Extrema of P-invariant functions on the Brillouin zone

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at a Colloquium in memory of Léon Vanhove

Abstract. This paper studies the number of extrema (and their positions) of a countinuous Morse function on the Brillouin zone, when it is invariant by the point group symmetry of the crystal. Forty years ago, Vanhove had shown the importance of this problem in physics, but he could use only the crystal translational symmetry. In that case Morse theory predicts at least eight extrema. With the added use of general symmetry arguments we show that this number is larger for six of the 14 classes of Bravais lattices; moreover it is possible to give the position of the extrema (and their nature) for 30 of the 73 arithmetic classes. This paper is written for a larger audience than that of solid state physicists; it also defines carefully the necessary crystallographic concepts which are generally poorly understood in the solid state literature.

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At the Colloquium in honor of Léon Van Hove it was very moving to speak of him who died one year before, and to hear all what was said of this great physicist by his friends and his wife. This is an expanded version of the given lecture. It starts from the exposition of a paper that Léon Van Hove wrote nearly forty years ago. This paper was extremely original and important; it is still often quoted.

0 Content.

This paper studies the extrema of continuous functions on the Brillouin zone when they have the symmetry of the point group of the crystal. It starts first by recalling an historical paper which emphasized the importance of such study.

1 One of the famous papers of Léon Van Hove.

In 1952 Léon Van Hove wrote a very original paper: "The occurence of singularities in the elastic frequency distribution of a crystal" (VHO53) which has become a classic. The frequency distribution function $g(\nu)$ is important for the thermodynamical, acoustical, optical properties of a crystal. A computation by E. Montroll (MON47), for a two dimensional square lattice had shown that $g(\nu)$ has two logarithmically infinite peaks [1]. M. Smollett (SMO52) had just extended this work, with the same type of lattice, for ionic crystals with long range Coulomb forces and obtained the same types of singularities. He had noted that these singularities were due to the *existence of saddle points for the function $\tilde{\nu}(k)$ expressing the frequency of an elastic plane wave in terms of its wave vector* [2] *k* of the Brillouin zone [3]. And Van Hove wrote: *The main object of the present paper is to point out that the existence of such saddle points in the $\nu(k)$ function, far from being accidental, is necessarily implied by the periodic structure of the lattice.* Indeed in part 3 of his paper he

[1] Remark that these physically very important analytic singularities did not appear in previous computations with the Born von Karman approach which replaces the "infinite" crystal by a finite one with periodic boundary conditions. Born von Karman approach is still widely used by solid state physicists, although it misses important topological aspects in physics; see e.g. BAC88, MIC92.

[2] In this introduction, italics indicate verbatim quotation of Van Hove's paper except that we use for the wave vectors, instead of q, the notation k which is traditional now.

[3] This paper wants to be very explicit and also to be written for a larger audience than that of solid state physicists. We precise that only the translational crystal symmetry is taken in account in Van Hove's paper and we give the definition of the Brillouin zone in this footnote and in the equation 5.3. The group of translational symmetries of the crystal in d (=2,3) dimensional space R^d, is a vector lattice L which is isomorphic to the additive group of sets of d integers: $\vec{t} = (t_1, \dots, t_d) \in L \sim Z^d \subset R^d$. The unitary irreducible representations of this Abelian group are of the form $\vec{t} \mapsto \exp(i\vec{k}.\vec{t})$ where $\vec{k}.\vec{t} = \sum_j k_j t_j$, $1 \le j \le d$, $t_j \in Z$ and the k_j are d real numbers defined modulo 2π which label the elements of $\hat{L}$ the set of irreducible representations of L. Remark that $\hat{L}$ is a group, isomorphic to U_1^d (that of the sets of d phases) that physicists call the Brillouin zone B and mathematicians, the "dual group" $\hat{L}$ of L. It is true that physicists consider also a geometric aspect of the Brillouin zone, as a fundamental domain of the dual lattice L^* of L, but for the physical problems considered here, only the group aspect of B is relevant (and too often forgotten in the physics literature). Indeed every function on the crystal may be developped in terms of the irreducible representations of L.

explains Morse theory and applies it to the function $\tilde{\nu}(k)$: in dimension d it must have at least 2^d extrema, all of them but two are saddle points. Van Hove finishes part 1 (the introduction) by predicting that in general, for dimension three, *$g(\nu)$ remains continuous whereas $dg/d\tilde{\nu}$ has infinite discontinuities*, [4] one at each extremum of $\tilde{\nu}(k)$.

In fact the "function" $\tilde{\nu}(k)$ has ad branches corresponding to the number of vibration modes of a crystal in d dimensions with a atoms per unit cell (whose volume is v). We denote by S_ν the ad-branch surface (of dimension $d-1$) of the Brillouin zone made of the points k satisfying the equation $\tilde{\nu}(k) = \nu$. Then:

$$g(\nu) = \frac{v}{ad} \int_B \delta(\nu - \tilde{\nu}(k)) d^d k = \frac{v}{ad} \int_{S_\nu} \frac{1}{|\nabla \tilde{\nu}(k)|} dS_\nu, \text{ with } |\nabla \tilde{\nu}(k)| = \sqrt{\sum_j \left(\frac{\partial \tilde{\nu}}{\partial k_j}\right)^2}. \qquad 1.1$$

From this equation, we see that when $\nabla \tilde{\nu}(k) = 0$ the corresponding singularity of $g(\nu)$ depends on the dimension. In section 2 of his paper Van Hove makes a more detailed study of these singularities for non degenerate extrema of $\tilde{\nu}(k)$, i.e.

$$\frac{\partial \tilde{\nu}(k)}{\partial k_i} = 0, \quad \det \frac{\partial^2 \tilde{\nu}(k)}{\partial k_i \partial k_j} \neq 0, \qquad 1.2$$

Van Hove shows that the function $g(\nu)$ has a logarithmic singularity for saddle points and a finite jump for a maximum or minimum in two dimensions; in three dimensions, it is the derivative of $g(\nu)$ which has an infinite singularity for any kind of non degenerate extremum of $\tilde{\nu}(k)$. In section 3 (the longest), Van Hove explains Morse theory and the application to his problem. Several times in the paper, and again in part 4, the conclusion, he points out that for special interactions there might be degenerate extrema with stronger singularities. He remarks [5] that the whole paper can be transposed to the density of states function for the electron energy bands. Indeed, few months before, a two dimensional computation of this density function by Coulson and Taylor (COU52) found the very singularities listed by Van Hove. Nowadays, these logarithmic singularities in the density of electron states might be a (partial) explanation of high temperature supraconductivity which is indeed two dimensional.

Van Hove did not study the influence of the point symmetry of the crystals, except that he remarked that *saddle points of the same type will often correspond to the same frequency*. This is right for about half of the possible crystal symmetries (for example for cubic P or trigonal crystal lattices) but, as we will show in this paper, for the other symmetries the function $\tilde{\nu}(k)$ must have more extrema.

Soon physicists tried to complete Van Hove paper by taking into account the crystal point symmetry (e.g. PHI56, PHI58), but this was not done systematically and was not very succesful. Indeed the physicists considered naturally the fundamental domain of the point group on the Brillouin zone: this is an orbifold, and they had to invent Morse theory for this case; it now exists but it is somewhat cumbersome. From 1969 I developped an efficient method for studying the extrema of functions invariant by some symmetry MIC70, MIC71 and applied it, often in collaboration, to different domains of physics: minima of Higgs potentials, symmetry change in second order phase transitions, Rydberg states of molecules, etc... One of these papers treat the irreducible representations of point groups: MIC78. I gave a general review of this method in MIC80 but nobody applied it to the present problem.

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4 In contradiction with Smollett who had announced logarithmic singularities for $g(\nu)$ in dimension three.

5 As pointed out long before by C. Herring, who is thanked in the paper.

It is time to do it in this paper! We will specialize the method to the particular problem here and be as self contained and elementary as possible. It will be even necessary to precise some points in crystallography which are often poorly or even wrongly explained, even in the best manuals: the relevant concept needed here is that of arithmetic class. We will give thorough explanations for dimension two, (less rich than dimension 3). Finally, for the 13, respectively 73 (in fact 31), arithmetic classes in 2 and 3 dimensions, we will give the minimal number of extrema of various kind for a continuous invariant function on the Brillouin zone, and its more general form. Nevertheless we will also be careful to help the reader who would wish to apply the same method to another problem, by indicating in foot notes more general mathematical properties than those strictly necessary here.

2 Morse theory.

Consider a smooth (=indefinitely differentiable) real valued function f on a real compact manifold M with a coordinate system [6] $\{x_i\}$, $1 \leq i \leq d = \dim M$. If at a point $m \in M$ of coordinates x_i the function satysfies an equation similar to 1.2: vanishing gradient, non vanishing determinant of the Hessian, we say that it has a non degenerate extremum. Then by a change of coordinates $\{x_i\} \mapsto \{y_i\}$, in a neighbourhood of m the function can be transformed into $f = \sum_i \varepsilon_i y_i^2$ with $\varepsilon_i = \pm 1$. The number of signs – is independent from the coordinate tranformation and it is called the Morse index μ of this non degenerate extremum: for instance $\mu = 0$ for a minimum, $\mu = d$ for a maximum and the intermediate values correspond to the different types of saddle points. A function on M with all its extrema non degenerate is called a Morse function. Let c_k the number of its extrema of Morse index k; these numbers are finite and satisfy the relations 2.3 and 2.4 below; these relations are expressed in terms of the Betti numbers of M. The Betti number b_k is defined as the rank of the k^{th} homology group of M. Intuitively b_k is the maximal number of k-dimensional submanifolds of M which cannot be transformed into one another or into a submanifold of smaller dimension; for instance for the sphere S_d of dimension [7] d, $b_0 = b_d = 1$ and all the others b_k vanish. More generally one has the Poincaré duality: $b_k = b_{n-k}$. It is interesting to introduce the Poincaré polynomial $P_M(t)$ of the manifold M:

$$d = \dim(M), \quad P_M(t) = \sum_{i=0}^{d} b_k t^k; \quad \text{e.g. } P_{S_d}(t) = 1 + t^d. \tag{2.1}$$

The Poincaré polynomial of a topological product of manifolds is the product of the Poincaré polynomials of the factors. For instance a d-dimensional torus is the topological product of d circles (1-dimensional spheres):

$$T_d = S_1^d \Rightarrow P_{T_d}(t) = (1+t)^d \Rightarrow b_k(T_d) = \binom{d}{k}. \tag{2.2}$$

For Morse functions on a compact manifold M it was known that:

$$\sum_{k=0}^{d} (-1)^{d-k}(c_k - b_k) = 0 \Leftrightarrow \sum_{k=0}^{d} (-1)^{d-k} c_k = \sum_{k=0}^{d} (-1)^{d-k} b_k \stackrel{\text{def}}{=} \chi(M); \tag{2.3}$$

[6] In general a single coordinate system cannot be defined on the whole manifold, but this is possible on the Brillouin zone.

