

PHYSICAL IMPLICATIONS OF CRYSTAL SYMMETRY AND TIME REVERSAL

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§0 Introduction.

To make Physics, one has to practice the art of making "good" approximations. Many physical systems have a symmetry defined with a very good approximation. That is the case of crystals. The physical predictions obtained from their symmetry can be applied to any specific problem of crystal physics whether of classical or quantic nature. Strangely enough many of these general predictions are still unknown or ... forgotten; most of those given here have been discovered recently; some are still unpublished.

Crystals are complicated systems for physicists and the models used for their study are rather coarse approximations. However if a model has the full symmetry of the crystal, the predictions of this model will satisfy all predictions of symmetry; so some physicists think that they have nothing to learn from symmetry that they cannot discover by their model. The answer to this objection is simple. First, by its generality and precision, the study of the consequences of symmetry belongs to the general culture of physicists; in fact it is a handicap to ignore it. More particularly we shall show that some predictions, although very specific and detailed, are model independent. They must be known in order to evaluate the nature of the model predictions: which ones are only a verification of a simple and general theorem of mathematics? Only the other ones can be specific to the model.

The title describes the aim of these lectures. They are made for all participants of the school (including those working in solid state physics!). The subject is too vast to be treated in two lectures. So we will precise explicitly how we restrict it; but we shall treat in full generality the selected types of problems:

- a) we shall deal only with periodic crystals ¹.
- b) we shall consider only stationary phenomena, so T (the time reversal symmetry) is valid and, to simplify ², we only study the phenomena for which spin effects can be neglected (that exclude for instance, all magnetic phenomena and the use of magnetic space groups).

For periodic crystals, all functions describing their physical properties have the periods of the crystal. However, most experiments measure the Fourier transforms of these functions, i.e. functions on the Brillouin zone. We will deal essentially with such functions for all 230 space groups; our results will also apply to the functions on our Euclidean space for the 73 symmorphic space groups. The summary of the paper is:

§1 recalls the fundamental concepts and tools for studying symmetry in general and particularly that of periodic crystals.

§2 studies the case of genuine functions. The results, without proofs (which have been

¹ Those called erroneously "quasi-crystals" are genuine crystals. Indeed they have a long range order; moreover their diffraction patterns are essentially made of bright peaks. These new crystals, discovered since 1984, can be considered as a particular case of modulated crystals (discovered in the seventies). They are quasi-periodic, i.e. their physical properties can be described by functions with a number of periods greater than the dimension of space. Hence crystallography in higher dimension can be one of the useful tools for their study. So in these lectures, all properties which are independent from dimension, are stated for dimension n .

² Subjects for theses should be left for the young generation!

recently published: [MIC96]), and their physical applications will be given here.

§3 will deal with multivalued functions. That corresponds to the important cases of vibrational spectra, energy band structures. . . I will present some history on it, recall or define the concepts playing the role of quantum numbers, and give a glimpse of the work presently in progress with J. Zak.

The two lectures were presented as seminar: one needs only to communicate the new ideas and the existence of precise results (very thorough for §2). The written version for a school must be a document worth to be studied carefully. However it is not written for specialists, but for a general audience similar to that of the school participants. It has two aims: 1) transmit the known general culture (essentially §1 and beginning of §2); indeed a solid state physicist needs to know what is relevant for him in mathematics, in crystallography, in mechanics....., in order to have a deep understanding of his subject. 2) to present the recent result in tables or figures that can be used effectively.

The author is conscious that, for lack of space, this text is very condensed; so readers should not be disappointed if they cannot grasp it at a first reading. The content is not perishable, so the reader who has learned more from the references or from books, may come back fruitfully to it.

§1 Fundamental tools for the study of symmetries. Periodic crystals.

We first recall few fundamental concepts of group actions and precise the notations used. It is a summary of the first section of [MIC95a] given at the last session of the school; we refer to it for more details and examples (and also to [MIC80]).

We write $H \leq G$ for H is subgroup of G ; the set of its conjugate subgroups, $[H]_G = \{gHg^{-1}, g \in G\}$, is called the conjugacy class of H . When it contains only H , that subgroup is called *invariant subgroup* of G and the traditional short hand is $H \triangleleft G$. The sets of G -elements gH (or Hg) are called a left (right) coset of H in G . We denote the set of cosets by $G : H$ ($H : G$). Notice that $\forall g \in G, gH = Hg \Leftrightarrow H \triangleleft G$: in that case, there is a natural group law on $G : H$; this group is called the quotient group and it is denoted by G/H . When a group G acts on a set M , we denote

by $G.m = \{g.m, \forall g \in G\}$ the orbit of m , i.e. the set of all transformed of m ,

by $G_m = \{g \in G, g.m = m\}$ the stabiliser of m . It is a subgroup of G (often called "little group" in the physics literature ³).

The stabilisers of an orbit form the conjugacy class $[G_m]_G$. Two orbits with same conjugacy class of subgroups belong, by definition, to the same *orbit type*. An example of orbit of type $[H]_G$ is the set of left cosets $G : H$ with the action of G on the cosets by left multiplication: $g.xH = gxH \equiv (gx)H$.

A *stratum* is the union of orbits of the same type. Equivalently, *two elements of M belong to the same stratum if, and only if, their stabilisers are conjugate in G .*

In the action of G on M , we denote the set of orbits by $M|G$ (those we shall meet are generally *orbifolds*, i.e. manifolds with some singularities) and the set of strata by $M||G$ (those we shall meet are all finite). Remark that the set of left (right) cosets $G : H$ can also be identified with the orbit space $G|H$ with the action of H on G by right (left) multiplication.

³ We prefer "stabiliser", used in the mathematics literature, because the word carries more meaning.

Example: G acts on its subgroups by conjugation (=inner automorphisms of G). In this action, the orbit of H is its conjugacy class $[H]_G$, the stabiliser G_H of H is called the *normalizer* of H in G and it is denoted by $N(G_H)$. We denote the set of subgroups of G by $\{\leq G\}$ and the set of conjugacy classes of subgroups of G by $\{[\leq G]_G\}$. It is the orbit space of this action ⁴

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

In a group action, the set of possible types of G -orbits can be identified to a subset of $\{[\leq G]_G\}$ (the set of conjugacy classes of the subgroup of G). That can be translated into a natural injection of the stratum space to $\{[\leq G]_G\}$:

$$M||G \xrightarrow{\phi} \{[\leq G]_G\}, \quad \phi \text{ injective.} \quad 1(2)$$

On the set $\{[\leq G]_G\}$ of conjugacy classes of G subgroups, there is a natural partial ordering, by subgroup inclusion up to a conjugation. Given this partial ordering, the injection ϕ defines a partial ordering on the the stratum space $M||G$. In physics, the role of this space is essential; indeed, its elements (the strata) correspond to the different symmetry types of the elements of M . In many theories of physics, physicists give names to the strata. For instance, in special relativity, in the action of the Lorentz group on the Minkowski space, the elements of the four strata are called: time-like, space-like, light-like and null vectors. The strata for the action of each of the 230 spaces groups (= crystallographic groups) on the 3 dimensional Euclidean space are called *Wyckoff positions* and are listed in the International Tables for Crystallography (=ITC).

Here is an abstract of §2 of [MIC95a]. It precises which concepts defined in the [ITC] are used here. In a vector space V_n , a lattice L is the Abelian group generated by the vectors $\{\vec{b}_i\}$ of a basis of space; note that the only condition that the basis vectors must satisfy is $\det(\vec{b}_i) \neq 0$. Every other basis of V_n can be obtained from $\{\vec{b}_i\}$ by a unique transformation $\vec{b}_i \cdot g^{-1}$, $g \in GL_n(R)$. So we can identify the set B_n of bases of V_n with an orbit of type $GL_n(R) : 1$. The different bases of the lattice L are obtained by: $\vec{b}'_i = \sum_j m_{ij} \vec{b}_j$ with $m_{ij} \in GL_n(Z)$. So, with the action of $GL_n(Z)$ on $GL_n(R)$ by left multiplication, we can identify the set \mathcal{L}_n of n -dimensional lattices with

$$\mathcal{L}_n = GL_n(R) | GL_n(Z) = GL_n(R) : GL_n(Z) \quad 1(3)$$

We are interested by the spaces V_n carrying an orthogonal scalar product that we denote by $\vec{a} \cdot \vec{b}$; it has the specific properties $\vec{a} \cdot \vec{a} \geq 0$, and $\vec{a} \cdot \vec{a} = 0 \Rightarrow \vec{a} = 0$. The action of the orthogonal group O_n on the bases of V_n ($\vec{b}_i \mapsto \vec{b}_i \cdot r^{-1}$ with $r^{-1} = r^T \in O_n$) defines its action on the lattices. The stabilisers are called *holohedries*. The strata are called in [ITC], the *Bravais crystallographic systems*. In dimension 3 there are 7 of them.

