RECENT RESULTS ON THE IMPLICATIONS OF CRYSTAL SYMMETRY AND TIME REVERSAL

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§0 Introduction.

I will report on recently obtained results, some of them not yet published, which are consequences of crystal symmetry and time reversal.

I will consider only periodic crystals. Their symmetry is a very good physical approximation which allows to make strong predictions. The ones I will present, apply to the results of many experiments: those which are expressed by functions on the Brillouin zone, invariant by the symmetry of the crystal. Time reversal invariance will be added in the case of stationary phenomena, but only in the approximation that direct spin effects can be neglected; i.e. we shall use only the 230 space groups and not the numerous "magnetic" or "Shubnikov" ones. By its generality and precision, the study of the consequences of symmetry belongs to the general culture of physicists; it can be a handicap to ignore them. It is true that a model which has the same symmetry will satisfy all its predictions. But the model independent consequences 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 symmetry conservation, which ones are specific to the model?

§1 Mathematical tools.

1a. *Some theorems on compact group actions.*

Symmetry appears in physics through the action of symmetry groups. I just recall some definitions to precise the notations. Let G be a group acting on a mathematical object M as subgroup of its automorphism group. 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 *stabilizer* of m. It is a subgroup of G (sometimes called "little group" in the physics literature). The stabilizers of an orbit form the conjugacy class $[G_m]_G$ of the subgroups of G conjugated to G_m. By definition, two orbits with same conjugacy class of stabilizers belong to the same *orbit type*. Given any H subgroup of G, an example of orbit of type $[H]_G$ is the set $G : H$ of the left cosets of H with the action of G on the cosets by left multiplication: $g.xH = gxH \equiv (gx)H$.

In a group action, a *stratum* is the union of the orbits of same type. Equivalently, *two elements of M belong to the same stratum if, and only if, their stabilizers are conjugated in the group G.*

In the action of G on M, the set of orbits is called the *orbit space*; we denote it by $M|G$.

We denote the set of strata by $M\|G$. This set is finite in most physical problems and it is very important to know it. For instance, there are four strata in the action of the Lorentz group on the Minkowski space: the time like, the space like, the light like vectors and the origin. The strata of the actions of the 230 crystallographic space groups on the space, are tabulated in the International Tables of Crystallography (=[ITC] under the heading "Wyckoff positions"; Bravais classes, crystallographic systems form stratum spaces (see (5) below), etc...

We consider from now on a smooth action of a compact group G on a real manifold M of finite dimension n. The stabilizers are closed subgroups of G. There is a natural partial order on the conjugacy classes of closed subgroups of G (by subgroup inclusion up to a conjugation). By averaging over the group a Riemannian metric on the manifold, one equips M with a G-invariant Riemannian metric; a particular example is a n-dimensional linear orthogonal representation of G. An action of G on M defines implicitly the action of G on the real functions defined on M. The functions which satisfy

$$\forall g \in G,\ \forall m \in M: \quad f(g.m) = f(m) \tag{1}$$

are the G-invariant functions. The sums, the products of G-invariant functions are G-invariant functions; so they form a ring that we denote by $\mathcal{F}_M^G$. If the G-invariant function f has an extremum at $m \in M$, all point of the orbit $G.m$ are extrema of the same nature.

We will use the following theorems for the smooth actions of compact groups on real manifolds.

Theorem 1. *There is a unique minimal stratum (i.e. with minimal symmetry): it is open and dense in M. The maximal strata (i.e. with maximal symmetry) are closed.*

Proof by D. Montgommery [MON56]. The minimal stratum is also called generic.

Theorem 2. *The gradient $\nabla f(m)$ at the point $m \in M$, of the G-invariant differentiable function f is normal to the orbit $G.m$ and tangent to the stratum $S(m)$ of m.*

Well known. We call *critical orbits* those orbits which are isolated in their strata (= no other orbits of the same type in a tubular neighbourhood of a critical orbit).