[7] An example of S_d is the boundary of the unit ball in the $d+1$ dimensional Euclidean space.

the integer χ is called the Euler Poincaré characteristic. Note that for a torus $\chi = 0$. Note also that χ and the total number of extrema are either both even or both odd [8]. To 2.3 Morse added the inequalities MOR27:

$$0 \leq \ell < d: \quad \sum_{k=0}^{\ell} (-1)^{\ell-k}(c_k - b_k) \geq 0 \qquad \Rightarrow c_k \geq b_k. \qquad 2.4$$

The last inequalities are *not* equivalent to Morse inequalities, but they give lower bounds to the number of extrema of a Morse function. For the Brillouin zone:

$$d = 2, \quad c_0 \geq 1, \ c_1 \geq 2, \ c_2 \geq 1; \qquad d = 3, \quad c_0 \geq 1, \ c_1 \geq 3, \ c_2 \geq 3, \ c_3 \geq 1. \qquad 2.5$$

From Poincaré duality one verifies that 2.3 and 2.4 yield the same conditions on c_k and c_{n-k}; it has to be so from the consideration of the pairs $f, -f$ of Morse functions. For the Brillouin zone, equations 2.3 and 2.4 are equivalent to:

$$d = 2, \quad c_0 - c_1 + c_2 = 0; \quad c_0 \geq 1 \leq c_2, \ c_0 + 1 \leq c_1 \geq c_2 + 1, \qquad 2.6$$

$$d = 3, \quad c_0 - c_1 + c_2 - c_3 = 0; \quad c_0 \geq 1 \leq c_3, \ c_1 \geq c_0 + 2, \ c_2 \geq c_3 + 2. \qquad 2.7$$

By looking at the set of points $m \in M$ for which $f(m)$ has a given value, one can define for continuous functions extrema and their type; for instance, by looking at a geographical map with level lines which are continuous (and have any type of singularities for their derivatives), one recognizes immediately a summit (around it, level lines are topologically equivalent to concentric circles) from a pass (two level lines intersect). So Morse theory has been extended to continuous Morse functions with singularities in their derivatives. It has also been extended to unbounded functions with values $+\infty$ or $-\infty$; these values can be replaced by finite maxima or minima respectively [9]. We do need these extensions for the applications to solid state physics.

3 Finite group actions on a compact manifold: the closed strata.

Symmetry groups enter in physics through their actions. Every mathematical structure M has a group of automorphism; an action of the group G on M is defined by a group homomorphism $G \xrightarrow{\theta} \mathrm{Aut}\, M$. For instance if M is a set, a vector space, an Euclidean space, a Hilbert space, a manifold, a Riemann manifold, etc... $\mathrm{Aut}\, M$ is respectively the group of permutations of the elements of M, the general linear group on M, the Euclidean group, the unitary group, the group of diffeomorphisms of M, the group of isometries of M , etc... The action is effective if $\ker\theta = 1$, i.e. no group element $\neq 1$ acts trivially on M. When M is a vector space, θ defines a linear representation of G (in that case we also say, when $\ker\theta = 1$ that the representation is faithfull). Instead of using $\theta(g)(m)$ for the transform of $m \in M$ by $g \in G$, we shell use the shorter notation $g.m$ when there are no ambiguity about the action of G which is considered.

Given a group action $G \xrightarrow{\theta} \mathrm{Aut}\, M$, one defines the *orbit* $G(m)$, the set of points of M transforms of $m \in M$. Remark that two distinct orbits have no common points. One also defines the *stabilizer* G_m, i.e. the set of elements of G which leave m fixed: $g.m = m$; they form a subgroup of G. Let $m' = h.m$; then $(hgh^{-1}).m' = m'$ for all $g \in G_m$: this shows that

$$G_{h.m} = hG_m h^{-1}. \qquad 3.1$$

[8] For instance $\chi(S_2) = 2$ and 2.3 tells for the earth: "the number of mountain summits minus the number of passes plus the number of lakes plus one (for all communicating oceans) is two"; a direct proof is easy.

[9] More recently Morse theory has also been generalized to functions invariant by a compact group (so finite groups are a particular case) WAS69. However this is not the best adapted method for our problem.

In a orbit the set of stabilizers form a conjugate class of G-subgroups. We say that orbits are of the same type when they have the same conjugate class of stabilizers [10] . The union of orbits of the same type is called a *stratum*; equivalently m' belongs to S_m, the stratum of m, if and only if $G_{m'}$ and G_m are conjugate. This decomposition in strata is the most natural and useful for physics since it corresponds to classify the points of M according to their symmetry. For instance the Wyckoff positions of the ICT (=international crystallographic tables HAH83) are the strata of the action of the space group on the $d = 2, 3$ dimensional Euclidean space [11]. Let us consider another example: the natural [12] three dimensional representation of $O_h \equiv m\bar{3}m$ (see the ICT), the symmetry group of the cube. It has $|O_h| = 48$ elements. Its seven strata are: the origin (stabilizer O_h), the 3 fourfold symmetry axes (perpendicular to the cube faces), the 4 threefold symmetry axes (=the diagonals of the cube), the 6 twofold symmetry axes (joining the middles of two opposite edges), all these axes with the origin removed (the corresponding stabilizers are: C_{4v}, C_{3v}, C_{2v}), the 3 symmetry planes parallel to the cube faces and the 6 symmetry planes, each containing two diagonals, without the origin and the rotation axes they contain, the corresponding stabilizers forming two distinct conjugation classes of groups C_s, and finally the three dimensional complement of the symmetry planes, which is the open dense stratum of points with trivial stabilizer [13].

We use the following notations for the set of orbits and the set of strata in the action of G on M:

$$\text{orbit space}: \ M|G; \qquad \text{stratum space}: \ M||G. \tag{3.2}$$

Remark that for a given group action, $M||G$ can be identified to a subset of $\{[.]_G\}$ the set [14] of conjugation classes of subgroups of G. There is a natural partial ordering of the subroups of a group defined from the inclusion: $H < K$ meaning that H is subgroup of K; this partial order on the set of G-subgroups has a unique maximal element G and a unique minimal element 1, the trivial subgroup of G. For finite groups [15] , there is also a partial ordering on the set $\{[.]_G\}$ by subgroup inclusion up to a conjugation. If there are no fixed points in the action of G on M, in general the stratum space will contain several maximal strata, i.e. strata with maximal symmetries. But it is a theorem [16] that for the action of a finite goup G on a manifold M, there is a *unique* stratum with minimal symmetry; moreover this stratum is open dense in M.

Let M be a compact smooth manifold of dimension d. The action of G on M transforms the tangent planes of M into themselves [17]. More precisely, if $T_m(M)$ denotes the tangent plane of M at m, the group element g transforms $T_m(M)$ into $T_{g.m}(M)$. In particular, this defines at each point $m \in M$ a linear representation of G_m on $T_m(M)$. A vector field on M is a function v which

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[10] Given a subgroup H of G and $g \in G$, one calls left, right cosets of H in G, the G-subsets gH, Hg. The set of left,right cosets are denoted respectively $G : H$, $H : G$. By multiplication on the left,right by elements of G, they form a G-orbit that we often consider as prototypes of the G-orbits whose conjugate class of stabilizers is that of H.

[11] Another example: in the action of the Lorentz group on space time(=Minkowski space), outside the zero vector (an orbit and a stratum by ifself) there are three strata, those of time-like, space-like and light-like vectors.

[12] In the solid state literature, this representation is also called the "vector" representation.

[13] For a detailed study of the orbits, strata, invariants and covariants vector fields of the representations of the closed subgroups of O_3, see JAR84.

[14] To explain this notation: { } means the set of elements defined inside the bracket; we denote by $[H]_G$ the class of subgroups conjugate to H in G and when we remplace H by a dot, we mean "any subgroup".

[15] More generally this is true for all groups G such any strict subgroup $K < G$ cannot be conjugate (in G) to one of its strict subgroup $H < K < G$.

[16] Finite groups are compact Lie groups of dimension zero. This theorem was first proven for compact groups in MON57. It has been extended in PAL61 to the actions of a non compact group, when all stabilizers are compact.

[17] Technically, one says that the action of G on M extends to $T(M)$, the tangent bundle of M.

associates to each point $m \in M$ a vector $v(m) \in T_m(M)$. A G-covariant vector field satisfies:

$$\forall g \in G,\ \forall m \in M,\ g.v(m) = v(g.m); \qquad 3.3$$

To a Riemaniann metric on M corresponds an orthogonal scalar product on each tangent plane. Averaging it by the finite (or compact) group yields an invariant Riemann metric; from now on we assume its existence.

We denote respectively by $T_m(G.m) \subseteq T_m(S_m) \subseteq T_m(M)$ the tangent plane at m of the orbit of m, the stratum of m, the manifold and by $N_m(G.m) \supseteq N_m(S_m)$ the corresponding normal planes; so $T_m(G.m) \overset{\perp}{\oplus} N_m(G.m) = T_m(S_m) \overset{\perp}{\oplus} N_m(S_m) = T_m(M)$. The gradient at m of any G-invariant function $f(m) = f(g.m)$, is orthogonal to the orbit and tangent to the stratum, i.e.

$$\nabla f(m) \in F_m = T_m(S_m) \cap N_m(G.m). \qquad 3.4$$

The natural d-dimensional orthogonal representation of G_m on $T_m(M)$ is reducible and respects the decomposition:

$$T_m(M) = T_m(G.m) \overset{\perp}{\oplus} F_m \overset{\perp}{\oplus} N_m(S_m). \qquad 3.5$$

This representation is trivial on F_m; on $N_m(S_m)$ it does not contain the trivial representation; the representation of G_m on $T_m(G.m)$ does not depend on the specific action of G on Ξ: it is the restriction of the adjoint representation of G to the subgroup G_m and to the subspace $G_m^{\perp}$ (where $\perp$ is defined by the Cartan Killing metric of the Lie algebra of the compact group G). When G is finite, $T_m(G.m) = 0$, and $N_m(G.m) = T_m(M)$ so equation 3.5 simplifies to

$$G \text{ finite},\ T_m(M) = T_m(S_m) \overset{\perp}{\oplus} N_m(S_m). \qquad 3.5'$$

Strata with maximal symmetry are closed. If they contain a finite number of orbits, at any of their point $F_m = 0$ and 3.4 shows that $\nabla f(m) = 0$. Those orbits isolated in their strata are called "critical"; indeed MIC71 *every one of them is an orbit of extrema for* **every** *G-invariant function* [18] on M. On every closed stratum containing an infinity of orbits, every G-invariant function has at least two orbits of extrema MIC70.