⁴ The equation 1(1) was labelled 1(3) in the set of lectures [MIC95a] given here two years ago, but a wrong equality was added: $= \{\leq G\}||G$. I wanted to give this erratum with my apologies. Obviously the stratum space is the set of conjugacy classes of the normalizers of the subgroups. For instance we ask the reader to check that for the group $B_2 \sim C_{4v}$, symmetry group of a square, the number of elements of the sets $= \{\leq G\}$, $\{\leq G\}|G$, $\{\leq G\}||G$ are respectively 10,8,3.

We need a more refined classification of lattice symmetries which was also introduced by Bravais [BRA850] somewhat empirically. Indeed the orbit $O_n.L$ corresponds to the different orientations of the same “intrinsic” lattice $L^{(i)}$. So the set $\mathcal{L}_n^{(i)}$ of n -dimensional intrinsic lattices can be identified with

$$\mathcal{L}_n^{(i)} = \mathcal{L}_n | O_n = GL_n(Z) : GL_n(R) : O_n, \quad 1(4)$$

where the last expression means double cosets. By the polar decomposition of matrices, $GL_n(R) : O_n$ can be identified to $\overline{\mathcal{C}_+}(Q_n)$, the (open) convex cone of positive matrices; that yields

$$\mathcal{L}_n^{(i)} = \overline{\mathcal{C}_+}(Q_n) | GL_n(Z). \quad 1(5)$$

One can obtain the same result by considering the Gram matrix $\vec{b}_i \cdot \vec{b}_j = q_{ij}(L)$, where $q(L) = q(L)^\top > 0$ is the basis dependent quadratic form associated to $L^{(i)}$. By the $GL_n(Z)$ action $q(L) \mapsto mq(L)m^\top$, $L^{(i)}$ corresponds to an orbit of the action of $GL_n(Z)$ on $\overline{\mathcal{C}_+}(Q_n)$, hence equation 1(5) ⁵. The strata of this action are the *Bravais classes*; we call the stabilisers *Bravais groups*. In dimension 3 there are 14 Bravais classes.

We denote by $\{BCS\}_n$ and $\{BC\}_n$ (n is the space dimension) respectively the sets of Bravais crystallographic systems and of Bravais classes. One remark is needed to explain the relation of these results with crystallography. We recall that an Euclidean space \mathcal{E}_n is a linear manifold, the orbit of R^n (the Abelian group of V_n) acting on the manifold \mathcal{V}_n formed by the vectors of V_n . This orbit is of type ⁶ $R^n : 1$, so it has the topology R^n . The orthogonal scalar product on V_n induces the Euclidean metric on \mathcal{E}_n . The Euclidean group (= the group of automorphisms of \mathcal{E}_n) is the semi-direct product $E_n = R^n \rtimes O_n$. An Euclidean lattice is an orbit of the subgroup $L < R^n$ on \mathcal{V}_n . Given an Euclidean lattice in \mathcal{E}_n , one reconstructs the results we have obtained by choosing a point of this Euclidean lattice as origin of the linear coordinates in \mathcal{E}_n .

Crystallographers call *arithmetic classes* ⁷ the set of conjugacy classes of finite subgroups of $GL_n(Z)$ and denote it by $\{AC\}_n$. The conjugacy classes in O_n of the same finite groups are usually called *geometric classes* and we denote here their set by $\{GC\}_n$. One proves (e.g. [MIC95a] §2-3) the existence of map:

$$\{AC\}_n \xrightarrow{\varphi} \{GC\}_n, \quad \varphi \text{ surjective, order preserving.} \quad 1(6)$$

Notice that φ maps the subset $\{BC\} \subset \{AC\}$ onto the subset $\{BCS\} \subset \{GC\}$. For dimension $n = 3$, $|\{AC\}_3| = 73$, $|\{GC\}_3| = 32$.

In solid state books the geometric classes are traditionnaly denoted by the Schönflies' notation and are well studied. Indeed they classify most of the macroscopic physical

⁵ The study of these orbits were made by number theory mathematicians of the XIX century under the name of *arithmetic theory of quadratic forms* without referring to lattices.

⁶ In the mathematic literature, orbits of type $G : 1$ are called principal orbits.

⁷ This name was used in crystallography before 1920. It is defined in the last edition of [ICT] p. 719.

properties of the crystals ⁸. Most of the other physical properties of a crystal do depend of its space group. For these 230 groups two notations are used in [ITC]. The Schönflies one distinguishes the groups corresponding to the same geometric class by an upper right index with sequential values; the “international” one (essentially due to Hermann and Maughin) is remarkable: with few letters and digits it contains so much information that one can reconstruct from it the space group law.

For the convenience of the reader we give in table 1 the names of the 7 elements of $\{BCS\}_3$ and the geometric class of their holohedry in both notations:

Bravais CS	triclinic	monoclinic	orthorhombic	tetragonal	rhombohedral	hexagonal	cubic
Schönflies	C_i	C_{2h}	D_{2h}	D_{4h}	D_{3d}	D_{6h}	O_h
ITC	$\bar{1}$	$2/m$	mmm	$4/mmm$	$\bar{3}m$	$6/mmm$	$m\bar{3}m$

Table 1: The seven Bravais crystallographic systems and the geometrical class of their holohedry:

The most important classification we shall need in these lectures is that given by the arithmetic classes; for them, the only available notation is the international one. For instance there are three arithmetic classes $P\bar{3}m1$, $P\bar{3}1m$, $R\bar{3}m$ which correspond by φ of 1(6) to the geometric class $D_{3d} = \bar{3}m$. Only the third one, $R\bar{3}m$, corresponds to a Bravais group and its holohedry is isomorphic to the geometric class group, i.e. the crystal belongs to the rhombohedral Bravais crystallographic system, while the crystals of the two first arithmetic classes belong to the hexagonal Bravais crystallographic system ⁹, so their holohedry $D_{6h} = 6/mmm$ is larger than the group of their geometrical classes. The list of the 73 arithmetic classes is given in table 2a.

For the convenience of the reader we reproduce here in Figure 1, a figure of [MIC95a] which gives explicitly the restriction of φ on $\{BC\}_3$.

One can define the space groups as *the discrete, topologically closed subgroups of E_n (the n -dimensional Euclidean group) which contain a lattice $L \in \mathcal{L}_n$ of translations*. One

⁸ Remark that the shape and aspect of the crystals depend essentially on the Bravais class, with some possibility to distinguish the arithmetic classes: e.g. garnet (cubic F = face centered) has easily the 14 face shape (6 squares, 8 hexagons) while iron sulfur crystals (Cubic P) can be perfect cubes. The orientations of the parallel strias on the cube faces reduce the cubic symmetry to a tetrahedral one. The shape of crystal was the first object of crystallography. The shape itself depends a lot on random-like effects influencing the growth but the values of the angles between the faces are much more regular. As A. Janner has shown, slightly curved faces prove a periodic modulation of the crystal.

⁹ Although the [ITC] notations correspond to the Bravais classification [BRA850], some vocabulary they use, e.g. “trigonal” geometric classes, is a remnant of an older classification [WEI816]. Each of these five trigonal geometric classes contains crystals with very different lattices, since they belong to two distinct Bravais crystallographic systems, each one containing a unique Bravais class, respectively the rhombohedral one and the hexagonal one. The five other crystallographic systems, are identical in the Weiss and Bravais classifications.