Theorem 3. *An orbit is critical $\Leftrightarrow$ It is an orbit of extrema for* **all** *functions of $\mathcal{F}_M^G$.*

Proof in [MIC71]. Let M be compact. Consider an invariant function $f \in \mathcal{F}_m^G$ and denote by f_S its rectriction to a maximal symmetry (and therefore closed) stratum. It reaches a maximal value and a minimal value on S. From the last statement of theorem 2, at any point m of this maximal stratum $\nabla f(m) = \nabla f_S(m)$. That proves another theorem of the same reference:

Theorem 3'. *Moreover, when M is compact,* **all** *functions of $\mathcal{F}_M^G$ have at least two orbits of extrema on any connected component S_α of the closed strata S, when S_α contains an infinity of orbits.*

In the particular case of a finite dimensional linear orthogonal representation of the compact group G on the vector space V_n, G. Schwarz has shown in [SCH75]:

Theorem 4. *The ring of invariant polynomials $\mathcal{R}_{V_n}^G$ is dense in the ring of invariant smooth functions.*

This theorem can be extended to some actions of G on M when a global system of coordinates exist. I do not know general theorems but it becomes obviously true in the case of the actions of the point groups on the Brillouin zone with an appropriate choice of the polynomial variables. Finally we remark that at any point $m \in M$ the action of G induces a linear representation of G_m on the tangent plane $T_m(M)$ of M at m. We will use it in the next subsection for theorem 5.

We shall need these five theorems only in the particular case of finite groups and compact manifolds. Then each orbit $G.m$ has a finite number of points, $|G.m|$, which is a divisor of $|G|$ (the number of elements of the group); more precisely: $|G.m||G_m| = |G|$. And the critical orbits are those belonging to strata of dimension 0. Hence we know the extrema common to all invariant functions. We will study in the next subsection what Morse theory can predict about the nature of these extrema.

§ 1b. *Morse theory of $\mathcal{F}_M^G$ when G is a finite group and M a compact manifold.*

Let us recall Morse theory in its simplest form. It applies to C^2 real functions with isolated extrema, i.e. at every extremum, their Hessian (= symmetric matrix of the second derivatives) has a non vanishing determinant. These assumptions are satisfied for most physical applications; it is also the case for the critical orbits we study since, for finite groups, their points are isolated. Given a function f, the number of negative eigenvalues of the Hessian at an extremum is called the Morse index of the extremum; we denote this index by i. For a minimum, $i = 0$ and $i = n = \dim M$ for a maximum. The intermediate values $0 < i < n$ are those of the Morse index for the different type of saddle points [1] Let c_i be the number of extrema of f with the index i; its Morse polynomial is:

[1] Morse theory is easily extended to continuous functions with discontinuous derivatives because the Morse index of their extrema is determined by the topology of the (continuous) level surfaces in the neighbourhood of an extrema.

$M_f(t) = \sum_{i=0}^{n} c_i t^i$. Similarly one defines the Poincaré polynomial $P_M(t)$ of the manifold M with its Betti numbers b_k as coefficients [2] . For instance, for a n-dimensional sphere $P_{S_n}(t) = 1 + t^n$. For a topological product of manifolds $M = M' \times M''$, $P_{M' \times M''}(t) = P_{M'}(t)P_{M''}(t)$; hence for a n-dimensional torus, since it is the topological product S_1^n of n circles,

$$P_{M' \times M''}(t) = P_{M'}(t)P_{M''}(t),\ P_{S_n}(t) = 1 + t^n,\ \Rightarrow P_{S_1^n} = (1+t)^n \tag{2}$$

The modern presentation of Morse theory can be expressed by the equation (see e.g. [DOU87] Vol 3, chap. 1 §20, theorem 2):

$$M_f(t) - P_M(t) = (1+t)Q(t); \quad Q \text{ coefficients are integers} \geq 0. \tag{3}$$

The inequalities satified by the coefficients of Q are the famous Morse inequalities. They imply $c_i \geq b_i$ (since the coefficients of the polynomial $M_f(t) - P_M(t)$ are ≥ 0) but they are stronger; for $t = -1$ (3) gives the equality $\sum_i (-1)^i (c_i - b_i) = 0$ known before Morse's work.

For functions invariant under the action of a compact (or finite) group, one can make stronger predictions on the nature of extrema; e.g.

Theorem 5. *If the linear representation of G_m on $T_m(M)$ is irreducible on the real and if m is an extremum of an invariant function f, this extremum is either a maximum or a minimum.*

Indeed, at each point m, the Hessian H_f of an invariant function commutes with G_m; that imposes a multiplicity structure on the spectrum of H_f. Since H_f is symmetric, when the representation of G_m is real irreducible, H_f is a multiple of the identity and its Morse index is either 0 or n.