For a crystal with point group P, these two results yield a minimum number μ of extrema for a P-invariant function on the Brillouin zone: it is the sum of the number of points of all critical orbits + the sum, for each closed stratum with an infinity of orbits, of $2|G.m|$ (where $|G.m|$ denote the number of points of the orbit $G.m$). Let us write this as an equation: we label the closed strata by the index α and denote them either $CS_\alpha^{\nu_\alpha}$ where ν_α is the (finite) number of its orbits, or CS_α^∞. Then the minimum number of extrema of any invariant functions for the action of P on the Brillouin zone is:

$$\mu = \sum_{\alpha, CS_\alpha^{\nu_\alpha} \in \mathcal{S}} \nu_\alpha |G.m_\alpha| + \sum_{\alpha, CS_\alpha^\infty \in \mathcal{S}} 2|G.m_\alpha| \qquad 3.6$$

where m_α is any point of CS_α and $\mathcal{S}$ is the stratum space. For many point groups P, μ is larger than 8 for $d = 3$ or 4 when $d = 2$. Moreover, for all point groups we will have to check if this minimal number μ of extrema is compatible with 2.6 and 2.7 (Morse inequalities) [19].

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[18] For instance: you know the symmetry of a problem and you write an invariant Lagrangian whose extrema give you the "good" spontaneous symmetry breaking; most likely you are on a critical orbit, and any invariant Lagrangian would have given you the same result as a verification of this theorem! So you have to test your model on more selective features.

[19] The method is similar to the one introduced in MIC78 for the invariant functions on the unit sphere of the irreducible representations of the point groups

We can extend the method of arguments we used for the gradient to the Hessian at $m \in M$

$$\mathcal{H}_{ij}(f(m)) \stackrel{\text{def}}{=} \frac{\partial f^2(m)}{\partial k_i \partial k_j} \tag{3.7}$$

of the invariant function f expressed in a local system of coordinates k_i of M. Indeed, at the point m, for any function, the Hessian is transformed by the isotropy group G_m as a quadratic form. So for an invariant function, it has to be invariant:

$$\forall g \in G_m,\ D(g)\mathcal{H}(f(m))D(g)^{-1} = \mathcal{H}(f(m)), \tag{3.8}$$

where $g \mapsto D(g) = D(g^{-1})^\top$ is the linear orthogonal representation of G_m on $T_m(M)$. When m belongs to a critical orbit, $F_m = 0$ and we have shown that this representation does not contain the trivial one. Moreover when G is finite, $T_m(G.m) = 0$ so $T_m(M) = N_m(S_m)$ and this representation might be irreducible on the real. If it is so, we have the lemma:

Lemma 3.1 *When the symmetry group G is finite, if at a point m of a critical orbit the orthogonal representation of G_m on $T_m(M) = N_m(S_m)$ is irreducible on the real, then $G.m$ is either an orbit of minima or of maxima for* **every** *G-invariant function.*

Indeed a (real) symmetric matrix which commutes (see 3.8) with every matrix of a group representation irreducible on the real must be a multiple of the identity [20] , so all eigenvalues of the Hessian are of the same sign.

4 Bravais classes, crystallographic systems, arithmetic classes, geometric classes.

Among its symmetries a periodic [21] ideal [22] crystal has a discrete translation group isomorphic to Z^d; it is a lattice that we denote by L (see footnote 3). In dimension d, the discrete group $L \sim Z^d$ is generated by a basis $\tilde{b} \equiv \{b_i\}$, $1 \leq i \leq d$ of the d-dimensional (real) vector space; we consider $\tilde{b}$ as the matrix of the d components of the d basis vectors. The condition of linear independence of the basis vectors is equivalent to $\det \tilde{b} \neq 0 \Leftrightarrow \tilde{b} \in GL_d(R)$. We shall denote by $\mathcal{B}_d$ the manifold of $GL_d(R)$; it describes also the set of bases of the d-dimensional vector space and the set of all bases of all d-dimensional lattices. All possible bases of L are obtained from $\{b_i\}$ by linear transformations $m\tilde{b} \equiv \sum_j m_{ij}b_j$ with integral coefficients which have an inverse with the same property: i.e. $m \in GL_d(Z)$. We can also say that two bases $\tilde{b}$, $\tilde{b}'$ generate the same lattice if, and only if, the matrices $\tilde{b}, \tilde{b}'$ are in the same right coset of $GL_d(Z)$ in $GL_d(R)$. Hence we can identify the set $\mathcal{L}_d$ of lattices with the orbit (the notation was defined in foot note 10)

$$\mathcal{L}_d = GL_d(Z) : GL_d(R) \tag{4.1}$$

which is a d^2-dimensional manifold. We can give another equivalent interpretation of the same facts: the maps on $GL_d(R)$, $g \xrightarrow{m} mg$ defined for all $m \in GL_d(Z)$ define an action of $GL_d(Z)$ on $\mathcal{B}_d$ and each orbit is the set of bases of a given lattice, so the manifold $\mathcal{L}_d$ of d-dimensional lattice is the orbit space:

$$\mathcal{L}_d = \mathcal{B}_d | GL_d(Z) \tag{4.1'}$$

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[20] We remind the reader that if this representation, irreducible on the real, is reducible on the complex, there are antisymmetric matrices commuting with all the matrix $D(g)$; their square is a symmetric matrix λI with $\lambda < 0$.

[21] Since 1984, SHE84 crystals with icosahedral point symmetry and many others have been discovered; they are not quasi-crystals but genuine crystals; however they are aperiodic, i.e. they have no translational symmetry.

[22] By ideal we mean that the defects and the boundaries are neglected so the crystal extends infinitly in all directions.

The orthogonal group [23] O_d acts on the manifold $\mathcal{L}_d$ of all lattices; the orbit $O_d.L$ of the lattices transformed of L can also be considered as the set of all possible positions of the "abstract" [24] lattice L; the latter can be given for instance by the Grammian of a basis (the dot denotes the orthogonal scalar product):

$$b_i.b_j = (\tilde{b}\tilde{b}^\top)_{ij}. \qquad 4.2$$

This matrix [25] does depend on the choice of basis of L but it is invariant by orthogonal transformations: $r \in O_d$ transforms the basis $\tilde{b}$ into $\tilde{b}r = \tilde{b}^{-1\top}$. Moreover the multiplication on the right of $\tilde{b} \in GL_d(R)$ by r can be applied to the right cosets of 4.1; it yields the explicit action of O_d on $\mathcal{L}_d$; so the double cosets $GL_d(Z) : GL_d(R) : O_d$ represent

$$\mathcal{L}_d^o = GL_d(Z) : GL_d(R) : O_d, \qquad 4.3$$

the set of all d-dimensional lattices up to an orthogonal transformation [26].

The lattice L is invariant by an orthogonal transformation $r \in O_d$ if the transformed basis $\tilde{b}' = \tilde{b}r$ is again a basis of L, i.e.

$$m \in GL_d(Z), \tilde{b} \in GL_d(R), r \in O_d, \qquad m\tilde{b} = \tilde{b}r. \qquad 4.4$$

which is equivalent to:

$$m\tilde{b}r^\top = \tilde{b} \Leftrightarrow m = \tilde{b}r\tilde{b}^{-1}. \qquad 4.4'$$

This shows that the symmetry group [27] H_L of the lattice L is the intersection in $GL_d(R)$ of $GL_d(Z)$ and a subgroup conjugated to O_d; therefore it is finite [28].

There are several interpretations of 4.3 in terms of group action $\tilde{b} \mapsto m\tilde{b}r$. It describes the action of the direct product $GL_d(Z) \times O_d$ on $\mathcal{B}_d$ (the manifold on $GL_d(R)$). The stabilizer of $\tilde{b} \in \mathcal{B}_d$ is the holohedry H_L given by 4.4' as a "diagonal" subgroup of $GL_d(Z) \times O_d$. We will respectively denote by H_L^z, H_L^o the projections of H_L on the two factors $GL_d(Z)$ and O_d. Equation 4.3 also describes the action of $GL_n(Z)$ on $GL_d(R) : O_d = \mathcal{C}^+(\mathcal{Q}_d)$ (see footnote 25); this action can also be written:

$$\forall m \in GL_d(Z), \forall q \in \mathcal{C}^+(\mathcal{Q}_d), \quad \tilde{b} = q \mapsto m\tilde{b}\tilde{b}^\top m^\top = mqm^\top. \qquad 4.5$$

The stabilizers are the H_L^z and by definition the strata of this action are the Bravais [29] classes BRA50; to summarize:

$$\mathcal{L}_d^o = \mathcal{C}^+(\mathcal{Q}_d)|GL_d(Z), \quad \{BC\}_d = \mathcal{C}^+(\mathcal{Q}_d)||GL_d(Z), \qquad 4.6$$

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[23] Of the Euclidean space in which lays the crystal.

[24] The situation is similar in elementary geometry: we can consider a triangle or this triangle independently of its position, i.e. up to an Euclidean transformation in the plane. This "abstract" triangle is then completly defined by the lengths of its three edges.

[25] Remark that $b_i.b_j$ is a positive quadratic form. The set of $d \times d$ positive quadrative forms is a convex cone $\mathcal{C}^+(\mathcal{Q}_d)$ in the d^2 dimensional vector space of $d \times d$ matrices. It is well known that the real symmetric positive matrices, e.g. $\tilde{b}^\top\tilde{b}$ have a unique real symmetric positive square root that we denote by $\sqrt{\tilde{b}^\top\tilde{b}}$ and any $\tilde{b} \in GL_d(R)$ have unique left and right polar decomposition: $\tilde{b} = r\sqrt{\tilde{b}^\top\tilde{b}} = \sqrt{\tilde{b}\tilde{b}^\top}r, \quad r \in O_d$. So $\mathcal{C}^+(\mathcal{Q}_d) = GL_d(R) : O_d$.