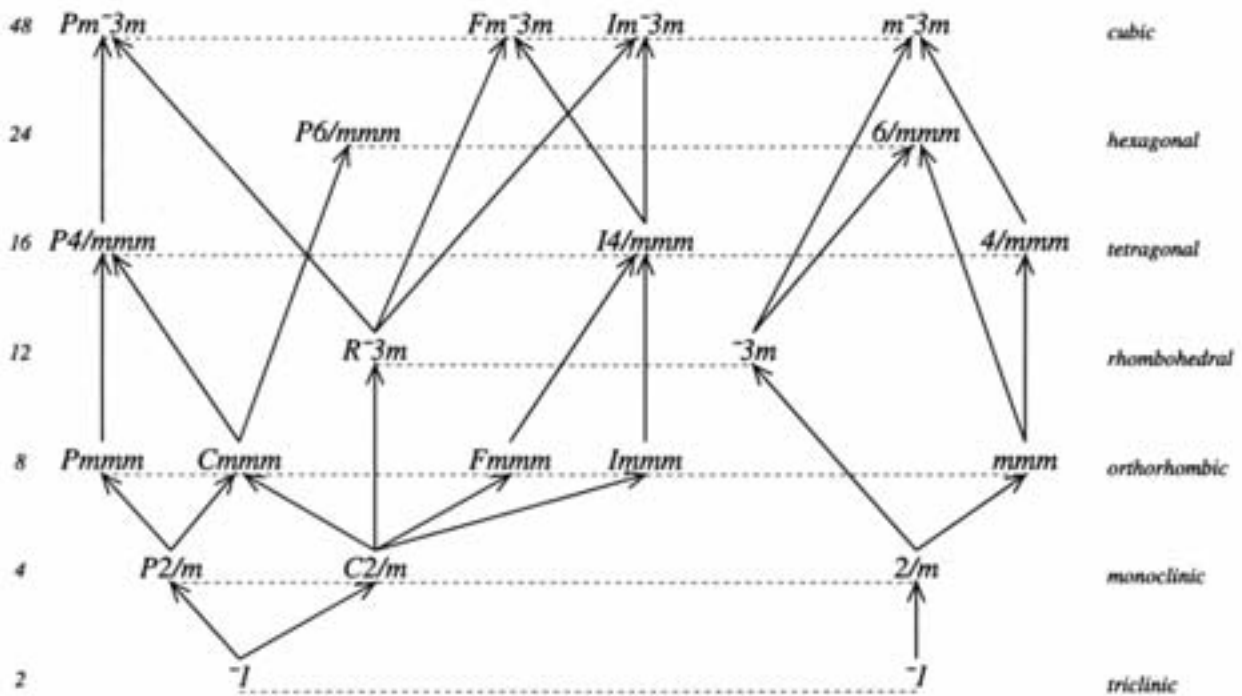


Figure 1. For three dimensional crystallography, the left diagram shows the partial order on $\{BC\}_3$, the set of the 14 Bravais classes and the right one shows the partial order on $\{CS\}_3$, the set of the 7 Bravais crystallographic systems. The dotted horizontal lines explicit the order preserving map φ' , restriction to $\{BC\}$ of the map φ defined in equation 1(6).

shows that L is invariant subgroup of the space group G and the quotient P is called the point group (we use the symbol \sim for group isomorphisms):

$$Z^n \sim L \triangleleft G; \quad G \xrightarrow{\theta} G/L = P \text{ finite}, \quad P < GL_n(Z). \quad 1(7)$$

We recall the construction of space groups (see e.g. [MIC89] for more details¹⁰). For each arithmetic class $[P]_{GL_3(Z)}$ one constructs the semi-direct product $G = L \rtimes P$. These groups are called symmorphic by the crystallographers. Cleverly, [ITC] use the same notation for an arithmetic class and its symmorphic group. It is a classical problem (second cohomology group; see e.g. [ASH65-68], [MOZ74] or the Polish book [MOZ76]) to construct all the other space groups belonging to the same arithmetic class. For the different positions of a crystal in the Euclidean space, the corresponding space groups form a conjugacy class $[G]_{E_3}$ of the Euclidean group. There is a domain of variations of external conditions such as temperature, pressure for which the “symmetry” of a crystal does not change through phase transition; but its space group, while staying a subgroup of E_3 , changes continuously by conjugation in Aff_3^+ , the connected affine group. So in crystallography, the *crystallographic symmetry classes* are defined by space groups as subgroups of $E(3)$ up to a conjugation by elements of Aff_3^+ ; there are 230 of them. It is an interesting

¹⁰ We want also to mention that the 4783 four-dimensional space groups have been determined by computer [BRO78]. For $n = 4$, $|\{AC\}_4| = 710$, $|\{GC\}_4| = 227$, $|\{BC\}_4| = 64$, $|\{BCS\}_4| = 33$.

theorem [BIE12] that, in any dimension n , two isomorphic space groups, subgroups of E_n , are conjugated in the affine group Aff_n . For $n = 3$ there are 219 isomorphic classes of space groups. So there are 11 “enantiomorphic” pairs of isomorphic space groups. For the chemical compounds whose crystals belong to these enantiomorphic crystal symmetries, the two space groups of the pair are equally represented in nature (for instance as macles). We shall give some examples of enantiomorphic pairs in 1(11).

There are ten geometric classes of cyclic subgroups of O_3 . In [ITC] the conjugacy classes of their generators are called *geometric elements*; the five rotations are denoted by their order: 1, 2, 3, 4, 6 and the five others, product of the rotations and the symmetry through the origin (represented by the matrix $-I_3$), are denoted by $\bar{1}, m, \bar{3}, \bar{4}, \bar{6}$ (the notation m is used, instead of $\bar{2}$, because this is a symmetry through a plane = a mirror). The preimage by φ (see 1(6)) of these 10 cyclic geometric classes are the 16 cyclic arithmetic classes:

$$P1, P2, C2, P3, R3, P4, I4, P6; P\bar{1}, Pm, Cm, P\bar{3}, R\bar{3}, P\bar{4}, I\bar{4}, P\bar{6}. \quad 1(8)$$

We shall call their generators *arithmetic elements* (strangely, they are not given names in [ITC]). All arithmetic classes of point groups are generated by such elements and with the translations one generates all symmorphic groups. Remark that 1(8) also lists 16 symmorphic space groups in [ITC] notation.

Since a translation leaves no point fixed, the stabilisers G_w of the space groups G do not contain pure translations. Hence (from 1(7))

$$G_w \sim \theta(G_w) \leq P. \quad 1(9)$$

In [MIC95a] we have proven that the intersection of stabilisers are stabilisers, that almost all points of the space have the trivial stabiliser 1, so they form the *generic stratum* (= generic Wyckoff position), which is open dense. One also proves that *The strata with maximal symmetry are topologically closed* or, equivalently, that *the conjugacy classes of maximal finite subgroups of G correspond to closed strata*. Since the symmorphic groups contains groups $\sim P$ as subgroups, from 1(9), they have as many closed strata with such stabilisers as there are conjugacy classes $[G_m]_G$, $G_m \sim P$; the number of these strata is $\leq 2^3 = 8$. The dimension of these strata is equal to the multiplicity of the trivial representation in the natural (= vector) representation of P . For instance, for the 16 symmorphic subgroups of 1(8), the maximal closed strata are of dimension $d = 3$ (=the whole space) for $P1$, $d = 2$ (=reflection planes) for Pm, Cm , $d = 1$ (=rotation axes) for $P2, C2, P3, R3, P4, I4, P6$ and $d = 0$ (=isolated points) for $P\bar{1}, P\bar{3}, R\bar{3}, P\bar{4}, I\bar{4}, P\bar{6}$. For non symmorphic groups, there are no stabilisers isomorphic to P . We call *non symmorphic* elements of G its non trivial elements $g \neq 1$ such that no element of its conjugacy class $[g]_G$ leaves fixed a point of space. In dimension 3, these are the glide reflections and the screw rotations. A glide reflection is a symmetry through a plane combined (after or before) by a translation $\frac{1}{2}\vec{\ell}$ where $\vec{\ell}$ is a *visible vector* of L (i.e. no vector $\lambda^{-1}\vec{\ell}$, λ integer $\neq 0$ belongs to the lattice). Then $g^2 = (\vec{\ell}, 1)$, i.e. the pure translation $\vec{\ell}$. A screw rotation r is a rotation of order ρ combined (after or before) with a translation $\frac{\mu}{\rho}\vec{\ell}$, $0 \leq \mu < \rho$ where the visible vector $\vec{\ell} \in L$ defines the rotation axis; the screw rotation r is denoted by the symbol ρ_μ in [ITC]:

$$r = \rho_\mu, \quad \rho = 1, 2, 3, 4, 6, \quad 1 \leq \mu < \rho, \quad r^\rho = (\mu\vec{\ell}, 1), \quad \vec{\ell} \text{ visible}. \quad 1(10)$$

The non symmorphic groups generated by L and one of these non symmorphic elements are denoted in [ITC] by:

$$Pc, Cc; P2_1, P3_1 \sim P3_2, P4_1 \sim P4_3, P4_2, P6_1 \sim P6_5, P6_2 \sim P6_4, P6_3. \quad 1(11)$$

This list of 13 non symmorphic space groups contains 4 enantiomorphic pairs ¹¹. As suggested by the comparison between 1(8) and 1(11), the [ITC] notation for non symmorphic space groups is obtained by replacing in the symbols of symmorphic groups (listed in table 2a) a rotation ρ by ρ_μ and a reflection m by c or a, b, d, n depending of the orientation of the glide vector (in the reflection plane) with respect to the other symmetry elements of the point group ¹². Indeed if a space group contains a non symmorphic element, it is a non symmorphic. Beware that the converse is not true, but the only exception is the non symmorphic space group $I2_12_12_1$; it contains only symmorphic elements.

We leave to the reader to check that the action of the space groups:

$$Pc, Cc, P2_1, P3_1 \sim P3_2, P4_1 \sim P4_3, P6_1 \sim P6_5 \quad 1(12)$$

on the Euclidean space is *free*, i.e. all stabilisers are trivial, so there is only one stratum, the generic one. As we had already noticed, that is also the case of $P1 \sim L$. There are 13 such groups; we leave as a practical exercise to find the 3 others by studying [ITC].

Since $L \triangleleft G$, the study of action of the space group G on the Euclidean space is equivalent to the study of the action of $P = G/L$ on $R^n/L \sim U_1^n$. Beware that the latter action, in the case of non symmorphic groups, does not preserve the group structure of U_1^n , but only its manifold structure, a n -dimensional torus. These actions are different for each of the 219 isomorphic classes of space groups. As we already said, their strata are tabulated in [ITC] under the heading "Wyckoff positions". Of course the points of a fundamental domain, e.g. the Voronoï cell, with the opposite faces identified, can also represent the points of the torus.