Of course extrema of the same orbits are of the same nature; so, for finite group actions, the c_i's are the number of points of a set of G-orbits. There are several studies of the "equivariant Morse theory"; I will summarize their conclusions for the cases of interest here by the requirement that Morse theory has to be applied not only to M but also to the topological closure of every stratum. Those compact closed subspaces are not necessarily submanifolds of M. So one may have to use the extension of Morse theory to manifolds with boundary, to orbifolds, or even to more complicated spaces (as union of manifolds). The required generalisation of Morse theory is explained in [GOR80]; however, in the cases studied below, we shall not really need it (only the closure of one dimensional strata are not submanifolds: e.g. set of circles with a common point).

§2 Extrema of functions on the Brillouin zone, invariant by the crystal symmetry and time reversal.

I first recall the basic facts of crystal symmetry classification. The symmetry group of a periodic crystal contains a lattice of translations. It is an Abelian group $L \sim Z^d$ where $d = 2, 3$ is the dimension of the space. The translations acts on our Euclidean space; the full symmetry of the crystal, called in physics the space group S, is a subgroup of the Euclidean group $Eu_d = R^d \rtimes O_d$. The translation lattice is an invariant subgroup of S and the corresponding quotient $P = S/L$ is the point group of the crystal. The point group P acts on L and must be a subgroup of Aut(L), the automorphism group of the lattice.

Let us introduce provisorily an orthonormal basis $\vec{e}_u.\vec{e}_v$ in our Euclidean space. Let $\{\vec{b}_j\}$ a set of d vectors generating the matrix (by addition and subtraction of vectors); so $L \ni \vec{\ell} = \sum_j \ell_j \vec{b}_j$, $\ell_j \in Z$. We denote by b the matrix of components of the $\vec{b}_j$'s, i.e. $b_{ju} = \vec{b}_j.\vec{e}_u$. Since the $\vec{b}_j$'s are

[2] This number b_k is the rank of the kth homology group of M in Z; intuitively it is the maximum number of k-dimensional submanifolds of M which cannot be deformed continuously into each other or into a submanifold of smaller dimension.

linearly independent, $\det b \neq 0 \;\Leftrightarrow\; b \in GL_d(R)$. Any other generating basis of the lattice must be of the form $\vec{b}'_i = \sum_j m_{ij}\vec{b}_j$ with the matrix $m \in GL_d(Z)$ (that implies $(\det m)^2 = 1$). By definition $r \in O_d$ is a sysmmetry of the lattice L when $r.L = L$; then the L basis b is transformed into br^{-1} which must be another basis of L:

$$r.L = L \Leftrightarrow br^{-1} = mb \Leftrightarrow r = b^{-1}m^{-1}b. \tag{4}$$

That shows that Aut(L) is finite [3] . Moreover we have two points of view for the symmetry of a lattice: the set of conjugacy classes of Aut L in O_d and in $GL_d(Z)$. The first stratum set is $\{CS\}_d$, the second one is $\{BC\}_d$ according to the names *Bravais crystallographic systems* and *Bravais classes* given to them in [ITC]. To be more explicit: we consider the set of lattices in dimension d: it is the orbit (set of cosets) $\mathcal{L}_n = GL_d(R) : GL_d(Z)$ and we study the orbits and strata of O_n on it. The orbit of a lattice, $O_d.L$, is the set of different positions of a same "intrinsic" lattice $L^{(i)}$; the latter is characterized by the Gram matrix [4] $q_{ij} = \vec{b}_i.\vec{b}_j$. Note that q depends on the basis b and that the change of basis $b \mapsto mb$, $m \in GL_d(Z)$ transforms q into $mqm^\top$. Hence an intrinsic lattice $L^{(i)}$ is an orbit of $GL_d(Z)$ acting on the set of q's that we denoted by $\mathcal{C}_d^+$. Indeed the $q(L)$'s are symmetric positive matrices; in the $d(d+1)/2$ dimensional vector space of $d \times d$ symmetric real matrices, the set of positive ones is a convex cone $\mathcal{C}_d^+$. Finally, explicit expressions for the two stratum spaces are:

$$\{CS\}_d = \mathcal{L}_d \| GL_d(R), \quad \{BC\}_d = \mathcal{C}_d^+ \| GL_d(Z). \tag{5}$$

In dimension $d = 2, 3$, $|\{CS\}_d| = 4, 7$, $|\{BC\}_d| = 5, 14$.