[26] Instead to consider the set $\mathcal{L}_d^o$, of position of lattices it is often more interesting to consider the set $\mathcal{L}_d^{od}$ of lattice up to a similitude (an orthogonal transformation and a dilation); for this replace O_d by the group of similitudes $O_d \times R^\times$.

[27] Wich is called the "holohedry" of L in crystallography.

[28] As an intersection of a discrete subgroup and a compact subgroup.

[29] In the same year 1850 appeared two works which stimulated the study of lattices: the Bravais classification of lattices in $d = 2, 3$ dimensions and the introduction by Hermite HER50 of the manifold $\mathcal{L}_d^o$ for an arbitrary dimension d and the search of densest sphere packing on lattices. Hermite did not use the word lattice, but the definition of $\mathcal{L}_d^o$ of 4.6.

where $\{BC\}_d$ is the set of Bravais classes in dimension d. For $d = 1, 2, 3, 4$ there are 1, 5, 14, 64 Bravais classes.

Finally 4.3 can also be interpreted as the action of O_d on $\mathcal{L}_d$ (defined in 4.1). The stabilizers are the H_L^o and the strata are called Bravais crystal systems [30] in the ICT (=international crystallographic tables **HAH83**):

$$\mathcal{L}_d^o = \mathcal{L}_d|O_d, \qquad \{BCS\}_d = \mathcal{L}_d||O_d. \tag{4.7}$$

In an ideal periodic crystal the atoms are not at rest: their motion around average positions increases as function of the temperature. The use "atom position" (or sometimes, "atom") is a short for this average of positions. To say that the group L (a lattice of translation vectors) is a symmetry of the (ideal) crystal means that for each atom position a, the orbit $L.a$ is an Euclidean [31] lattice. If the crystal contains only one Euclidean lattice of atom positions, its symmetry group (one says its space group) is the semi-direct product $G = L \rtimes H_L^z$. But in the general case a crystal contains several Euclidean lattices of atoms of different kinds and the space group G is the largest subgroup of the Euclidean group which transforms the Euclidean lattices of identical atoms into themselves. In general G is not a semi-direct product (crystallographers say G is not "symmorphic"). By its definition, the discrete translation group L is an invariant subgroup of G and the quotient $P_z = G/L$ is a subgroup of H_L^z.

In crystallography, the conjugation class of P_z in $GL_d(Z)$ is called an arithmetic class. Conversely, any finite subgroup F of $GL_d(Z)$ leaves invariant some positive definite quadratic forms; indeed, it is easy to prove that q^F defined from any positive quadratic form q by:

$$F < GL_d(Z), \quad q = q^\top > 0, \quad q^F = \sum_{m \in F} mqm^\top; \tag{4.8}$$

is F-invariant; it is also definite positive as a sum of definite positive quadratic forms. So the set $\{AC\}_d$ of arithmetic classes in dimension d is the set of conjugation classes of finite subgroups of $GL_d(Z)$. Jordan JOR80 showed that this set is finite for any d. The number of arithmetic classes (which is also the number of symmorphic space groups) is respectively [32] 2, 13, 73, 710 for $d = 1, 2, 3, 4$. For a given dimension d, there is a partial ordering on the arithmetic classes (by subgroup inclusion up to a conjugation). The number of maximal arithmetic classes is respectively 1, 2, 4, 9, 17 for the first five dimensions. Maximal arithmetic classes are Bravais classes.

Finite subgroups of $GL_d(Z)$ are conjugate in $GL_d(R)$ to subgroups of O_d. One can prove that finite subgroups of O_d, conjugated in $GL_d(R)$ are conjugated [33] in O_d. So there is a natural map

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[30] In the crystallographic literature, there are several inequivalent definitions of crystallographic systems ($=CS$); the first introduced one, in 1815, is due to Weiss WEI15; that introduced here (=BCS) is often called French crystallographic system, e.g. BRO78. These two definitions are not equivalent for the distribution of crystal space groups among the different crystallographic systems, but they define the same list of holohedries H_L^o so the sets $\{CS\}$ and $\{BCS\}$ have the same number of elements in any dimension: explicitly 1, 4, 7, 33 for $d = 1, 2, 3, 4$.

[31] A Euclidean lattice is a closed discrete subset set of points in an Euclidean space which is an orbit of a vector lattice. As for the Euclidean space itself, the Euclidean lattice has no distinguished point, (no origin), so it is not a group!

[32] Curiously, many mathematiciens give 70 for the number of arithmetic classes in dimension 3: e.g. WEY52, SPE56, NEW72.

[33] Here is the proof. Assume $g, g' \in O_d$ conjugate by $s \in GL_d(R) : g' = sgs^{-1}$. Let $s = rt$, $r \in O_d$, $t = \sqrt{s^\top s} = t^\top$ the polar decomposition of s. Then $I = g'^\top g' = (s^\top)^{-1} g^\top t^2 g s^{-1}$, i.e. $t^2 = g^{-1} t g g^{-1} t g$. Since the positve square root of t^2 is unique, $t = g^{-1} t g$, i.e. $gt = tg$ and $g' = sgs^{-1}$ becomes $g' = rgr^{-1}$.

ϕ between the arithmetic classes and the conjugation classes of finite subgroups of O_d. It is an order preserving map between these two partially ordered sets. Those in the image of ϕ are called "geometric classes" in crystallography. In the correspondence:

$$\{AC\} \xrightarrow{\phi} \{GC\}; \quad \phi(P_z) = P_o, \qquad 4.9$$

often several arithmetic classes correspond to the same geometric class; beware that if the latter is a holohedry $P_o = H_L^o$, all the arithmetic classes in the preimage $\phi^{-1}(P_o)$ are not necessarily Bravais classes. As we will see, this already occur for $d = 3$. In dimension $d = 1,2,3,4$, the number of geometric classes is respectively 2, 10, 32, 227. For the dimensions $d = 2,3$ the ICT (international crystallographic tables) distinguish the different arithmetic classes mapped by ϕ to the same geometric class; first one letter is added in front of the symbol of the geometric class in order to distinguish the different possible types of lattices: this letter is p or c in dimension 2 and one of the letters P, C, F, I, R in dimension 3. When this is not sufficient, some permutation is made among the elements (letters or digits) of the geometric class symbol [34] ; for an example in dimension 2, see 6.6.

5 **Strata of the action of the point group P_z on the Brillouin zone.**

Before specializing to dimension 2,3, we want to give some general reults on this subject. Let $P_z < GL_d(Z)$ be the arithmetic class of a crystal. As soon as a basis $\tilde{b}$ of the vector space R^d is chosen, P_z is represented by a set $\{m\}$ of integral matrices which define a linear representation of P_z; it transforms the translation lattice L in itself; P_z acts on the dual space R^{d*} of R^d by the contragredient representation: $m \mapsto (m^\top)^{-1} \equiv (m^{-1})^\top$ and transforms in itself the dual lattice L^*, which is defined by:

$$\vec{k} \in L^* \Leftrightarrow \forall \vec{t} \in L, \; \vec{t}.\vec{k} \in 2\pi Z. \qquad 5.1$$

Indeed:

$$\forall \vec{t} \in L, \forall \vec{k} \in L^*, m \in H_L^z, \; m\vec{t}.(m^\top)^{-1}\vec{k} = \vec{t}.\vec{k}. \qquad 5.2$$

The contragredient representation of P_z, that we denote by $(P_z^\top)^{-1}$, might belong to an arithmetic class distinct from that of P_z and both correspond to the same geometric class. We have recalled in footnote 3 that dual group $\hat{L} = R^{d*}/L^* \sim U_1^d$ is called the Brillouin zone (denoted by B here):

$$B \stackrel{\text{def}}{=} \hat{L} = R^{d*}/L^* \sim U_1^d. \qquad 5.3$$

However most physicists consider B *only* as a fundamental domain of L^*, i.e. as a geometric realisation of the orbit space $R^{d*}|L^*$. The group $(P_z^\top)^{-1} < GL_d(Z) \sim \mathrm{Aut}(U_1^d)$ defines the natural action of P_z on the Brillouin zone. One obtains explicitly this action for all arithmetic classes by restriction of the action of the holohedry H_L^z for each Bravais class. Given an R^d basis: $\{b_i\}$ which generates L, one defines the dual basis $\{b_j^*\}$ of R^{d*} by

$$b_i.b_j^* = \delta_{ij}. \qquad 5.4$$

In this basis the components of the vectors $\vec{k} \in L^*$ are multiples of 2π. And from the definition of the Brillouin zone recalled in 5.3, its elements, that we denote by k are described by a set of d real numbers defined modulo 2π. That correponds to an additive notation for the group B. For

[34] In dimension 3, the maximum number of arithmetic classes mapped by ϕ on the same geometric class is 5. This occurs for $C_{2v} = mm2$; the corresponding arithmetic classes are: $Pmm2, Cmm2, Amm2, Fmm2, Imm2$ (the use of the A lattice occurs only in this case).

instance its elements of order 2 are defined by the equation $2k = 0$ (in multiplicative notation they are the square roots of the identity); their components are either zero or π. So there are 2^d elements which satisfy $2k = 0$, the origin 0, invariant by the holohedry and the $2^d - 1$ elements of order 2 which must be transformed into each other by H_L^z.

There are dozens of physics books which give the complete list of little groups and orbits which appear in the action of the holohedry on B for the 14 Bravais classes, but strangely enough, they give only the geometric class of these little groups although, in cases of ambiguity, physics requires the knowledge of their arithmetic class! This is hard to understand since there are symbols, universally adopted by all crystallographers, for labelling the arithmetic classes. It is worthwhile to add several other facts related to the sociology of crystallographers and physicists. The "international" symbols (devised by Hermann and Mauguin) used by the ICT for labelling the 230 space groups contain enough information for reconstructing exactly the group law [35] , but many physicists prefer to use the original symbols of Schönflies or, for some Russians, of Fedorov, although this symbols are an arbitrary sequential labelling of the space groups of a given geometric class. Moreover the ICT have fixed an arbitrary but universal labelling for the strata (=Wyckoff positions) appearing in the action of the 230 space groups on R^d, $d = 2, 3$. Alas! they do not deal with the 14 Brillouin zones (and with space group representations). Except that the 0 element of B is labelled by Γ in all physics books (is that a progress?), there are no common notations for the strata of the 14 Brillouin zones. And the relations among these strata are never mentionned; they are due to the natural partial ordering [36] of the 14 Bravais classes, but very few physics books give this ordering or they give it with an error: the holohedry H_L^z of the trigonal lattice is not a subgroup of that of the hexagonal lattice [37]; an equivalent error is to pretend that one can deform continuously the hexagonal lattice directly into the trigonal lattice, in contradiction with the original Bravais paper BRA50.