§2 Functions on the Brillouin zone invariant by the space groups and time reversal.

Given a lattice $L \subset V_n$, the set of vectors of V_n whose scalar products with all vectors of L are integral, is also a lattice, called the *dual lattice*; it is denoted by L^* in the mathematical literature. Physicists prefer to consider $2\pi L^*$ (every vector of L^* is multiplied by 2π); they call it the *reciprocal lattice*. If $\{\vec{b}_j\}$ is a basis of L , the dual basis,

$$\{\vec{b}_i^*\}, \quad \vec{b}_i^* \cdot \vec{b}_j = \delta_{ij}, \quad 2(1)$$

generates the dual lattice L^* . Correspondingly $q(L^*) = q(L)^{-1}$. Let P a finite subgroup of $GL_n(Z)$; it defines an arithmetic class as well as an action of P on L . The corresponding action on L^* is defined by the contragredient representation of P :

$$GL_n(Z) \supset P \ni p \mapsto (p^{-1})^\top = (p^\top)^{-1}. \quad 2(2)$$

¹¹ The seven other pairs also correspond to the exchange $\rho_\mu \leftrightarrow \rho_{\rho-\mu}$ in a space group symbol.

¹² The first letter for the space group symbol, P, C, F, I, A as indicated in table 2a, is related to the Bravais class of the lattice L , with A which occurs in a unique arithmetic class, as a particular case of C .

For $n = 3$ the representation of P and its contragredient one are equivalent on Z for 65 of the 73 arithmetic classes. The non equivalent pairs are the F and I classes for the orthorhombic and cubic system. The list of these 3 + 5 pairs are:

$$Fmmm \leftrightarrow Immm, F222 \leftrightarrow I222, Fmm2 \leftrightarrow Imm2, \quad 2(3a)$$

$$Fm\bar{3}m \leftrightarrow Im\bar{3}m, F432 \leftrightarrow I432, F\bar{4}3m \leftrightarrow I\bar{4}3m, Fm\bar{3} \leftrightarrow Im\bar{3}, F23 \leftrightarrow I23. \quad 2(3b)$$

Every unitary irreducible representation (= unirrep) of the translation group L is one dimensional and has the form:

$$L \ni \vec{\ell} \mapsto e^{i\vec{k} \cdot \vec{\ell}}, \quad \vec{k} \bmod 2\pi L^*. \quad 2(4)$$

Equivalently, with a choice of basis:

$$\vec{\ell} = \sum_j \nu_j \vec{b}_j, \quad \vec{k} = \sum_j \kappa_j \vec{b}_j^*, \quad \vec{\ell} \mapsto e^{i \sum_j \kappa_j \nu_j}, \quad \nu_j \in Z, \quad \kappa_j \bmod 2\pi. \quad 2(4')$$

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

$$\vec{k} = \vec{k}^{(1)} + \vec{k}^{(2)} \bmod 2\pi L^* \Leftrightarrow \kappa_j \equiv \kappa_j^{(1)} + \kappa_j^{(2)} \bmod 2\pi. \quad 2(5)$$

This group is called the *dual group* by the mathematicians and the *Brillouin zone* (= BZ) by the physicists. Of course the points of a fundamental domain of the reciprocal lattice, e.g. its Voronoï cell, can represent the elements of BZ . The action of the space group on BZ is defined through the contragredient representation of $G/L = P$ on the reciprocal lattice. It is the same action for the space groups belonging to the same arithmetic class; so we have only 73 actions to study. These actions respect the group structure of the Brillouin zone \hat{L} . For instance \hat{L} has seven distinct elements of order 2; they satisfy:

$$\vec{k} \neq 0, \quad 2\vec{k} = 0 \Leftrightarrow \kappa_j = 0 \text{ or } \pi, \quad \sum_j |\kappa_j| \neq 0. \quad 2(6)$$

These elements form on BZ , a union of orbits of the space group G .

We denote by G_k, P_k the stabilisers of \vec{k} in the space group and the point group. The strata of the action of the space groups on BZ have been computed in many books without remarking that, with the help of 2(3), they can be read directly from the [ITC] compilation of Wyckoff positions from the symmorphic groups. The generic (open, dense) stratum corresponds to $P_k = 1, G_k = L$. From any representation \vec{k} of the translation group L one obtains by induction a representation of the space group G :

$$\text{Ind}_L^G(\vec{k}). \quad 2(7)$$

In appendix A we give an explicit computation of the matrix elements of these unirreps of G of dimension $|P|$ (= the number of elements of P). It shows that the matrix elements are *analytic functions on BZ* . Representations induced from two \vec{k} 's belonging to the same

orbit $G\vec{k}$ are equivalent; those induced from \vec{k} 's of the generic stratum are irreducible. Those induced from the other \vec{k} 's are reducible; from their reduction one obtains **all** unirreps of G . It is important to note that by reduction the matrix elements are defined only on each stratum of BZ . For non symmorphic groups, for some strata of dimension 1 or 2, the matrix elements are no longer analytic on the closure of the stratum, but only on a covering of it. That phenomenon was discovered by Herring [HER42] on two examples of space groups. We shall give more systematic examples at the end of §3 and show the important physical consequences of this phenomenon.

Another construction of all unirreps of space groups was made by Seitz [SEI36]; we recall it with the improvements made in [HER42]. Given a $\vec{k} \in \hat{L}$, we denote by $\ker \vec{k}$ and $\text{Im } \vec{k}$ the kernel and the image of this unirrep of L ; then $\text{Im } \vec{k} = L / \ker \vec{k}$ and $\ker \vec{k} \triangleleft G_k$. Herring introduced the group $P(\vec{k}) = G_k / \ker \vec{k}$. It is a central extension of $\text{Im } \vec{k}$ by P_k , i.e. $\text{Im } \vec{k} \leq C(P(\vec{k}))$, the center of $P(\vec{k})$; it splits into the direct product $P(\vec{k}) = \text{Im } \vec{k} \times P_k$ when G is symmorphic. For the computation of $P(\vec{k})$ when G is a non symmorphic group we refer to [MIC83] and to appendix A. One calls *allowed* unirreps of $P(\vec{k})$ those in which the subgroup $\text{Im } \vec{k}$ is represented faithfully. They are also the allowed representations of G_k . The induction from G_k to G of these allowed representations yields **all** unirreps of G .

We want to study the properties of functions on BZ implied by their invariance under the space group G , i.e. $\forall p \in P, f(\vec{k}) = f(p^\top \cdot \vec{k})$. We also require the invariance under T , the time reversal, when spin coordinates do not intervene explicitly. For a real observable function this requires $f(\vec{k}) = f(-\vec{k})$. This is already required from P invariance when P contains $-I_3$; that is the case for 24 arithmetic classes. For the other we replace the point group P by the one generated by P and $-I_3$. For convenience to the reader we give explicitly this substitution in table 2a. An equivalent table can be found implicitly in [ITC] under the heading: Patterson symmetry ¹³.

Examples of such invariant functions are the electron energy for a simple band, i.e. with a unique branch (in that case [NEN83] proves that the function is analytic), the Fermi surface energy of the electrons,... To study the invariance of such functions we have to study only 24 cases. Moreover, using 2(3), the same study can be used for the functions on the Euclidean space when G is symmorphic. That was done for instance in [WIG33] for metallic sodium: one atom per fundamental cell ¹⁴ of $Im\bar{3}m$. In that paper it was already remarked that at the points of a symmetry plane, a rotation axis, the gradient of invariant functions was in the plane or on the axis. More generally one can prove (see [MIC71] for the exact assumptions) that the gradient of an invariant function on a manifold is tangent to the stratum ¹⁵. The orbits isolated in their stratum are called *critical orbits* because they are orbits of extrema for **any** invariant differentiable function. In our problem that is the case of the symmetry centers and, more generally, of the points of strata of zero dimension. Moreover if the linear representation of the stabiliser P_k at such a critical

¹³ That symmetry appears in diffraction pattern when one measures only the intensity.

¹⁴ As far as I know, that paper was the first to use the Voronoï cell in physics, hence the name of Wigner-Seitz cell often used in physics literature.

¹⁵ So this theorem can be applied to the action on any space group on BZ and also on the direct space, thanks to the last paragraph of §1.