When the crystal of a chemical element has only one atom per fundamental cell of its lattice L (e.g. the alkaline metals), its space group is the semi-direct product $L \rtimes \mathrm{Aut}(L)$. The crystal space group S is a subgroup of it when there are several atoms in the fundamental cell of L and the point group $P = S/L$ can be any subgroup of Aut(L). So the conjugacy classes of all possible point groups are the conjugacy classes $[P]_{GL_d(Z)}$ of all finite subgroups $P \in GL_d(Z)$; they are called *arithmetic classes*, [ITC] p. 719. The macroscopic aspects of the symmetry of a crystal are essentially classified by the corresponding $[P]_{O_d}$ classes; they are called the *geometric classes.*
In dimension $d = 2, 3$, $|\{AC\}_d| = 13, 73$, $|\{GC\}_d| = 10, 32$.
The number of arithmetic classes corresponding to the same geometry class varies from 1 to 2, 1 to 5, in dimension 2, 3. The usual notation for the arithmetic classes is that of [ITC]; it is good and we shall use it. To each arithmetic class $[P]_{GL_d(Z)}$ corresponds a unique space group, semi-direct [5] product $L \rtimes P$. There may also correspond other space groups [6] with same quotient S/P.
For $d = 2, 3$ the number of space groups per arithmetic class varies from 1 to 3, 1 to 16.

Diffraction experiments (with X-rays, neutrons, electrons,...) by periodic crystals show the *reciprocal lattice* $2\pi L^*$ where L^* is the dual lattice [7]

$$L^* = \{\vec{\ell}^* : \forall \ell \in L, \vec{\ell}^*.\vec{\ell} \in Z\}. \tag{6}$$

It is interesting to use for L^* the dual basis of that of L:

$$\vec{b}_i^*.\vec{b}_j = \delta_{ij}, \quad \text{then} \quad q(L^*) = q(L)^{-1}. \tag{7}$$

[3] As intersection of the compact O_d and the discrete $b^{-1}\,GL_d(Z)\,b$ subgroups of $GL_d(R)$.

[4] That explains why we introduced the orthonormal basis $\vec{e}_u$ "provisorily"

[5] These 13, 73 space groups are said to be "symmorphic" in crystallography.

[6] They are called non-symmorphic groups in crystallography, non trivial extensions in mathematics.

[7] This concept was also introduced by Bravais, [BRA850].

We are interested by experiments measuring the functions over the Brillouin zone, i.e. the Fourier transforms of functions over the space of L. The Brillouin zone (=BZ) is the dual group of the translation lattice: it is generally denoted in mathematics by $\hat{L}$ and it is isomorphic to U_1^d. Let us be more explicit for some readers. In the Euclidean geometry, to perform the Fourier transform of functions we use the unitary irreducible representations $\vec{k}$ of the translation group: $R^d \ni \vec{x} \mapsto \exp(i\vec{k}.\vec{x})$. The set of the representations $\vec{k}$ is a group, that of the reciprocal vector space $\sim R^d$. The situation is different for the lattice of translations:

$$L \ni \ell \xrightarrow{\vec{k}} e^{i\vec{k}.\vec{\ell}} = e^{i(\vec{k}+\vec{K}).\vec{\ell}}, \quad \forall \vec{K} \in 2\pi L^*. \tag{8}$$

This shows that the set of unitary irreducible representations of the translation lattice L is the set $\{\vec{k} \bmod 2\pi L^*\}$. It is a group isomorphic to $R^d/2\pi L^* \sim U_1^d$ and it is called the Brillouin zone of L (in shorthand we will write: $BZ(L)$).