We now prove the lemma:

Lemma 5.1 *Every P_z-invariant function on the Brillouin zone has an extremum at each of the 2^d points defined by $2k = 0$ when the arithmetic class P_z contains $-I$.*

As we have seen the set of these 2^d elements of the group B is a union of orbits of P_z; we show that they are isolated in their stratum and therefore critical. Indeed no other point of B satisfies $2k = 0 \Leftrightarrow -k = k$, so no other point of B has a little group containing $-I$.

In 2 dimensions, $-I_2$ is the rotation by π and in 3 dimensions, $-I_3$ is the symmetry through the origin. In any dimension it belongs to the holohedry of every lattice. In dimension $d = 2, 3$ there are respectively 7, 23 arithmetic classes for which this lemma applies. Moreover for 7 arithmetic classes in dimension 2 and 15 (that of the cubic crystal system) in dimension 3, the group of integral matrices P_z is irreducible on the real, so we can apply the lemma 3.1 to the point $0 \in B$ and to the other points of the critical orbits which have an irreducible little group.

6 Minimal number of extrema of P-invariant Morse functions on the dimension 2 Brillouin zone.

The elements of finite order of O_2 are the rotations by $2\pi/k$ with k a positive integer, and the conjugation class of reflections through an axis, i.e. the orthogonal matrices of determinant 1 and trace 0. The ITC denote the rotations by [38] k and any reflection by m and they use the same symbols for the cyclic groups they generate; the Schönflies notations for these groups (very much used in molecular physics) are respectively C_k, C_s. The other finite subgroups of O_2 form the

[35] Although they are made of 2 to 7 charaters: letter, digit or /.

[36] Obtained by restriction of the ordering of the arithmetic classes.

[37] See figure 7.1; that is true only of their geometric class.

[38] Here we shall sometimes use r_k instead of k.

conjugation classes of dihedral groups generated by a non trivial rotation k and any reflection m; these groups have $2k$ elements and are denoted by km (although mm is preferred to $2m$) in ICT and C_{kv} in Schönflies notations. A necessary condition for a rotation to be conjugated, in $GL_2(R)$, to an element of $GL_2(Z)$ is that tr$k = 2\cos(\pi/k)$ be an integer; this restricts the values of k to $k = 1, 2, 3, 4, 6$. This condition is sufficient as the existence of the representative matrices shows [39]:

$$r_6 = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}, \quad r_4 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad r_3 = r_6^2 = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad r_1 \equiv I = -r_2, \qquad 6.1$$

To summarize: *The 10 geometric classes in two dimensions are:*

$$1 = C_1, \; m = C_s, \; 2 = C_2, \; mm = C_{2v}, \; 3 = C_3, \; 3m = C_{3v},$$

$$4 = C_4, \; 4m = C_{4v}, \; 6 = C_6, \; 6m = C_{6v}\,. \qquad 6.2$$

In two dimensions there are 13 arithmetic classes because there are 3 pairs of arithmetic classes whose image by ϕ are only 3 geometric classes:

$$\phi(pm) = \phi(cm) = m; \quad \phi(pmm) = \phi(cmm) = mm; \quad \phi(3m1) = \phi(31m) = 3m. \qquad 6.3$$

We do not give here a proof of the uniqueness of the arithmetic class for the other seven geometric classes, but we explain each of the three exceptions; indeed this is absolutely necessary for an understanding of crystallography by the non specialist.

i) The matrices:

$$m_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -m_y, \quad m_{xy} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -m_{\bar{x}\bar{y}} \qquad 6.4$$

are not conjugate in $GL_2(Z)$. Indeed the largest common divisor of the elements of an integral matrix is invariant by conjugation in $GL_d(Z)$; the largest common divisors of the elements of $I_2 + m_x$ and $I_2 + m_{xy}$ are respectively 2 and 1. We leave to the reader the proof that there are only two arithmetic classes of reflections: for the most general integral reflection matrix: $\begin{pmatrix} a & b \\ c & -a \end{pmatrix}$, $a^2 - bc = 1$, these two classes are given by the value of $a + b + c \equiv \bmod 2$. These two classes correspond to symmetries through the coordinate axes or through their diagonals and they are respectively denoted by pm, cm in ICT.

ii) The group $C_{2v} = mm$ is generated by two orthogonal symmetries; therefore both belong to the same arithmetic class: either pm or cm, and they generate respectively the groups of the arithmetic classes pmm or cmm. These are two Bravais classes. The first one is that of the "rectangular" lattices: any such lattice is generated by two orthogonal vectors $t_1.t_2 = 0$ of different lengths; its vectors are $t = \mu_1 t_1 + \mu_2 t_2, \mu_i \in Z$. The Bravais class of the sublattice defined by $\mu_1 + \mu_2 \in 2Z$ (i.e. an even number) is cmm; indeed t_1, t_2 do not belong to this new lattice, but $t_1 \pm t_2$ form a basis and these vectors are exchanged, eventually up to a sign, by the reflections of axis t_1 and t_2.

iii) The group $6m = C_{6v}$ has two conjugate classes of 3 reflections (their axes are labelled c, c', c'' and a, b, d in fig. 6.2), each one generates a subgroup $3m = C_{3v}$. These two subgroups are not conjugated in $6m = C_{6v}$ but they are conjugated in O_2; we prove that they are not conjugated [40]

[39] Of course we could have chosen $r_3 = -r_6$.

[40] Indeed, by multiplication by one of the elements of these two $3m = C_{3v}$ subgroups, the O_2 transformation which conjugates them can always be transformed into a rotation by $\pi/6$; such rotation of order 12 cannot be represented by an integral matrix. We also give in the text another, more explicit proof in order to show to the reader the use of integers, so important in crystallography and so ignored in solid state physics text books.

in $GL_2(Z)$. Given two finite group representations $G \ni g \mapsto d_1(g)$, $g \mapsto d_2(g)$, and an arbitrary matrix z, one easily verifies:

$$s(z) = \sum_{g \in G} d_1(g) z d_2(g^{-1}) \;\Rightarrow\; d_1(g)s(z) = s(z)d_2(g) \qquad 6.5$$

Moreover any intertwinning matrix s can be obtained this way: put $z = s|G|^{-2}$ where $|G|$ is the number of elements of G. Here the two representations we consider are the two integral representations of $3m$, generated respectively by r_3, m_{xy} and $r_3, -m_{xy}$ respectively and z is the most general integral matrix $z = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. Then $s(z) = u - m_{xy} u m_{xy}$ with $u = z + r_3 z r_3^{-1} + r_3^{-1} z r_3$; explicitely: $s = (a + 2b - 2c - d)\begin{pmatrix} -1 & 2 \\ -2 & 1 \end{pmatrix}$; whatever the value of the integers a, b, c, d, the determinant of $s(z)$ is a multiple of 3, so $s(z) \notin GL_2(Z)$ and there is no integral matrix which conjugates these two representations of $3m$ on the integers. Following the convention of ICT, we label the two arithmetic classes isomorphic to the geometric class $3m = C_{3v}$ by:

$$p31m = \langle r_3, m_{xy} \rangle, \quad p3m1 = \langle r_3, -m_{xy} \rangle. \qquad 6.6$$

A coordinate independent distinction between these two arithmetic classes is the following property: the space group $L \rtimes p3m1$ is the group generated by the reflections through 3 axes containing the sides of an equilateral triangle [41].

In figure 6.1 we give the two partially ordered sets $\{AC\}_2$ and $\{GC\}_2$ and the order preserving map ϕ.

There are 4 holohedries (they are underlined in fig. 6.1); indeed the two maximal classes $6m$ and $4m$ are holohedries; since $t \in L \Rightarrow -t \in L$, every lattice has the symmetry group $2 = C_2$. To have more symmetry one may add either a reflection or the rotation 3. In the first case the multiplication by $r_2 = -I_2$ gives the orthogonal reflection so the holohedry is $mm = C_{2v}$. As we have already seen, there correspond two Bravais classes pmm, cmm. When the lengths of the orthogonal vectors t_1, t_2 (used above) become equal, the symmetries of these two lattices become both identical to $4m = C_{4v}$ whose Bravais class is denote $p4m$. When the rotation 3 is added to the generic lattice with minimal symmetry 2, it gets the symmetry 6 and it is easy to prove that it has also reflection axes so its holohedry is $6m = C_{6v}$. The table 6.1 gives the traditional names of the 4 crystallographic systems.

Bravais class	$p2$	pmm cmm	$p4m$	$p6m$
Holohedry	$2 = C_2$	$mm = C_{2v}$	$4m = C_{4v}$	$6m = C_{6v}$
Crystallographic system	diclinic	orthorhombic	quadratic	hexagonal

Table 6.1. **Crystallographic systems, holohedries and Bravais classes in two dimension.**

We make the choice of basis corresponding to the matrices of 6.1 and 6.4. The 12 element group $p6m$ is generated by the matrices r_6, m_{xy}, while the 8 element group $p4m$ is generated by r_4, m_{xy}. These last two matrices are orthogonal and therefore equal to their contragredient; $(r_6^\top)^{-1} = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}$. The other P_z groups are subgroups of these two. So we need only to study the action of $p4m$ and $p6m$ on their respective Brillouin zones; we obtain the action of the other groups by restriction.

Outside the generic two dimensional stratum, the action of $p4m$ on B defines 4 strata, 2 of dimension 0, composed of 4 points that we give with their little groups:

$$p4m: \; k_O = (0,0), \; k_R = (\pi, \pi); \quad pmm: \; k_A = (\pi, 0), \; k_B = (0, \pi), \qquad 6.7$$

[41] Among the 17 space groups in dimension 2, only 4 are generated by reflections; they are the symmorphic groups of the arithmetic classes $pmm, p3m1, p4m, p6m$; they are the Weyl group of the Kac Moody Lie algebras $\tilde{A}_1 \times \tilde{A}_1, \tilde{A}_2, \tilde{B}_2, \tilde{G}_2$.

