller list of Herring groups that have been called the skeleton Herring groups.

Since the G_k are themselves space groups, the next section can be applied for finding their unirreps.

8.3. The irreducible representations of a space group G

We will be very short on this subject since many books deal with it. Several formulas written here are more concise and elegant and few are not in the physics textbooks. The method to build the unirreps of the space group G is by induction from those of subgroups with the same translations. Before doing it, we want to recall some properties of the induction method along lines not found in physics textbooks.[68]

To simplify we first consider the case of a finite group G and its sugroup H. The complex valued functions on the group which satisfy

$$\phi(g_1 g_2) = \phi(g_2 g_1) \Leftrightarrow \phi(g_1 g_2 g_1^{-1}) = \phi(g_2)\,, \tag{134}$$

form a finite-dimensional Hibert space $\mathscr{H}_G$ with the Hermitian scalar product

$$\langle \varphi, \phi \rangle_G = |G|^{-1} \sum_{g \in G} \varphi(g)\phi(g)\,. \tag{135}$$

Labelling the unirreps of G by α, their characters χ_G^α form an orthonormal basis of $\mathscr{H}_G$. Restricting the functions $\phi \in \mathscr{H}_G$ to the subgroup $H < G$ defines the linear operator

$$\mathscr{H}_G \overset{\mathrm{Res}_H^G}{\rightarrow} \mathscr{H}_H\,. \tag{136}$$

[68] We advise the remarkable small book by Serre (1977).

By definition, its adjoint operator is the induction operator

$$\mathscr{H}_H \overset{\mathrm{Ind}_H^G}{\to} \mathscr{H}_G; \quad \mathrm{Ind}_H^G = (\mathrm{Res}_H^G)^\dagger \ . \tag{137}$$

From this definition we have immediately the Frobenius reciprocity

$$\langle \mathrm{Ind}_H^G \chi_H^\rho, \chi_G^\alpha \rangle_G = \langle \chi_H^\rho, \mathrm{Res}_H^G \chi_G^\alpha \rangle_H \ . \tag{138}$$

From the associativity of the linear maps we obtain the theorem of induction by step

$$\begin{aligned} &H < H_1 < H_2 < \cdots < H_{m-1} < H_m < G \\ &\Rightarrow \mathrm{Ind}_H^G = \mathrm{Ind}_{H_m}^G \mathrm{Ind}_{H_{m-1}}^{H_m} \ldots \mathrm{Ind}_{H_1}^{H_2} \mathrm{Ind}_H^{H_1} \end{aligned} \tag{139}$$

and from the other fundamental properties of linear maps

$$\mathrm{Ind}_H^G(\chi_H^\rho \oplus \chi_H^\sigma) = \mathrm{Ind}_H^G \chi_H^\rho \oplus \mathrm{Ind}_H^G \chi_H^\sigma \ . \tag{140}$$

To construct an induced representation from H to G one chooses representatives of the left cosets $G{:}H$

$$G = \bigcup_j s_j H \ . \tag{141}$$

Then, given a representation $h \mapsto D(h)$ of H, one obtains the induced representation of G as block matrices

$$\Delta = \mathrm{Ind}_H^G D, \quad \Delta_{j\ell}(g) = \begin{cases} D(s_j^{-1} g s_\ell) & \text{if } s_j^{-1} g s_\ell \in H \ , \\ 0, & \text{otherwise} \ . \end{cases} \tag{142}$$

Obviously that formula can be extended to finite-dimensional representations of a subgroup H of finite index in G. That is the case of the space group G and a subgroup H containing the subgroup L of translations. Let us first induce from a one-dimensional unirrep $\hat{k}$ of the translation group L. We choose as representatives of the L-cosets, the elements $\{\boldsymbol{v}(A_i), A_i\}$ defined in Eq. (113), where the A_i are the elements of the point group P. Then Eq. (142) yields

$$\Delta = \mathrm{Ind}_L^G \hat{k}: \quad \Delta_{j\ell}(\{\boldsymbol{t}, I\}) = \delta_{j\ell} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_j \cdot \boldsymbol{t}}, \quad \boldsymbol{k}_j = (A_j^\top)^{-1} \boldsymbol{k} \ , \tag{143}$$

$$\Delta_{j\ell}(\{\boldsymbol{v}(A), A\}) = \begin{cases} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_j \cdot \boldsymbol{z}(A, A_\ell)} & \text{if } A_j = A A_\ell \ , \\ 0 & \text{otherwise} \end{cases} \tag{144}$$

with the vector $\boldsymbol{z}(A, A_\ell)$ defined in Eq. (115). Remark that the matrix elements of these representations are analytic functions on BZ.