In solid state physics, BZ's were introduced as the fundamental cell of the lattice $2\pi L^*$ with symmetry $\mathrm{Aut}(L^*)$ in [BRI31]. They are defined as the set of points nearest to the origin than to any other point of the lattice; their boundary corresponds to an equality of distance (to the origin and to another lattice point). Obviously the origin is symmetry center of the cell. The torus topology is obtained by identifying opposite faces. These cells had been introduced in the XIXth century. Dirichlet was first to study them in 2 dimensions; for 3 Bravais classes: diclinic (generic case), c-orthorhombic and hexagonal, the cells are an hexagon with a symmetry center and inscriptible in a circle; for the 2 other Bravais classes, p-orthorhombic, quadratic, they are rectangles, squares. In dimension 3, they were studied by Fedorov [FED885] who found the 5 combinatorial types of these centrosymmetric polyhedrons with 6,8,12,12,14 faces respectively; all faces have a symmetry center and either 4 or 6 edges. For 3 Bravais classes the lattices may have 3 different combinatorial types of cells, for 2 other Bravais classes, 2 types and for the 9 others, a unique type (see e.g. [DEL74] or [MIC95]). Here we need only the BZ group law $\sim U_1^d$; so, to obtain general results, we do not need to consider several different cases corresponding to the different types of Brillouin cells of a space group. Since, by definition, the translations of L act trivially on $BZ(L)$, a space group S acts on its $BZ(L)$ only through its point group $P = S/L$, i.e. the action depends only on the arithmetic class. This action preserves the group law of BZ; for instance, for any $m > 0$, the number of elements which satisfy $m\vec{k} \equiv 0 \bmod 2\pi L^*$ is m^d and for each m they form a union of P-orbits.
Time reversal, T, tranforms a unitary irreducible representation of the translation lattice L, into its complex conjugate, i.e. it exchanges $\pm\vec{k} \bmod 2\pi L^*$ on the BZ. The only BZ elements invariant by this transformation satisfy $-\vec{k} \equiv \vec{k} \bmod 2\pi L^*$, equivalent to $2\vec{k} \equiv 0 \bmod 2\pi L^*$; as we have seen there are 2^d of them. Since the elements in a neighbourhood of every such points is not invariant by the exchange $\vec{k} \leftrightarrow -\vec{k}$, by theorem 3 we obtain:

Lemma 1. *The 2^d points of the Brillouin zone satisfying $2\vec{k} \equiv 0 \bmod 2\pi L^*$ are extrema of every continuous function invariant by S and T.*

Forty five years ago, in a famous paper using Morse theory, Van Hove [VHO53] pointed out the existence of at least 2^d extrema for every Morse function on BZ and he showed how they are related to what is now called the Van Hove singularities. He did not used T invariance, so he did not know their positions. Several papers, as [PHI56-58] extended this study to some space groups. Since that time it seems that this problem has been completely forgotten. I gave its general solution last year in a short note [MIC96]; the results were presented in two tables which are reproduced here as tables 1 ($d = 2$) and 2 ($d = 3$). A correction has been made in the last case (common to $Im\bar{3}$, $Im\bar{3}m$) of the second table: by a stupid oversight I had not applied theorem 5 to it.

As said before, for $d = 2, 3$ there are 13, 73 arithmetic classes, each one corresponding to a different action of the points groups. For the 7, 24 classes containing $-I_d$, T invariance does not

cr. syst.	sg	Bc	arithm. class		$k=0$	$2k=0$	$3k=0$	nb	$0,2$	1	$2,0$	$Q(t)$
diclinic	2	6	$p2$	$p1$	O	R,A,B		4	1	$1,1$	1	0
ortho-	5	4	pmm	pm	O	R,A,B		4	1	$1,1$	1	0
rhombic	2	6	cmm	cm	O	R,AB		4	1	2	1	0
square	1	4	$p4$		$[O]$	$[R],AB$		4	[1]	2	[1]	0
	2	4	$p4m$		$[O]$	$[R],AB$		4	[1]	2	[1]	0
hexa-	2	6	$p6$	$p3$	$[O]$	RAB	$[CC']$	6	[2]	3	[1]	1
gonal	3	6	$p6m$	$p3m1$ $p31m$	$[O]$	RAB	$[CC']$	6	[1]	3	[2]	t

Table 1. *Extrema common to all functions on the two dimensional Brillouin zone, invariant by the crystallographic group and time reversal.*
Column 1 gives the crystallographic system; each contains one Bravais class except the orthorhombic one which contains two: *pmm* and *cmm*. Column 2 gives the number of corresponding space groups. Column 3 indicates the number of sides of the geometrical Brillouin cell. Columns 4,5 list respectively the arithmetic class containing $-I$, and those which yield that arithmetic class when $-I$ is added to them. Column 6,7,8 list the critical orbits. When the Brillouin cell has 6 sides, the 3 points satisfying $2k=0$ are the middle of them; the 2 points $3k=0$ represent the 6 vertices. We choose R to correspond to the pair of shrinking symmetric edges when the Brillouin zone is transformed into a 4 side one (rectangle). Then R represents the four vertices and is invariant by the full point group. The points of the orbits between [ ] have to be maxima or minima because the stabilizer acts as a 2-dimensional representation irreducible on the real. Column 9 gives the minimal number of extrema. Columns 10 to 12 give the critical orbits of extrema, labelled by their number of points, with a given Morse index. Column 13 gives the corresponding $Q(t)$ (defined in (3)).

give stronger consequences. For the other classes, adding T invariance is equivalent to replace the point group by the direct product $P \times Z_2(-I_d)$. So we have only 7+24 applications of Morse theory to work out, with the method sketched at the end of §1b, in order to obtain the complete solution. The strata of the action of P on BZ where first given in the fundamental paper [BOU36] for the 3 cubic Bravais classes. For the other ones they have been given in many books (at least for $d=3$) with different notations for the geometric elements of the Brillouin cells.