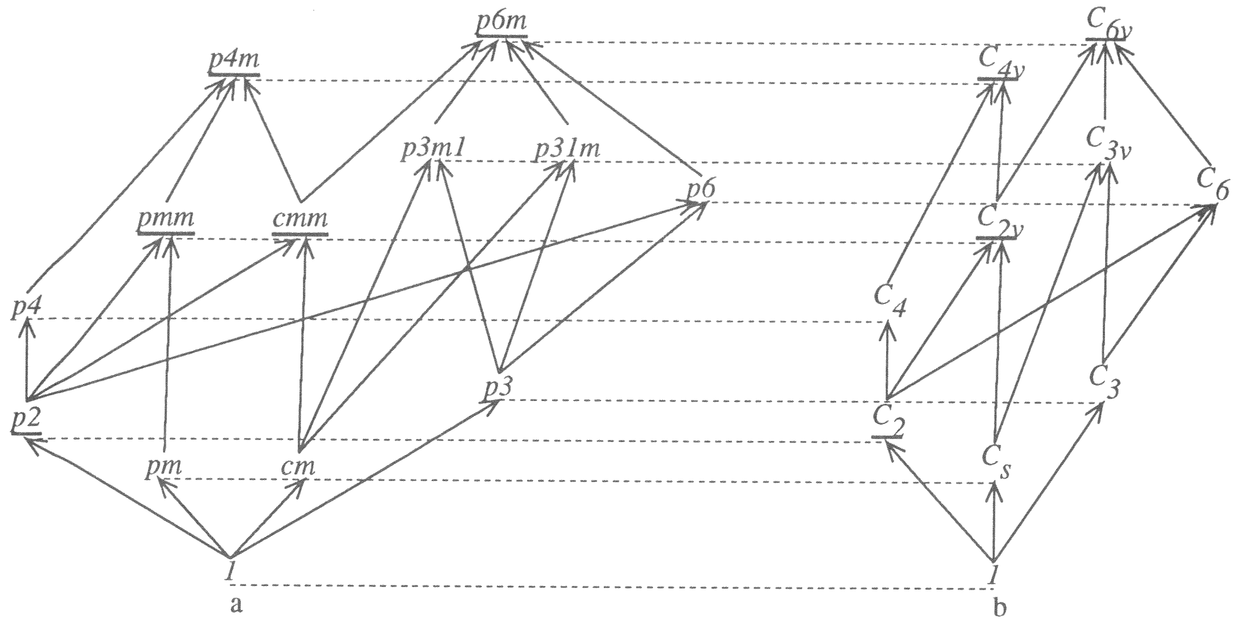

Figure 6.1(a,b). For two dimensional crystallography, the diagram a) shows the partial order on $\{AC\}$, the set of the 13 arithmetic classes and b) shows the partial order on $\{GC\}$, the set of the 10 geometric classes. The dotted horizontal lines explicit the order preserving map $\{AC\} \xrightarrow{\phi} \{GC\}$. The underlined arithmetic classes are the five Bravais classes and the underlined geometric classes are the four holohedries. We use for the arithmetic classes the only existing notation: that of ICT; we use the Schönflies notation for the geometric classes in order to help the reader to make the translation from this notation to that of the ICT.

and 2 strata of dimension 1, composed of 6 circles minus that four points:

$$0 \neq k,\ -\pi < k < \pi, \quad pm:\ a = (k,0),\ a' = (k,\pi);\ pm':\ b = (0,k),\ b' = (\pi,k),$$

$$cm:\ c = (k,k),\ cm_-:\ d = (k,-k). \qquad 6.8$$

The little groups of these one dimensional strata are 2 element groups generated by one reflection:

$$pm = \langle m_x \rangle, \quad pm' = \langle m_y \rangle, \quad cm = \langle m_{xy} \rangle, \quad cm_- = \langle -m_{xy} \rangle. \qquad 6.9$$

The groups pm, pm' and cm, cm_- form two pairs of conjugate little groups.

Outside the generic two dimensional stratum, the action of $p6m$ on B defines 5 strata, 3 of dimension 0, composed of 6 points (the first four ones are defined in 6.7):

$$p6m:\ k_O; \quad cmm:\ k_R,\ cmm':\ k_B,\ cmm'':\ k_A; \quad p31m:\ k_C = (\frac{2\pi}{3}, \frac{2\pi}{3}) = -k_{C'} \qquad 6.10$$

and 2 of dimension 1, composed of 6 circles minus those six points:

$$0 \neq k,\ -\pi < k < \pi, \quad cm_-:\ d = (k,-k), \quad cm'_-:\ b = (0,k), \quad cm''_-:\ a = (k,0), \qquad 6.11$$

for the first stratum, and for the second one, with $0 \neq k \neq \pm\frac{2\pi}{3}$):

$$cm:\ c = (k,k)\ -\pi < k < \pi, \qquad 6.12$$

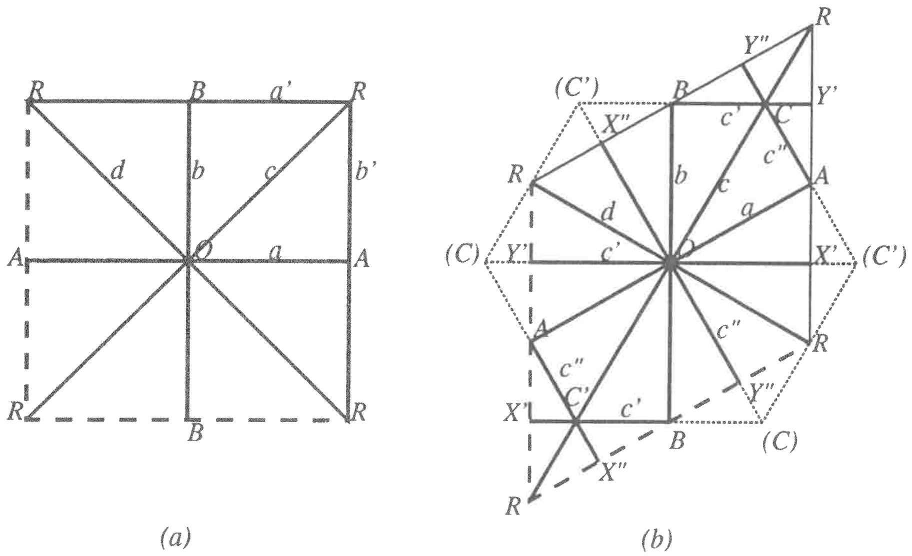

Figure 6.2(a,b). These figures a) and b) show the strata of the Brillouin zones of the maximal arithmetic classes $p4m$ and $p6m$ respectively. In these two Brillouin zones the points and the axes with the same coordinates bear the same label; e.g. AOA, BOB are the coordinates axes. The cooordinates are defined modulo 2π so, on the drawing, they are limited by $-\pi < k_i \leq \pi$, $i = 1, 2$. The figures respect the space metric (so the $p6m$ zone is a rhomb). The Brillouin zones are Abelian groups with neutral element O. The closure of the one dimensional strata form conjugation classes of one parameter subgroups:
$p4m$ Brillouin zone: $\bar{a} \cup \bar{a}', \bar{b} \cup \bar{b}'$ (these 2 conjugated subgroups have 2 connected components) and c, d;
$p6m$ Brillouin zone: c, c'(path $OX'BY'O$),c'' (path $OX''AY''O$) and d, a, b.
With the added dotted lines, fig. b) gives also the hexagonal Voronoï cell. It is otained by translating four triangles $CAY'R$, $CBY"R$, $C'AX'R$, $C'BX"R$ by 2π along the coordinate axes.

$$cm' : c' = \begin{cases} (-2(k+\pi), k) & \text{when } -\pi < k \leq -\frac{\pi}{2}, \text{ BC'X'} \\ (-2k, k) & \text{when } -\frac{\pi}{2} \leq k \leq \frac{\pi}{2}, \; X'OY' \\ (-2(k-\pi), k) & \text{when } \;\; \frac{\pi}{2} \leq k < \pi, \; Y'CB \end{cases} \qquad 6.12'$$

$$cm'' : c'' = \begin{cases} (k, -2(k+\pi)) & \text{when } -\pi < k \leq -\frac{\pi}{2}, \; AC'X" \\ (k, -2k) & \text{when } -\frac{\pi}{2} \leq k \leq \frac{\pi}{2}, \; X"OY" \\ (k, -2(k-\pi)) & \text{when } \;\; \frac{\pi}{2} \leq k < \pi, \; Y"CA \end{cases} \qquad 6.12''$$

The little groups of these one dimensional strata are 2 element groups generated by one reflection:

$$cm = \langle s \rangle, \quad cm' = \langle s' \rangle, \quad cm'' = \langle s'' \rangle, \quad cm_- = \langle -s \rangle, \quad cm'_- = \langle -s' \rangle, \quad cm''_- = \langle -s'' \rangle,$$

$$s = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s' = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}, \quad s'' = \begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}. \qquad 6.13$$

The groups cm, cm', cm'' and cm_-, cm'_-, cm''_- form two triplets of conjugate little groups. Finally the triplet of conjugate little groups of d, b, a are defined as

$$cmm = cm \times cm_-, \quad cmm' = cm' \times cm'_-, \quad cmm'' = cm'' \times cm''_-. \qquad 6.14$$

Figure 6.2 a,b show this decomposition in strata for these two Brillouin zones. The table 6.2 gives the strata composition for the action of the 12 non trivial arithmetic classes P_z. From figure 6.1 we remark that cmm and its subgroups $cm, p2, p1$ belong to both $p4m$ and $p6m$ Brillouin zones.