2	($P\bar{1}$)	$P1$;	5	($R\bar{3}m$)	$R32, R3m$;
8	($P2/m$)	$P2, Pm$;	4	$P\bar{3}$	$P3$;
5	($C2/m$)	$C2, Cm$;	7	$P\bar{3}1m$	$P312, P31m$;
30	($Pmmm$)	$P222, Pmm2$;	7	$P\bar{3}m1$	$P321, P3m1$;
15	($Cmmm$)	$C222, Cmm2, Amm2$;	9	$P6/m$	$P6, P\bar{6}$;
5	($Fmmm$)	$F222, Fmm2$;	18	($P6/mmm$)	$P622, P6mm, P\bar{6}m2, P\bar{6}2m$;
9	($Immm$)	$I222, Imm2$;	5	$Pm\bar{3}$	$P23$;
9	$P4/m$	$P4, P\bar{4}$;	10	($Pm\bar{3}m$)	$P432, P\bar{4}3m$;
40	($P4/mmm$)	$P422, P4mm, P\bar{4}2m, P\bar{4}m2$;	3	$Fm\bar{3}$	$F23$;
5	$I4/m$	$I4, I\bar{4}$;	8	($Fm\bar{3}m$)	$F432, F\bar{4}3m$;
14	($I4/mmm$)	$I422, P4mm, I\bar{4}m2, I\bar{4}2m$;	4	$Im\bar{3}$	$I23$;
2	$R\bar{3}$	$R3$;	6	($Im\bar{3}m$)	$I432, I\bar{4}3m$;

Table 2a. Arithmetic classes (in dimension 3) obtained by adding $-I_3$. Number of corresponding space groups. This table gives the application, by adding $-I$, of the 73 three dimensional arithmetic classes onto the 24 ones containing $-I$ (columns 2,5). In physical applications $-I$ might also represent the effect of time reversal on the Brillouin zone. For the labels of the arithmetic classes and for the order in their listing, we follow the “International Tables for Crystallography” [ITC]. The 14 arithmetic classes of the Bravais groups are between (). Columns 1 and 4 give the number of space groups corresponding to these 24 cases.

point is irreducible, all invariant functions have a maximum or minimum at these points. Table 2b lists the critical points of BZ in the 24 cases to be studied; among them we find $\vec{k} = 0$ and the 7 points which satisfy 2(6), as critical points for each of the 24 cases.

We can say more on the extrema, their nature, their number by using Morse theory. That was made for the first time by Van Hove [VHO53] using only the periodicity of the function. [PHI56],[PHI58] tried to do more for some space groups. Let us explain first Morse theory. It applies to real continuous functions with non degenerate extrema ¹⁶, i.e. the Hessian (= symmetric matrix of the second derivative) has a non vanishing determinant. Those assumptions are satisfied for most physical applications. The number of negative eigenvalues of the Hessian at an extremum is called the Morse index of the extremum (it is 0 for a minimum and n (= the dimension of the manifold) for a maximum. Let c_k the number of extrema of index k of the function f ; its Morse polynomial is: $M_f(t) = \sum_{k=0}^n c_k t^k$. Similarly one defines the Poincaré polynomial $P_M(t)$ of the manifold M with its Betti numbers as coefficients; for instance, for a n -dimensional torus, $P_M = (1+t)^n$. The modern presentation of Morse theory can be expressed by the equation (see e.g. [DOU87]

¹⁶ Their definition can be extended to continuous functions with discontinuous derivatives: e.g. [GOR80].

Extrema common to all functions on the Brillouin zone
invariant by the crystallographic group and time reversal

cs	arithm. class	0	$2k=0$	$4k=0$	$3k=0$	$6k=0$	nb	0,3	1,2	2,1	3,0	$Q(t)$
tc	$P\bar{1}$	1	1, 1, 1, 1, 1, 1				8	1	1+1+1	1+1+1	1	0
^m 6	$P2/m$	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
^{or} 6	$Pmmm$	1	1, 1, 1, 1, 1, 1				8	1	1+1+1	1+1+1	1	0
8	$Cmmm$	1	1, 1, 1, 2, 2				8	1	1+2	1+2	1	0
"	$Fmmm$	1	1, 1, 1, 4				8+(2)	$\frac{1}{1+1}$	$\frac{4}{4}$	$\frac{1+1+(2)}{1+(2)}$	$\frac{1}{1}$	$\frac{t}{1, t^2}$
14	$Immm$	1	1, 2, 2, 2	2 W			10	$\frac{1}{2}$	$\frac{2+2}{2+2}$	$\frac{2+2}{1+2}$	$\frac{1}{1}$	$\frac{t}{1, t^2}$
tt	$P4/m$	1	1, 1, 1, 2, 2				8	1	1+2	1+2	1	0
6	$P4/mmm$	1										
14	$I4/m$	1	1, 2, 4	2 P			10	$\frac{1}{2}$	$\frac{4}{4}$	$\frac{2+2}{1+2}$	$\frac{1}{1}$	$\frac{t}{1, t^2}$
$\overline{12}$	$I4/mmm$	1										
rh	$R\bar{3}$	1	1, 3, 3				8	1	3	3	1	0
14	$R\bar{3}m$	1										
hx	$P\bar{3}$	1	1, 3, 3		(2)c	(2)c	8+(4)	$\frac{1}{(2)}$	$\frac{(2)+3}{(2)+3}$	$\frac{(2)+3}{1+3}$	$\frac{1}{(2)}$	$\frac{2t}{1+t, t(1+t)}$
8	$P\bar{3}1m$	1						$\frac{(2)}{(2)}$	$\frac{(2)+3}{1+3}$	$\frac{1+3}{1+3}$	$\frac{1}{(2)}$	$\frac{1+t^2}{1+t^2}$
8	$P\bar{3}m1$	1	1, 3, 3	2 K	2 H	12		$\frac{1}{2}$	$\frac{2+3}{2+3}$	$\frac{2+3}{1+3}$	$\frac{1}{1}$	$\frac{2t}{1+t, t(1+t)}$
	$P6/m$	1						$\frac{2}{2}$	$\frac{2+3}{1+3}$	$\frac{1+3}{1+3}$	$\frac{1}{2}$	$\frac{1+t^2}{1+t^2}$
	$P6/mmm$	1						$\frac{2}{2}$	$\frac{1+3}{1+3}$	$\frac{1+3}{1+3}$	$\frac{2}{2}$	$\frac{1+t^2}{1+t^2}$
cu	$Pm\bar{3}$	[1]	[1], 3, 3				8	[1]	3	3	[1]	0
6	$Pm\bar{3}m$	[1]										
14	$Fm\bar{3}$	[1]	3, 4	(6)c			8+(6)	$\frac{[1]}{[1]}$	$\frac{3}{4}$	$\frac{(6)}{(6)}$	$\frac{4}{3}$	$\frac{3t^2, 3}{t+2t^2, 2t+t^2}$
14	$Fm\bar{3}m$	[1]	3, 4	6 W			14	$\frac{[1]}{[1]}$	$\frac{3}{4}$	$\frac{6}{6}$	$\frac{4}{3}$	$\frac{3t^2, 3}{t+2t^2, 2t+t^2}$
12	$I\bar{3}m$	[1]	[1], 6	[2]P			10+(6)	$\frac{[2]}{[2]}$	$\frac{(6)}{6}$	$\frac{6}{(6)}$	$\frac{[1]+[1]}{[1]+[1]}$	$\frac{1+2t+t^2}{1+2t+t^2}$
	$Im\bar{3}m$	[1]										

Table 2b. Minimum number of extrema and their positions for the functions on the 3-dimensional Brillouin zone, invariant by the crystallographic group and time reversal. Column 2 lists the 24 arithmetic classes obtained from table 1. Column 1 recalls their crystallographic systems (cs) and the combinatorial type of their Brillouin cell: 14, $\overline{12}$, 12, 8, 6 (numbers indicating their number of faces). " is a short for {14, $\overline{12}$, 12}.

Columns 3 and 4 give the critical orbits $\vec{k} = 0$ and among the 7 vectors $2\vec{k} = 0$ in BZ ; they are listed by their number of points. With the same notation, columns 5,6,7 (depending on the order of \vec{k}) give the other critical orbits when they exist (they are followed by an upper case label not universally used). The points of critical orbits between [] have to be maxima or minima because their stabiliser acts as an irreducible 3-dimensional representation.

Columns 5,6,7 may also contain one non critical orbit required by Morse theory (their number of points is between { } or { }).

Column 8 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 (); this occurs with (2) for the orthorhombic F Bravais class and with (6) for the Cubic I Bravais class, so the minimal number of extrema is 16 for the latter case. For two arithmetic classes of hexagonal P, there is a 2-component closed stratum (corresponding to two “vertical” edges of the hexagonal prism); each orbit (of the infinite family of them) has a point in each connected component (only the “horizontal” components of k satisfy $3\vec{k} = 0$). On this stratum, there must be 2 orbits of 2 extrema (the Morse index for the two orbits must differ by 1): each orbit is indicated by {2}c. Because the arithmetic class $Fm\bar{3}$ has only 3 critical orbits, Morse theory requires more extrema; since there is a stratum whose closure contains six circles meeting at $\vec{k} = 0$, there must be an orbit of 6 extrema on them (one extremum on each circle); they are indicated by {6}.

Columns 9 to 12 give the orbits of extrema with a given Morse index.

The last column gives the corresponding polynomial $Q(t)$.