Tables 1, 2 show that the extrema common to all invariant functions have known positions and in 2, 7 cases, their number is larger than 4, 8. Moreover, for 6 other 3-dimensional cases Morse theory requires for each function the existence of at least 2,4 or 6 other extrema (their stratum is known when the number of these extrema is the smallest possible). Finally, in dimension 2, for the square and hexagonal systems we know that the center and the 4, 6 vertices of the Brillouin cell (respectively 1 point orbit, 2 point orbit of the BZ) are maxima or minima of all invariant functions; the middle of the edges are also critical points and, for functions on BZ with the minimal number of extrema (4,6 respectively), these critical points have Morse index 1 (saddles). The $d=3$ cubic system contains 3 Bravais classes: P, F, I; we know for the 8, 14, 10 critical extrema common to all functions the position of those which have to be maxima-minima (see table 2): the sign cannot be determine by symmetry arguments but by the physics dynamics! The full geometrical discussion (similar to the one done here for $d=2$) for the five types of Brillouin cells is postpone to a future publication (soon available).

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	1,1,1,1,1,1,1				8	1	$1+1+1$	$1+1+1$	1	0
m 6	$P2/m$	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
or 6	$Pmmm$	1	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				$8+(2)$	1 $1+1$	4 4	$1+1+(2)$ $1+(2)$	1 1	t $1,t^2$
14	$Immm$	1	1,2,2,2	2 W			10	1 2	$2+2$ $2+2$	$2+2$ $1+2$	1 1	t $1,t^2$
tt 6	$P4/m$ $P4/mmm$	1	1,1,1,2,2				8	1	$1+2$	$1+2$	1	0
14 $\overline{12}$	$I4/m$ $I4/mmm$	1	1,2,4	2 P			10	1 2	4 4	$2+2$ $1+2$	1 1	t $1,t^2$
rh 14 12	$R\bar{3}$ $R\bar{3}m$	1	1,3,3				8	1	3	3	1	0
hx 8	$P\bar{3}$ $P\bar{3}1m$	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 $\{2\}$	$2t$ $1+t, t(1+t)$ $1+t^2$
8	$P\bar{3}m1$ $P6/m$ $P6/mmm$	1	1,3,3		2 K	2 H	12	1 2 2	$2+3$ $2+3$ $1+3$	$2+3$ $1+3$ $1+3$	1 1 2	$2t$ $1+t, t(1+t)$ $1+t^2$
cu 6	$Pm\bar{3}$ $Pm\bar{3}m$	[1]	[1],3,3				8	[1]	3	3	[1]	0
14	$Fm\bar{3}$	[1]	3,4	$\{6\}c$			$8+\{6\}$	[1] [1]	3 4	$\{6\}$ $\{6\}$	4 3	$3t^2, 3$ $t+2t^2, 2t+t^2$
14	$Fm\bar{3}m$	[1]	3,4	6 W			14	[1] [1]	3 4	6 6	4 3	$3t^2, 3$ $t+2t^2, 2t+t^2$
12	$I\bar{3}m$ $Im\bar{3}m$	[1]	[1],6	$[2]P$			$10+(6)$	[2] [2]	(6) 6	6 (6)	$[1]+[1]$ $[1]+[1]$	$1+2t+t^2$

Table 2. 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 exists (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 stabilizer 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 $Q(t)$.

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§3 The general form of functions on the Brillouin zone invariant by S.

This section presents the strategy and some results of a work in progress with Jaisam Kim and Boris Zhilinskii; the manuscript will soon be finished. We study the 7, 24 rings of functions $\mathcal{F}^P_{BZ}$ and give a minimal set of generators for 7, 16 of them.