a'	b'	a	b	d	c	O	R	A	B	C	C'	c'	c''	closed strata
pm	(1)	pm	(1)	(1)	(1)	(pm)	(1)	(pm)	(1)					$\bar{a}, \bar{a}'$
(1)	(1)	(1)	(1)	(1)	(1)	$p2$	$p2$	$p2$	$p2$	(1)	(1)	(1)	(1)	O, R, A, B
(1)	(1)	(1)	(1)	(1)	cm	(cm)	(cm)	(1)	(1)	(1)	(1)	(1)	(1)	$\bar{c}$
(1)	(1)	(1)	(1)	cm_-	cm	cmm	cmm	$p2$	$p2$	(cm)	(cm)	(1)	(1)	O, R, AB
pm	pm'	pm	pm'	(1)	(1)	pmm	pmm	pmm	pmm					O, R, A, B
(1)	(1)	(1)	(1)	(1)	(1)	$[p4]$	$[p4]$	$p2$	$p2$					$[O], [R], AB$
pm	pm'	pm	pm'	cm_-	cm	$[p4m]$	$[p4m]$	pmm	pmm					$[O], [R], AB$
		(1)	(1)	(1)	(1)	$[p3]$	(1)	(1)	(1)	$[p3]$	$[p3]$	(1)	(1)	$[O], [C], [C']$
		(1)	(1)	(1)	(1)	$[p6]$	$p2$	$p2$	$p2$	$[p3]$	$[p3]$	(1)	(1)	$[O], RAB, [CC']$
		cm'_-	cm''_-	cm_-	(1)	$[p3m1]$	(cm_-)	(cm'_-)	(cm''_-)	$[p3]$	$[p3]$	(1)	(1)	$[O], [CC']$
		(1)	(1)	(1)	cm	$[p31m]$	(cm)	(cm'')	(cm')	$[p31m]$	$[p31m]$	cm'	cm''	$[O], [C], [C']$
		cm'_-	cm''_-	cm_-	cm	$[p6m]$	cmm	cmm'	cmm''	$[p31m]$	$[p31m]$	cm'	cm''	$[O], RAB, [CC']$

Table 6.2: *Brillouin zone strata for the actions of the 12 arithmetic classes $P_z \neq 1$ in dimension 2.* The last but one column headlines list the connected components of the non generic strata (see fig. 6.2 a,b and equations 6.7 to 6.14 for their definition). In these columns the table gives the little groups $P_k < GL_2(Z)$ for each stratum of the Brillouin zone. P_z leaves fixed the origin O, so it is given in the 7th column. The last column indicates the closed strata. Except for the arithmetic classes pm, cm, these strata contain only critical orbits; they are given by their points and the orbits are separated by a ",". These orbits are between [ ] when the representation of the stabilizer on the tangent plane is irreducible on the real; then P_k is also between [ ] in the previous columns.
The symbol of P_k is between ( ) in a column when the corresponding part of the Brillouin zone is not a connected component of a stratum but only a strict subset of it. The two element subgroups (generated by one reflection) pm, pm', cm, cm_- and cm, cm', cm'', cm_-, cm'_-, cm''_- are defined in equations 6.9 and 6.13 respectively and the subgroups cmm, cmm', cmm'' in 6.14.
The maximal Bravais classes $p4m, p6m$ have distinct Brillouin zones; this explains the blanks in the table. The Bravais class cmm (to which correspond the arithmetic classes $cmm, cm, p2, 1$) is smaller than both maximal ones.

From table 6.2 (see also fig. 6.1) we can reach the following
Conclusion: *The minimum number of extrema for a P_z invariant Morse function f on the Brillouin zone is 4 (one maximum, one minimum, 2 saddle points) for the 8 arithmetic classes $\leq p4m$ and 6 (1 or 2 maxima, 2 or 1 minima and 3 saddle points) for the 5 arithmetic classes $\geq p3$..*

For each arithmetic class we can give more details and precise for invariant functions with the minimum number of extrema where those are located:
$p4m, p4, pmm$: for these arithmetic classes there are 4 critical points on 3 critical orbits: O, R and the orbit AB. So A and B must be saddle points and therefore the minimum and the maximum are either O, R or R, O. Lemma 3.1 requires that for any $p4m$ or $p4$ invariant function.
$cmm, p2$: any permutation of the critical points O, R, A, B corresponds to the four extrema: one maximum, one minimum, two saddle points.

cm: the circle $\bar{c}$ is the only closed stratum. At each point $k \in \bar{c}$ the normal $N_k(\bar{c})$ is orthogonal to the gradient and is an eigendirection of the Hessian; the correponding eigenvalue has a fixed constant sign for all $k \in \bar{c}$. The restriction of f to $\bar{c}$ has one maximum and one minimum; so this corresponds for the whole function to a saddle point and either a maximum or a minimum. It is possible for f to have only 2 other extrema outside $\bar{c}$.
pm: there is one closed stratum with two connected components, the circles $\bar{a}, \bar{a}'$. By the same argumentation than the previous case there must be a saddle point on each circle and the maximum on one of them and the minimum on the other.
1: only the translational symmetry; this is the case considered by Van Hove.
$p6m, p6$: from lemma 3.1 we know that the two points of the critical orbit C, C' are either maxima and minima, then O is the unique minimum or maximum; the critical orbit R, A, B carries the 3 saddle points.
$p3m1$: same conclusion as the preceding case for C, C' and O. The three saddle point form one 3 point orbit; so each of the 3 circle $\bar{d}, \bar{a}, \bar{b}$ carries a saddle point; those could again be R, AB.
$p31m$: same as the previous case for the 3 saddle points, except that they must be on the circles c, c', c'' (they still can be R, A, B); any permutation of the three fixed points O, C, C' must carry one maximum and two minima.
$p3$: same as the previous case for the three fixed points. The rest of B is the generic stratum; it is made of 3 point orbits; anyone can carry the three saddle points.

7 Minimal number of extrema of holohedry invariant functions on the dimension 3 Brillouin zone.

For dimension 3 we first give in table 7.1 the name of the 7 crystallographic systems, their corresponding holohedry and Bravais classes. Those different classes carry the same label that their holohedry H_L^z which is distinguished from the crystallographic system holohedry H_L^o by adding one of the letters P, C, F, I, R in front of the symbol for H_L^o.

BC	P	$P\ C$	$P\ C\ F\ I$	$P\ I$	P	R	$P\ F\ I$
H_L^o	$\bar{1} = C_i$	$2/m = C_{2h}$	$mmm = D_{2h}$	$4/mmm = D_{4h}$	$R\bar{3}m = D_{3d}$	$6/mmm = D_{6h}$	$m\bar{3}m = O_h$
CS	triclinic	monoclinic	othorhombic	tetragonal	trigonal	hexagonal	cubic

Table 7.1. *The 14 Bravais classes (BC) and the 7 crystallographic systems (CS) in dimension 3.* **The holohedries H_L^o of the crystallographic systems are given in ICT and Schönflies notations. For the Bravais classes, we indicate only the first letter (=type of lattice) of their symbol. To have the full symbol one must add the H_L^o symbol in ICT notation.**

In figure 7.1 we give the partial ordering of the sets $\{BC\}$ of Bravais classes and $\{CS\}$ of the crystallographic systems with the increasing map ϕ' between them. Indeed, by their holohedries (defined as little groups) $\{BC\} \subset \{AC\}$ and $\{CS\} \subset \{GC\}$; they acquire by restriction the natural order of $\{AC\}$ and $\{GC\}$; the restriction of the map $\{AC\} \xrightarrow{\phi} \{GC\}$ (defined in 4.9) to $\{BC\}$ defines $\{BC\} \xrightarrow{\phi'} \{Cs\}$.

As we announced after 4.9, the preimage of $\{AC\} \xrightarrow{\phi} \{GC\}$ for a holohedry H_L^o is not necessarily a set of Bravais classes H_L^z. Indeed

$$\phi^{-1}(\bar{3}m = D_{3d}) = \{R\bar{3}m, P\bar{3}m1, P\bar{3}1m\}; \qquad 7.1$$

Of these 3 arithmetic classes, only the first is a lattice holohedry: that of the unique lattice ($R\bar{3}m$) of the trigonal system [42].

[42] There is some confusion in many physics books about this lattice and the distinction between the trigonal

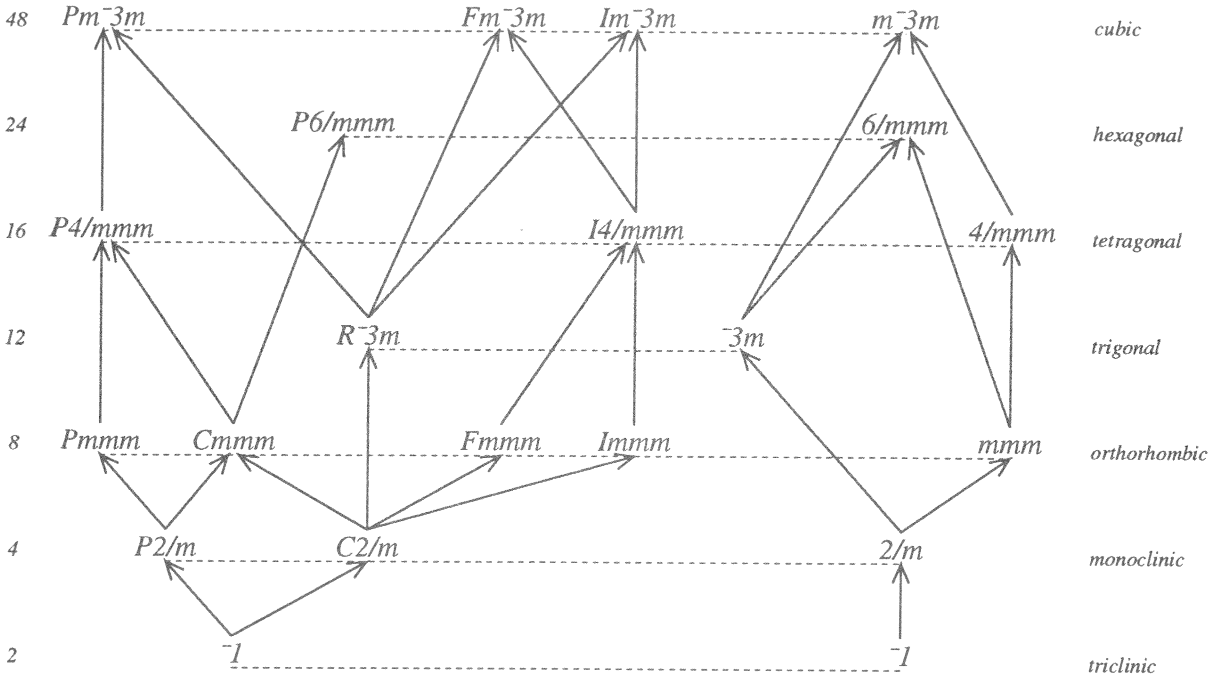

Figure 7.1. For three dimensional crystallography, the diagram a) shows the partial order on $\{BC\}$, the set of the 14 Bravais classes and b) shows the partial order on $\{CS\}$, the set of the 7 Bravais crystallographic systems. The dotted horizontal lines explicit the order preserving map ϕ', the restriction to $\{BC\}$ of the map ϕ defined in equation 4.9.