Vol 3, chap. 1 §20, theorem 2):

$$M_f(t) - P_M(t) = (1+t)Q(t); \quad Q \text{ coefficients are positive integers.} \quad 2(8)$$

In our case, Morse theory should be applied to the topological closure of every stratum ¹⁷ on BZ . The results we obtained are given in table 2b.

§3 Space group and time reversal invariance for multivalued functions.

We use here the short hand $muf(\vec{k})$ for multivalued functions on BZ . A $muf(\vec{k})$ can be considered as a union $\cup_i f_i(\vec{k})$ of b distinct functions on BZ but there is arbitrariness in defining them ¹⁸.

The two main physical applications are the study of the energy $muf \omega(\vec{k})$ corresponding to the vibrations of the atoms of the crystal and the energy $E(\vec{k})$ of the bound states of the electrons. One can neglect the perturbation, due to the presence of the neighbouring atoms, to the electronic states for the closed shell of the crystal atoms ¹⁹; so we consider only the electrons in the non closed shells (in short, the *valence electrons*). These

¹⁷ Those of dimension 1 may not be manifold (e.g. a set of circles meeting in a unique point); the application of Morse theory can be done intuitively in that case, without the need of the generalisation of [GOR80]!

¹⁸ For most solid state books a convention is made (under the name of “labelling of bands”). Van Hove [VHO53] already doubted of the interest of this convention. We shall not make one, but some convention may be very natural when we know better their structure; e.g. some muf might be transformed in an analytic function on a covering of BZ (e.g. 3(4)).

¹⁹ For them, the corresponding muf are nearly constant.

two mvf 's on BZ are most important for the study of the thermodynamical and physical properties (e.g. electrical conductivity) of the crystals. Each mvf defines a set of hypersurfaces (called the *graph* of the mvf) in the 4-dimensional space of coordinates, the three κ_j 's (defined in 2(4')) of BZ and the energy value. For $\omega(\vec{k})$ the f_i 's are generally called branches of bands; there are three branches which satisfy

$$\omega(\vec{0}) = 0 \quad 3(1)$$

they belong to the *acoustic band*. But for the valence electrons, the graph of $E(\vec{k})$ is often called "a band structure" and each f_i is often called a band; however one also used the expressions "composite bands" and "simple bands". We will use the vocabulary of bands made from branches, currently used for vibrations, also for electron energy.

Of course space group ($=G$) and time reversal ($=T$) symmetry conditions do not apply separately to the different branches of a mvf , but they apply globally to its graph; e.g. it is periodic in the κ_j with period 2π . The direct extension of the §2 results to these mvf is difficult to do presently ²⁰ and, in my opinion, it is not advisable to try it. Indeed we should first have a more detailed knowledge of the general frame of the physical theory; for instance for $E(\vec{k})$, G and T invariances applied to a Schrödinger equation problem ²¹. The corresponding program was explained in the fundamental paper [BOU36]: let us quote three sentences of its introduction:

Thus far the group theory of the B-Z is not different from the group theory of any other system. But while in atoms, molecules, etc., the characteristic values of (1) [= the eigen values of the Schrödinger equation for bound states] are well separated, the characteristic values of (1) for a crystal form a continuous manifold.... [for example the graph of the energy E on BZ].

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.

The investigation of the "topology" of representations will be essentially the subject of this paper, from the mathematical point of view.

The last quote is the last sentence of the introduction. This paper ²² started the program by recalling the proof of the continuity of the energy as function of \vec{k} and by giving the *compatibility conditions* imposed by continuity on the unirreps of G_k when \vec{k} sweeps BZ . As the next step along its program, that paper announced Herring's thesis whose summary appeared a year after in two papers [HER37]. The first one shows the importance of using "corepresentations" (i.e. using also antiunitary operators) for the group generated by G and T ; it gives theorems for the sticking of two branches of an

²⁰ The generalisation of Morse theory to mvf 's is not finished and too involved for our needs.

²¹ In §2 we did not use it.

²² This paper is much quoted, but very little read! The notations introduced by the authors for the strata on the Cubic P, F, I Brillouin cells and for the unirreps of their G_k 's are still currently used. But I observed that the great majority of solid state physicists ignore the emphasis of this paper on the "topology of representations". Indeed this is quite a foreign idea to the users of Born von Karman groups with a BZ replaced by a finite set of points. Prof. R. Dirl in his 3rd lecture proposes an explicit method to perform the continuous limit.

mvf. The second one discusses the *accidental* contacts or crossings of *mvf*'s branches, i.e. those not due to symmetry; so they can disappear when one changes continuously the potential in the Schrödinger equation. That leads to the study of the existence of gap between branches, which has a great physical importance (it is necessary for insulators or semi-conductors). With changing external conditions (e.g. temperature or pressure) the two branches may meet ²³. That was the basis of the prediction in [WIG35] that under high pressure solid hydrogen will be metallic; this has been verified this year (more than sixty years after!) at Livermore. We can extend the concept of "changes in the potential" by going down a column of the Mendeleev table. C as diamond, Si, Ge have a common crystal structure: the cubic (non symmorphic) space group $Fd\bar{3}m$, with 2 atoms per fundamental cell, on an orbit of the Wyckoff position a (stabiliser $F\bar{4}3m \sim T_d$). Their Fermi surface corresponds to the upper end of the energy spectrum $E(\vec{k})$ of the valence band. Diamond is an insulator because the gap with the conduction band is about 6ev while it is 1.1ev and .7 ev for Si and Ge respectively; the last two (with precise doping of impurities) can be excellent semi-conductors. The crystal structure of Bi, lower in the next Mendeleev column, is obtained from the previous by a slight elongation along the cube diagonal; so it is rhombohedral: space group $R\bar{3}m$ with 2 atoms in Wyckoff position c (stabiliser $R3m \sim C_{3v}$). It is a metal (or semi-metal); when pressure is increased, the gap appears at about 25 Kbars.

Obviously, the first step for studying the complicated "band structures" obtained in experiments is to try to decompose them into simpler system by "removing" the accidental degeneracy until one obtains "indecomposable elements" which are so simple that one can classify them. De Cloizeaux ([CLO63] p. 561) gave the obvious definition for the indecomposable band structures: *their graph should always be connected*. He called the latter bands and their components: branches and showed that their symmetry was described by an induced representation. In his thesis, Herring had emphasized the the electron energy bands and the vibration bands have some similarity in their mathematical structure. The band classification was first made for the vibrations. Indeed, it was natural to extend to crystals the group theoretical method introduced by [WIG30] for molecules. I am not able presently to retrace the history of the statement very clearly given for instance in the textbook [STR67]:

the space of eigen states corresponding to the mvf $\omega(\vec{k})$ carry the representation:

$$\oplus_w \text{Ind}_{G_w}^G V(G_w); \quad V(G_w) \text{ is the vector representation of } G_w, \quad 3(2)$$

and the direct sum is over all Wyckoff positions occupied by atoms. If n is the number of atoms by fundamental cell, the number of branches is $3n$. [STR67] does not speak of induced representation; the translation in the form 3(1) is done in [MIC82] which also gives the explicit reduction in unirreps of G_k for each $\vec{k} \in BZ$. Eq. 3(1) yields the connectivity of the 3 branches for $n = 1$ and many exemples of the 6 branches for $n = 2$ are given in

²³ The meeting of two branches is a sufficient condition for destroying the gap between the two connected intervals (on the real line) of their energy spectrum; however it is not a necessary condition since the two branches have no common points when the common part of the values of the *mvf* $E(\vec{k})$ comes from separated domains of BZ .

[MIC95b]. A full study will be made; in the general case the total vibration spectrum is the union of several indecomposable bands.

Intuitive classifications of electron energy bands were made by assuming their relation with atomic electron orbitals. Zak [ZAK80] was the first one to show that the *band representation*, i.e. the representation of the space group G on the Hilbert space of the Schrödinger equation solutions corresponding to the band was an induced representation of the form of $3(2)$, in which the Wyckoff positions w might be a position of atoms, but more generally they have to be determined by the nature of the physics as well as the representation of G_w (instead to be restricted to the vector representation). With that clear formulation of the nature of the band representations, Zak was able to define non ambiguously the decomposition of band structures! Indeed a band structure is decomposable if its band representation is a direct sum of band representations. He called “irreducible” the band representations which cannot be decomposed ²⁴ into a direct sum of band representations. He added (on p. 1026) “The irreducible band representations serve as *elementary* building bricks in the symmetry definition of bands in solids”. That is the qualificative we used in our later common publications. Bands whose band representations are elementary are simply called here *elementary bands*. Furthermore [ZAK80] gave necessary conditions for elementary band representations: it is induced from a *unique* Wyckoff position w which satisfies the two conditions 1) it has maximal symmetry ²⁵, 2) the representation of the stabiliser G_w is irreducible. These two conditions are not sufficient; an example showing it was found by [EVA84]. Moreover, distinct elementary band representations can be equivalent: the first example was found by [ZAK82] in the study of the diamond like structure.