These representations of G have dimension $|P|$. When $\hat{k}$ is in the open dense stratum of BZ (i.e. $G_k = L$) these representations are irreducible. We notice, since $P_k^z = 1$, that all $\boldsymbol{k}_j$ are different so any matrix C which commutes with all the diagonal matrices of Eq. (143) must be diagonal. Let us first consider the symmorphic group of the arithmetic class P^z; then all $\boldsymbol{z}(A, A_\ell)$ vanish and the matrices of Eq. (144) are permutation matrices (independent of $\boldsymbol{k}$). Their commutations with the diagonal C permutes the elements of C; so C is an intertwinning matrix, invariant by these permutations, only if it is a multiple of I. The proof can be extended to the non-symmorphic groups.

When P_k^z is not trivial, the (unitary) induced representations $\mathrm{Ind}_L^G \hat{k}$ are reducible. It has been proven (Mackey, 1970) that the decomposition into unirreps of all these representations yields the complete set of unirreps of G. For symmorphic groups we have already noticed that the matrices of Eq. (144) are independent of $\boldsymbol{k}$ and they form the regular representation of P^z. The decomposition of the induced representation into irreducible components is easy to do. For non-symmorphic groups the reduction into unirreps may not preserve the analyticity of the matrix elements on BZ. Indeed $\boldsymbol{k}$ may be replaced by $\boldsymbol{k}/m$, $m = 2,3,4,6$ in the exponential, so the analyticity is preserved only on a covering of BZ. That introduces the monodromy of representations that we have introduced earlier (e.g. Eqs. (124)–(125)).

Let us consider now the representations of G_k of the form $\mathrm{Ind}_{L^k}^{G_k}\boldsymbol{k}$; their dimension is $|P_k|$. From Eq. (143) we see that the matrices representing the translations are $\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot t)}I$, i.e. multiple of the identity. For the symmorphic G_k, in the decomposition of this induced representation into irreducible representations, the multiplicity of the obtained unirreps is equal to their dimension. This extends to the non-symmorphic G_k.

Eq. (139) shows that the induction can be made by step. Mackey (1970) also proved that by inducing from G_k to G a unirrep of G_k, one obtains a unirrep of G and all unirreps of G are obtained by induction from all unirreps of all G_k's for all orbits $\in BZ|P^z$. So all unirreps of G are finite-dimensional; their dimension is a divisor of $|P|$. For non-symmorphic groups, the monodromy groups merge some unirreps into an orbit; the convention to distinguish them by labels is artificial and not useful.

We finish this chapter by a small digression about the $\boldsymbol{z}(A,B)$ introduced in Eq. (115). The associativity of the group law applied to Eq. (114) imposes the condition

$$\boldsymbol{z}(A,B) - \boldsymbol{z}(A,BC) + \boldsymbol{z}(AB,C) - A\boldsymbol{z}(B,C) = 0\ . \tag{145}$$

We already noted, at the beginning of this section that a change of origin of coordinates modifies the $\boldsymbol{v}(A)$'s but leaves the $\boldsymbol{z}(A,B)$'s invariant; it is interesting that Eq. (144) depends only on the $\boldsymbol{z}(A,B)$'s. However there is still some freedom to choose the $\boldsymbol{v}(A)$'s by adding to it an arbitrary translation $\boldsymbol{c}(A)\in L$ of the lattice. We denote with a' the new vector functions

$$\begin{aligned} &\boldsymbol{v}'(A) - \boldsymbol{v}(A) = \boldsymbol{c}(A)\in L \\ &\qquad\Rightarrow \boldsymbol{z}'(A,B) - \boldsymbol{z}(A,B) = \boldsymbol{c}(A) - \boldsymbol{c}(AB) + A\boldsymbol{c}(B)\ . \end{aligned} \tag{146}$$

The right-hand expressions of Eq. (115) and of the last equality of Eq. (146) look alike but their meanings are very different: in Eq. (115) the $\boldsymbol{v}(A)$'s are vectors of the Euclidean space while in Eq. (146) the $\boldsymbol{c}(A)$'s are lattice vectors. It is convenient and natural to take the $\boldsymbol{v}(A)$ inside the fundamental domain defined by the basis vectors generating L; then the $\boldsymbol{z}(A,B)$ are uniquely defined.

Eqs. (115)–(117) and (145)–(146) are basic expressions of the theory of cohomology. This algebraic aspect of crystallography is treated in Ascher and Janner (1965) and Ascher and Janner (1968). The first set of lectures on cohomology of groups given in a Physics summer school, is of Michel (1964).

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