Since we study only the invariance under the holohedries of the Bravais classes, we know from the lemma 5.1 that in each Brillouin zone, the 8 points solutions of $2k = 0$ belong to critical orbits. One of these orbits is the point $k = 0$; we give the partition in orbits of the 7 points of order 2 in table 7.2 where we also list the other critical orbits: they occur in 5 of the Bravais classes. Only the point groups of the cubic systems have 3 dimensional (real or complex) irreducible representations; in table 7.2 we put between [ ] the five critical points with an irreducible little group; according to lemma 3.1, they have to be maxima or minima.

We see from table 7.2 (column 8) the list of 8 Bravais classes for which there exist holohedry invariant functions on the Brillouin zone with only 8 extrema: one maximum, one minimum and three saddle points of Morse index 1 and 2:

$$\geq 8: \quad \text{triclinic}P; \quad \text{monoclinic}P, C; \quad \text{orthorhombic}P, C; \text{tetragonal}P; \quad \text{trigonal}R; \quad \text{cubic}P. \qquad 7.2$$

For three other Bravais classes we have a minimum of 10 extrema including 8 or 7 saddle points (hence more than the Van Hove number of singularities):

$$\geq 10 = (1,4,4,1) \text{ or } (2,4,3,1): \quad \text{orthorhombic}F, \text{ orthorhombic}I; \text{ tetragonal}I. \qquad 7.3$$

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and hexagonal system. The ICT class these two systems in one "family", each of the five other 3-dimensional crystallographic systems forming a family by itself. But do not confuse crystallographic systems and families! The latter concept has been introduced in order to have a map from $\{GC\}$ the set of geometrical classes, to the set of crystallographic families $\{CF\}$: it can be defined in any dimension as the least coarsed set obtained from $\{BCS\}$ such that the map exists! This shows that this family concept is not very deep and I regret that the ICT have adopted it.

crys. sys	Bravais class	0	$2k=0$	$4k=0$	$3k=0$	$6k=0$	nb	$0,3$	$1,2$	$2,1$	$3,0$
triclinic	$P\bar{1}$	1	$1,1,1,1,1,1,1$				8	1	$1+1+1$	$1+1+1$	1
monoclinic	$P2/m$	1	$1,1,1,1,1,1,1$				8	1	$1+1+1$	$1+1+1$	1
"	$C2/m$	1	$1,1,1,2,2$				8	1	$1+2$	$1+2$	1
orthorhom.	$Pmmm$	1	$1,1,1,1,1,1,1$				8	1	$1+1+1$	$1+1+1$	1
"	$Cmmm$	1	$1,1,1,2,2$				8	1	$1+2$	$1+2$	1
"	$Fmmm$	1	$1,1,1,4$				$8+2$	1	4	$1+1+2$	1
								$1+1$	4	$1+2$	1
"	$Immm$	1	$1,2,2,2$	$2(W)$			10	1	$2+2$	$2+2$	1
								2	$2+2$	$1+2$	1
tetragonal	$P4/mmm$	1	$1,1,1,2,2$				8	1	$1+2$	$1+2$	1
"	$I4/mmm$	1	$1,2,4$	$2(P)$			10	1	4	$2+2$	1
								2	4	$1+2$	1
trigonal	$R\bar{3}m$	1	$1,3,3$				8	1	3	3	1
hexagonal	$P6/mmm$	1	$1,3,3$		$2(K)$	$2(H)$	12	1	$2+3$	$2+3$	1
								2	$2+3$	$1+3$	1
								2	$1+3$	$1+3$	2
								3	$2+3$	$1+2$	1
cubic	$Pm\bar{3}m$	[1]	$1,3,3$				8	1	3	3	1
"	$Fm\bar{3}m$	[1]	$3,4$	$6(W)$			14	1	3	6	4
								1	4	6	3
"	$Im\bar{3}m$	[1]	$1,6$	$[2](P)$			$10+6$	1	6	$1+6$	2
								2	6	6	$1+1$

Table 7.2. *List of the critical orbits of the Brillouin zone B for the actions of holohedries of the 14 Bravais classes, according to the order of $k \in B$; number and Morse index of extrema of H_L^z invariant continuous functions with minimum number of extrema.*

Lemma 5.1 proves that under the action of its holohedry, every Brillouin zone has at least 8 critical points: $k=0$ and the 7 points of order 2; column 4 gives their distribution into orbits. Five Brillouin zones have more critical points: thier orbits are listed (with their usual label) in columns 5,6,7. The points between [ ] have to be maxima or minima (lemma 3.1). The eighth column gives the minimum number "nb" of extrema of invariant functions, giving the number of critical points plus, for two Brillouin zones, the smallest orbit of extrema which must necessarily be added. The last four columns give the number of extrema with a given Morse index.

There is at least one type of saddle point with multiplicity 4, either as 2 two-point orbit for orthorhombic$I$ or as a four-point orbit for the two other Bravais classes.

For orthorhombic$F$ there must always be some extrema on a non critical orbit; the smallest such orbits have 2 points, their little groups are $C2$. In the repartition of this orbit and the five critical ones among the different Morse indices for extrema, in table 7.2 one can exchange $1+1$ and 2. All possible orbit repartitions among the extrema (in minimal number) of Morse index $0,1,2,3$ or $3, 2, 1, 0$ are:

$$\geq 10 = (1,4,1+1+2,1) = (1+1,4,1+2,1) = (2,4,1+1+1,1): \quad \text{orthorhombic}F. \qquad 7.4$$

For the three last Bravais classes the minimum number of extrema is respectively 12, 14, 16 corresponding to a minimum of saddle points of 8,9 or 10, 9 or 10, and 12 or 13. For the hexagonal Bravais class, in the table 7.2 one can permute 3 and $1+2$, so all possible decompostions into orbits are:

$$\geq 12 = (1,2+3,2+3,1) = (2,2+3,1+3,1) = (2,1+3,1+3,2) = (3,2+3,1+2,1) =$$

$$= (1+2,2+3,3,1): \quad \text{hexagonal}P. \qquad 7.5$$

Remark that for the cubic$I$ Bravais class, one of the 6 point orbit is not critical and its little groups are $I4mm$.

We already pointed out (see table 7.2) that, in the three Bravais classes of the cubic system, the point $k=0$ is either a maximum of a minimum for every H_L^z invariant function and this is also the case for the 2 point of the orbit P of the Bravais class cubic$I$. For invariant functions with the minimum number of extrema, the point $k=0$ has also to be a maximum or a minimum in the trigonal$R$ Bravais class.

In crystallography, there is a natural map $\{AC\} \xrightarrow{\gamma} \{BC\}$ from the arithmetic classes to the Bravais classes MIC89. Given an arithmetic class $[P_z]$, the little groups of the action of P_z on the Brillouin zone are obtained from those, denoted here by H, of the action of the holohedry $H_L^z \in \gamma([P_z])$ as the intersection $P_z \cap H$. If these little groups are all non polar (i.e. their vector representation does not contain the trivial representation), every critical point in the action of the holohedry on the Brillouin zone is a critical point for the action of P_z; and no other critical point can appear. So we can immediatly extend to these arithmetic classes the results we have otained for the 14 Bravais classes. These means that we know the minimum number of extrema (and their positions) of P_z invariant functions for the arithmetic classes listed in table 7.3.

P cubic	: $Pm\bar{3}m$ $=O_hP$	$P\bar{4}3m$=T_dP	$P432$ $=OP$	$Pm3$ $=T_hP$	$P23 = TP$
F cubic	: $Fm\bar{3}m$ $=O_hF$	$F\bar{4}3m$=T_dF	$F432$ $=OF$		
I cubic	: $Im\bar{3}m$ $=O_hI$	$I432$ $=OI$	$Im3$ $=T_hI$		
P hexagonal	: $P6/mmm$ $=D_{6h}P$	$P622$ $=D_6P$	$P6/m$=$C_{6h}P$	$P\bar{3}m1$= one of the $D_{3d}P$	
R trigonal	: $R\bar{3}m$ $=D_{3d}R$	$R\bar{3}$ $=C_{3i}R$			
P tetragonal	: $P4/mmm$ $=D_{4h}P$	$P422$ $=D_4P$	$P4/m$=C_{4h}	$P\bar{4}2m$= one of the $D_{2d}P$	
I tetragonal	: $I4/mmm$ $=D_{4h}I$				
P orthorhombic:	$Pmmm$ $=D_{2h}P$	$P222$ $=D_2P$			
C orthorhombic:	$Cmmm$ $=D_{2h}C$				
F orthorhombic:	$Fmmm$ $=D_{2h}F$				
I orthorhombic	: $Immm$ $=D_{2h}I$				
P monoclinic	: $P2/m$ $=C_{2h}P$				
C monoclinic	: $C2/m$ $=C_{2h}C$				
P triclinic	: $P\bar{1}$ $=C_iP$				

Table 7.3 List of the 30 arithmetic classes with known positions of the extrema of invariant Morse functions on the Brillouin zone, when these functions have the minimum possible number of extrema; these

extrema are on the critical points. Among these 30 classes there are the 14 Bravais classes; they are listed in the second column.

In this paper I have not completly fulfilled the program announced in its title since I have determined the minimum number of extrema of P_z invariant functions on the Brillouin zone for only 30 of the 73 arithmetic classes: they are those for which the position of the extrema are known (they are at the critical points). The trivial class $P1$ was treated by Léon Van Hove, but taking account time reversal the result is in fact similar to the Bravais class $P\bar{1}$, i.e. the eight extrema are at the points $k = 0$ and $2k = 0$. Indeed the treatment of the other arithmetic classes is more interesting to physicists when more physical input is introduced. I intend to do it in a lengthy paper or in a book. Meanwhile this paper has treated completly the mathematical problem for dimension two; and it gives to the reader all the tools to treat the other 42 arithmetic classes in dimension three!

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During a one month sojourn at the Technion (Haifa, Israel), I had the opportunity to repeat this lecture. I am grateful to the Physics department of the Technion for its warm hospitality.