In 1987, with Bacry, we established the complete classification of elementary band representations: [BAC88]. All band representations satisfying conditions 1) and 2) are elementary except 40 of them belonging to 25 space groups: they all occurs for the two dimensional representations of stabilisers isomorphic to $322 = D_3$, $422 = D_4$, $622 = D_6$, $\bar{4}2m = D_{2d}$. Among the elementary band representations there are 152 equivalent pairs: 57 at the same w and 37 at different w 's for some unirreps of G_w and 62 for all G_w unirreps for 17 pairs of Wyckoff positions in 14 space groups. For this last class of equivalent representations a (Berry phase like) topological invariant seems to distinguish them [MIC92]. Using a well known Mackey's formula (eq. (20) of [BAC88]) for the reduction of band representations ²⁶ that paper gives the explicit decomposition of an elementary band representation on G_k for all points of BZ . For $G_k = 1$ (corresponding to the generic stratum) the multiplicity b is the number of branches of an elementary band:

$$b = \frac{|P|}{|G_w|} \dim \rho(G_w). \quad 3(3)$$

²⁴ That is a very confusing term, because these infinite dimensional band representations are reducible (by a direct integral) into the finite dimensional unirreps of G .

²⁵ We have stated after 1(9) that “Wyckoff position with maximal symmetry” is equivalent to either: a) the stabiliser G_w is a maximal finite subgroup of G , or b) the stratum with stabilisers in $[G_w]_G$ is topologically closed.

²⁶ We assumed (and I hope to prove it!) that Frobenius reciprocity (see the appendix) can be extended to space groups; that assumption also extends to them the Mackey's formula.

For instance for diamond, Si, Ge, the valence band and the first conduction band are both elementary 4 branch bands; their symmetry²⁷ is respectively “ $w = c$ trivial representation of $G_w \sim D_{3d} = R\bar{3}m$ ” and “ $w = c$ 1 dimensional representation of $G_w \sim D_{3d} = R\bar{3}m$ with kernel D_3 (so its image is $\{1, -1\}$)” (J. Zak, private communication).

The next evident step in the program of [BOU36] on the topology of representations on BZ is the conjecture:

The graph of an elementary band is connected²⁸ that Zak and I have formulated and are trying to prove²⁹. Here we prove it for the 13 non-symmorphic groups of 1(11). We denote by ℓ the visible³⁰ lattice vector defining the glide vector $\frac{1}{2}\vec{\ell}$ for Pc, Cc or the screw rotation axis for the other space groups of 1(11). As any visible vector, $\vec{\ell}$ can be chosen as a vector basis of the lattice; we denote by $\vec{\ell}^*$ the conjugate vector in the dual basis (defined in 2(1)) and by $k' \bmod 2\pi$ the corresponding coordinate in BZ . In the unirrep $k'\vec{\ell}^*$ of the translation lattice L , the translation $\vec{\ell}$ is represented by $e^{ik'}$. We have called r in 1(10), a non-symmorphic generator of the groups in 1(11). From 1(10) we obtain that r is represented by

$$r \mapsto e^{\lambda 2\pi i / \rho} e^{ik' \mu / \rho}, \quad 0 \leq \lambda < \rho, \quad 3(4)$$

in the ρ -dimensional induced representation $\text{Ind}_L^G(k'\vec{\ell}^*)$ (defined in 2(7)). One verifies that these ρ branches, labelled by λ , form 1-dimensional inequivalent unirreps of G_k on the circle \mathcal{C} of coordinate k' on BZ . After a complete cycle on \mathcal{C} , $k' \mapsto k' + 2\pi$ which, from 3(4), is equivalent to $\lambda \mapsto \lambda + \mu$. That is the phenomenon of holonomy of the G_k unirreps found in [HER42]. Let us first consider the case $\mu = 1$; i.e. we study only the 9 non-symmorphic groups of 1(12). As we have pointed out, the full space is their unique Wyckoff position; therefore they have a unique equivalence class of elementary band representations. Its ρ branches are continuous functions of the representative of r in 3(4). They form a unique analytic function of k' on the ρ -fold covering of \mathcal{C} so the graph of the elementary band on \mathcal{C} is connected on \mathcal{C} and, a fortiori, on BZ .

For each of the 4 other groups of 1(11) there are several closed Wyckoff positions; each one is a rotation axis with an infinity of finite orbits. Each closed Wyckoff position yields μ different elementary bands and the connexity of their graph is again a direct consequence of 3(4). Since all non-symmorphic space groups but one ($I2_12_12_1$) contain as subgroup at least one of the 13 space groups of 1(11), the proof of the graph connexity of their elementary bands is easy to extend to them. It is verified directly for $I2_12_12_1$ from the compatibility conditions on the edges on BZ .

To end these notes, let us consider in detail, for the unique elementary band of $P4_1$, its graph over \mathcal{C} . This circle contains two points, $k' = 0$ and $k' = \pi$, invariant by time reversal T . At $k' = 0$, r is represented by $\exp(i\lambda\pi/2)$; then T requires the contact of the branches with complex conjugate values, i.e. for $\lambda = 1, 3$. At $k' = \pi$, r is represented

²⁷ We give it by the sequence: w , and the unirrep of G_w .

²⁸ Very natural conjecture since an elementary band is by definition indecomposable; see above.

²⁹ Our proof for non-symmorphic groups seems in good shape, but we have some difficulty for some symmorphic groups.

³⁰ Concept defined before 1(10).

by $\exp(i(2\lambda + 1)\pi/4)$; then T requires the contact of the branches of the pairs $\lambda = 0, 3$ and $\lambda = 1, 2$. Taking in account the holonomy of the G_k representations and the global symmetry of the graph over C for $k' = -k' \bmod 2\pi$, one obtains Figure 2 for two possible schematic shapes of this graph. They are topologically distinct; their difference is explained in the caption of figure 2.

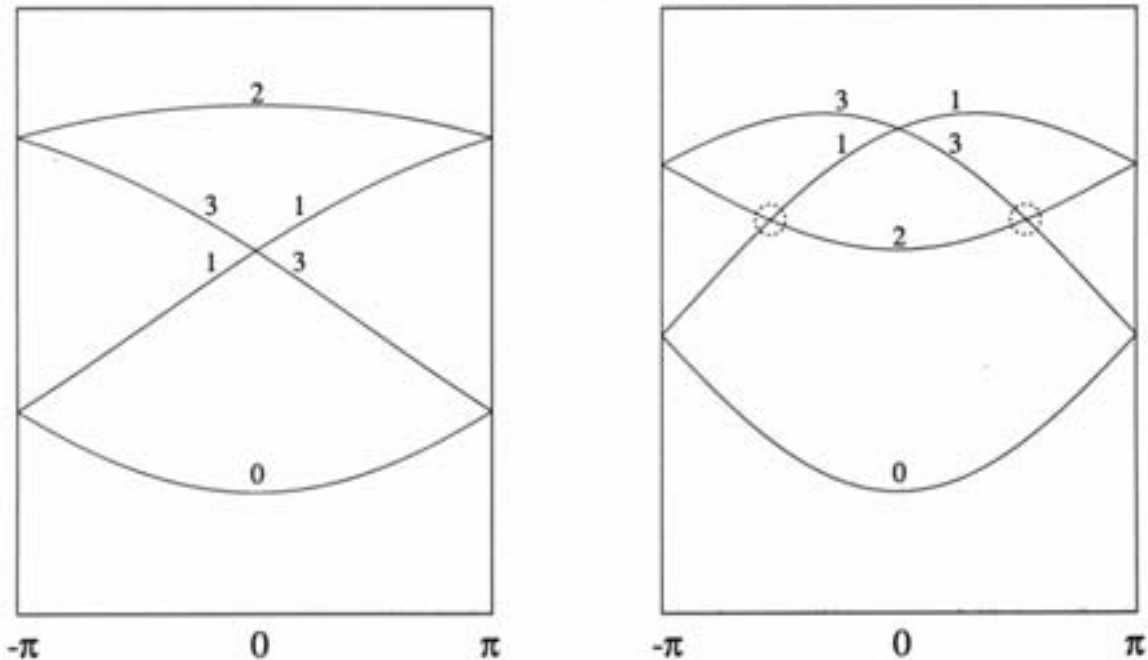


Figure 2. Two possible topologies for the graph of electron energy $E(k')$ above the circle on BZ corresponding to the skew rotation axis for the unique elementary band of the space group $P4_1$.

The left diagram corresponds to the (increasing or decreasing) order $\lambda = 0, 1 = 3, 2$ for the energy levels at $k = 0$, the right one corresponds to the different order $\lambda = 0, 2, 1 = 3$. In the two cases T invariance requires two contact points at $k' = \pi$ and one at $k' = 0$. The second case b has two more contact points, with same $E(k')$ value, at the symmetric coordinates $\pm k'$ with $0 < |k'| < \pi$. These two contacts are required by the topology (continuity of $E(k')$) but are *accidental* since by variation of the potential one might replace the order of the energy levels at $k' = 0$ in the right diagram by that of the left diagram.