The BZ's are tori, so they have a global system of coordinates. As we said after theorem 4 the extension of this theorem applies to them; hence we can limit ourselves to rings of polynomials. There are theorems of Mostow [MOS57] and Palais [PAL57] which tell that a smoth action of a compact group on a compact manifold can be linearized. We did it and found that the dimensions of the linear representations we obtained for our problems are: 4,6 for $d = 2$ and 6,8,12 for $d = 3$. The rings have so many generators for the F and I Bravais classes that we do not intend to study them (at least in our announced paper).

We first recall what is known for the ring of polynomial invariants for n-dimensional vector space V_n on which the finite group G acts through a linear orthogonal representation ρ by summarizing a Molien paper [MOL897] one hundred years old. The character $\chi^{(m)}(g)$ of the m^{th} completely symmetrized tensor power of this representation is given by the generating function:

$$\sum_{m=0}^{\infty} \chi^{(m)}(g) t^m = \det(I_n - t\rho(g))^{-1}. \tag{9}$$

If x_j, $1 \leq j \leq n$ are the coordinates of V_n, the coordinates of the m^{th} order completely symmetrized tensor of the representation are homogeneous n variable polynomials of degree m. We denote by R_m the vector space of these polynomials; then

$$\dim R_m = \binom{m+n-1}{m}. \tag{10}$$

The dimension r_m of the subspace R_m^G of invariant polynomials is obtained by taking the component of $\chi^{(m)}$ on the character $\chi(g) = 1$ of the trivial representation. We denote by M_G the generating function of r_m; using 2(1) we obtain the Molien function:

$$r_m = \dim R^G_m = |G|^{-1} \sum_{g \in G} \chi^{(m)}(g), \text{ so } \sum_{m=0}^{\infty} r_m t^m = M_G(t) = |G|^{-1} \sum_{g \in G} \det(I_n - t\rho(g))^{-1}. \quad (11)$$

It is a rational function of t of the form:

$$M_G(t) = N_G(t)/D_G(t), \quad (12)$$

with

$$D_G(t) = \prod_{i=1}^{n}(1 - t^{d_i}), \ \prod_{i=1}^{n} d_i = \beta|G|, \ 1 \leq \beta \in Z, \quad N_G(t) = 1 + \sum_{s=1}^{\nu} \gamma_s t^s, \ 0 \leq \gamma_s \in Z. \quad (13)$$

It is known now that a form of the Molien function [8] corresponds to the structure of Macauley algebras, i.e. the ring of invariant polynomials R^G is a $N_G(1) = (1+\nu)$-dimensional free module over a polynomial ring $P_n[\theta_i]$. Explicitly there exist n algebraically invariant polynomials θ_i of degrees:

$$1 \leq i \leq n, \ \text{degree}(\theta_i) = d_i, \quad (14)$$

and $P_n[\theta_i]$ is the ring of n-variable polynomials. The basis of the module is formed by $N_G(1)$ homogeneous G-invariant polynomials φ_α, with $\varphi_0 = 1$ and γ_s polynomials are of degree s. These invariant polynomials φ_α form a ring:

$$0 \leq \alpha, \beta, \gamma \leq \nu, \qquad \varphi_\alpha \varphi_\beta = \sum_\gamma p_{\alpha\beta\gamma} \varphi_\gamma, \quad p_{\alpha\beta\gamma} \in P_n[\theta_i]; \quad (15)$$

i.e. the coefficients $p_{\alpha\beta\gamma}$ are polynomials in variables θ_i. So the algebra R^G is the set of polynomials:

$$\theta_i, \varphi_\alpha \in P_n[x_1, \ldots, x_n], \quad R^G = \{\sum_{\alpha=0}^{\nu} p_\alpha(\theta_i)\varphi_\alpha\}, \quad \text{with } \varphi_0 = 1, \quad (16)$$

where the p_α are arbitrary n variable polynomials. The module determined by n algebraically independent polynomials θ_i and ν polynomials ϕ_α satisfying (15), is denoted here by:

$$\theta_i, \varphi_\alpha \in P_n[x_1, \ldots, x_n], \quad R^G = P_n[\theta_1, \ldots, \theta_n] \bullet (1, \varphi_1, \ldots, \varphi_\nu). \quad (17)$$

Remark that the explicit expressions of the polynomial invariants depend on the basis chosen for V_n.