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§6 Appendix.

The space groups are discrete subgroups of the Euclidean group E_n . To write the group law of the latter we choose an origin on the Euclidean space E_n . Then every element of E_n can be written as the product of first, an orthogonal transformation A and second, of

a translation t . We write such an element ³¹ $\{t, A\}$. Its action on the point $x \in \mathcal{E}_n$ is:

$$\{t, A\}.x = Ax + t. \quad A(1)$$

The Euclidean group is the semi direct product: $E_n = R^n \rtimes O_n$; its group law is:

$$\{s, A\}\{t, B\} = \{s + At, AB\}, \quad \{s, A\}^{-1} = \{-A^{-1}s, A^{-1}\} \quad A(2)$$

As we have seen in §1 a space group G is a discrete subgroup of the Euclidean group, containing L , a lattice of translations, as invariant subgroup; the quotient $G/L = P$ is the point group. The majority of space groups are non symmorphic (i.e. are not semi-direct products) and P cannot be identified with a subgroup of G . In that case we have to choose a section for the homomorphism $G \xrightarrow{\theta} P$ of the equation 1(7), i.e. a map ³² $P \xrightarrow{\tau} G$ such that $\sigma \circ \tau = I_P$ the identity map on P . For any $A \in P$, $\tau(A)$ is an element $\{v(A), A\} \in E_n$. When the translation $\{v(A), I\}$ does not belong to the translation subgroup L , the translation $v(A)$ is called a non-primitive translation ³³. The product of two elements of the space group $G < E_n$ is given by:

$$\{s + v(A), A\}\{t + v(B), B\} = \{s + At + v(AB) + z(A, B), AB\} \quad A(3)$$

with the definition:

$$z(A, B) \stackrel{def}{=} v(A) - v(AB) + Av(B) \in L \quad A(4)$$

The function $v(A)$ depends of the choice of origin in the Euclidean space; indeed if we translate this origin by the translation $x = o o'$, we make a conjugation in E_n by the element $\{-x, 0\}$:

$$\{s' + v'(A), A\} = \{-x, 0\}\{s + v(A), A\}\{x, 0\} = \{s + v(A) - (I - A)x, A\}$$

$$\text{i.e. } v'(A) = v(A) - (I - A)x \quad A(5)$$

From this equation and the definition A(4) it is easy to verify that the function $z(A, B)$ is independent from the choice of origin. This important property makes this function very useful in physical applications; by contrast, because they depend on an arbitrary choice of origin of the physical space, the imprimitive translations cannot appear explicitly in the general equations governing physical phenomena. From the convention $v(I) = 0$, the function $z(A, B)$ satisfies:

$$z(I, A) = 0 = z(A, I) \quad A(6)$$

³¹ In the solid state literature it seems to be a tradition to write the elements $\{A, t\}$, although A is performed before t and the usual convention of product of operators or group elements from left to right: $g_1 g_2$ means first g_1 then g_2 . Here we cannot adopt this incoherence.

³² which cannot be a group homomorphism.

³³ When $\{v(A), I\} \in L$, one can choose the section τ such that $v(A) = 0$. However the only convention we require here is $v(I) = 0$, because it is independent from the choice of origin.

Moreover, the associativity of the space group law requires:

$$z(A, B) - z(A, BC) + z(AB, C) - Az(B, C) = 0 \quad A(7)$$

We shall refer to the two variable function $z(A, B)$ defined on P and valued in L as a *cocycle* since it is the mathematical name of such functions satisfying A(6) and A(7). Note that a cocycle has still some arbitrariness. Indeed instead of the section τ we could have chosen $\tau'(A) = \tau(A) + c(A)$, $c(A) \in L$, the cocycle is changed into $z'(A, B)$ given by:

$$z'(A, B) - z(A, B) = b(A, B) = c(A) - c(AB) + Ac(B). \quad A(8)$$

The particular cocycles of the form given by the last equality, are called coboundaries. For a given arithmetic class (i.e. a given action of P on $Z^3 \sim L$) the different possible cocycles (by addition of their value) form a group denoted by $Z^2(P, L)$ and the coboundaries form the subgroup $B^2(P, L)$. The "second cohomology group" mentionned after 1(7) is the quotient $H^2(P, L) = Z^2(P, L)/B^2(P, L)$. A simpler notation than that of A(3), independant of the choice of origin is used in the text (e.g. in 1(10)). With it, the space group law is written:

$$(s, A)(t, B) = (s + At + z(A, B), AB). \quad A(9)$$

The corresponding law for the stabiliser G_k is given by the matrices:

$$A, B \in P_k, \quad (e^{i\vec{k} \cdot \vec{s}} A)(e^{i\vec{k} \cdot \vec{t}} B) = e^{i\vec{k} \cdot (\vec{s} + \vec{t} + \vec{z}(A, B))} AB. \quad A(10)$$

Replacing the exponentials of translations by their value yields the Herring group $P(\vec{k})$ (defined in the paragraph after 2(7)).

We now recall the definition and fundamental properties of induced representations. We first consider the case of a finite group G and its subgroup H . The complex valued functions on the group which satisfy:

$$\phi(g_1 g_2) = \phi(g_2 g_1) \Leftrightarrow \phi(g_1 g_2 g_1^{-1}) = \phi(g_2), \quad A(11)$$

form a finite dimensional Hilbert space \mathcal{H}_G with the Hermitean scalar product:

$$\langle \varphi, \phi \rangle_G = |G|^{-1} \sum_{g \in G} \bar{\varphi}(g) \phi(g). \quad A(12)$$

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

$$\mathcal{H}_G \xrightarrow{\text{Res}_H^G} \mathcal{H}_H. \quad A(13)$$

By definition, its adjoint operator is the induction operator:

$$\mathcal{H}_H \xrightarrow{\text{Ind}_H^G} \mathcal{H}_G; \quad \text{Ind}_H^G = (\text{Res}_H^G)^\dagger. \quad A(14)$$

From this definition we have immediatly the Frobenius reciprocity:

$$\langle \text{Ind}_H^G \chi_H^\rho, \chi_G^\alpha \rangle_G = \langle \chi_H^\rho, \text{Res}_H^G \chi_G^\alpha \rangle_H. \quad A(15)$$

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

$$H < H_1 < H_2 < \dots < H_{m-1} < H_m < G \Rightarrow \text{Ind}_H^G = \text{Ind}_{H_m}^G \text{Ind}_{H_{m-1}}^{H_m} \dots \text{Ind}_{H_1}^{H_2} \text{Ind}_H^{H_1}, \quad A(16)$$

and from the other fundamental properties of linear maps:

$$\text{Ind}_H^G \chi_H^\rho \oplus \chi_H^\sigma = \text{Ind}_H^G \chi_H^\rho \oplus \text{Ind}_H^G \chi_H^\sigma, \quad \text{Ind}_H^G \chi_H^\rho \otimes \chi_H^\sigma = \text{Ind}_H^G \chi_H^\rho \otimes \text{Ind}_H^G \chi_H^\sigma, \quad A(17)$$

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

$$G = \cup_j s_j H. \quad A(18)$$

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

$$\Delta = \text{Ind}_H^G D, \quad \Delta_{j\ell}(g) = \begin{cases} D(s_j^{-1} g s_\ell) & \text{if } s_j^{-1} g s_\ell \in H; \\ 0, & \text{otherwise.} \end{cases} \quad A(19)$$

Obviously that formula can be extended to finite dimensional representations of a subgroup H of finite index³⁴ in G . For instance the induction of the unirreps \vec{k} of the translation subgroup L to the whole space group G is straightforward:

$$\Delta_{j\ell}(t) \equiv \Delta_{j\ell}((t, I)) = \delta_{j\ell} e^{i\vec{k}_j \cdot t}, \quad k_j = (S_j^T)^{-1} k, \quad A(20)$$

$$\Delta_{j\ell}((0, S)) = \begin{cases} e^{i\vec{k}_j \cdot \vec{r}(S, S_\ell)}, & \text{if } S_j = S S_\ell; \\ 0, & \text{otherwise} \end{cases} \quad A(20')$$

In a d -dimensional allowed unirrep of $P(\vec{k})$ (which is also an allowed unirrep of G_k) the translations are represented by multiples of the unit matrix ζI_d with $\zeta \in \text{Im } \vec{k}$. The induction to G is straightforward.

Equation A(19) could also be used for the induction to the space-group G of a representation of the finite subgroup G_w ; it yields infinite matrices. Frobenius reciprocity cannot be defined by A(15); however its definition has been extended to locally compact groups in the mathematical literature. The space groups are a particular (trivial) case of such groups and we had assumed e.g. in [BAC88] that it was valid and that we can use the expressions written as scalar product of characters of finite representations. I hope to study more thoroughly this problem.

³⁴ That is $G : H$ is a finite set.