This choice depends on the coordinates on the BZ. The bases $\vec{b}^*_i$ in the reciprocal space satisfy the following conditions: the middle of the two basis vectors coincide with the middle of an edge of the Brillouin cell and $\vec{b}^*_1.\vec{b}^*_2 \leq 0$. The 2 coordinates of the points in the BZ are the angles $k_i \bmod 2\pi$; we use the shorthand $c_i = \cos k_i$, $s_i = \sin k_i$. I have no place to explain here the choice of bases for $d = 3$ and, in all cases, the linearization of the actions of the point groups which produces the representation $\rho(P)$. Let R^P the ring of polynomials invariant by $\rho(P)$. In V_n the image of the BZ is an algebraic variety defined by $n - d$ polynomial equations which are sometimes non homogenuous: they form an ideal $\mathcal{B}$ of R^P. The quotient $R^P/\mathcal{B}$ is the ring of invariant polynomials

[8] That is not necessarily the most simplified form of this rational function.

	class	θ_1	θ_2	φ_1	φ_2	φ_3
	$p1$	c_1	c_2	s_1	s_2	$s_1 s_2$
*	$p2$	c_1	c_2	$s_1 s_2$		
	pm	c_1	c_2	s_1		
*	pmm	c_1	c_2			
	cm	$c_1 + c_2$	$c_1 c_2$	$s_1 + s_2$	$s_1 s_2$	$c_1 s_2 + c_2 s_1$
*	cmm	$c_1 + c_2$	$c_1 c_2$	$s_1 s_2$		
*	$p4$	$c_1 + c_2$	$c_1 c_2$	$(c_1 - c_2) s_1 s_2$		
*	$p4mm$	$c_1 + c_2$	$c_1 c_2$			
	$p3$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_1^{-+}	ϕ_2^{--}	$\phi_3^{+-} = \phi_1^{-+} \phi_2^{--}$
	$p3m1$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_1^{-+}		
	$p31m$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_2^{--}		
*	$p6$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$	ϕ_3^{+-}		
*	$p6mm$	$c_1 + c_2 + c_1 c_2 - s_1 s_2$	$c_1 c_2 (c_1 c_2 - s_1 s_2)$			

$$\phi_1^{-+} = s_1 + s_2 - (c_1 s_2 + c_2 s_1), \quad \phi_2^{--} = (c_1 - c_2)(s_1 + s_2) - (c_1 + c_2 - 2c_1 c_2)(s_1 - s_2),$$

$$(\phi_1^{-+})^2 = 1 - 2\theta_1 + \theta_1^2 - 4\theta_2. \quad (\phi_2^{--})^2 = 2 + 4\theta_1 + \theta_1^2 + 20\theta_2 - 2\theta_1^3 + 20\theta_1\theta_3 - \theta_1^4 + 4\theta_1^2\theta_2 - 4\theta_2^2$$

Table 3. *Modules of invariant polynomials on the Brillouin zone for the 13 arithmetic classes in dimension 2.* Time reversal restricts to the seven cases indicated by * .
Remark the compatibility with the chain of subgroups $p2 < cmm < p6m$, and $cm < p3m1$. Let us denote by $cm' = Z_2(-(cm))$ the group generated by the reflection through an axis orthogonal to that of the reflection of (cm); its invariants are obtained from those of cm by changing s_2 into $-s_2$. So we remark also the compatibility with $cm' < p31m$.
This table should be quoted as table 8 of the paper *The algebra of real invariant functions on the Brillouin zone* by J.S. Kim, L. Michel, B. Zhilinskii (to be published).

in c_i, s_i on BZ. We found that these rings are also modules. Here I will give only the final result for the 13 2-dimensional arithmetic classes: see table 3. It is interesting to check how the invariants given in this table satisfy table 1.

§4 Conclusion.

The applications of the results presented here are obvious. What seems to me more important is to point that these results apply to functions only and that in physics we observe also multivalued functions; I have already given some results for them in [MIC97] explaining the work I am doing with Josuah Zak. The branches of multifunctions describe the branches of vibration or electron energy bands in solids. For the latter, Zak [ZAK80] has introduced the concept of *elementary band representations*: they are induced from an irreducible representation $\rho(S_w)$ of the stabilizer in S of a point w belonging to a maximal (closed) stratum (=Wyckoff position) of our space. This necessary condition is not sufficient; a complete classification of the equivalence classes of these representations has been given in [BAC88] (we should have included time reversal and considered *corepresentations*) as well as the number b of branches: $b = \dim(\rho(S_w)).|P|/|G_w|$. Presently Zak and I are trying to prove the conjecture: *The graph of an elementary band is connected.*

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