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Symmetry, invariants, topology. I

Symmetry, invariants, topology. Basic tools

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Abstract

Elementary concepts of group actions: orbits and their stabilizers, orbit types and their strata are introduced and illustrated by simple examples. We give the unified description of these notions which are often used in the different domains of physics under different names. We also explain some basic facts about rings of invariant functions and their module structure. This leads to a geometrical study of the orbit space and of the level surfaces of invariant functions (e.g. energy levels of Hamiltonians). Combining these tools with Morse theory we study the extrema of invariant functions. Some physical applications (not studied in other chapters) are sketched. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

This chapter introduces the basic concepts and the basic tools to be used in this issue of Physics Reports. The linear representations of groups are a particular case of group actions. The non-linear actions appear naturally in physics: for instance the action of the Euclidean group on the space is not a linear action! That is generally the case for the action of the symmetry group G of a physical problem on the configuration space or on the space of dynamical variables.

In Section 2 we explain the fundamental concepts for the study of group actions. The action of a group G on a space M (let us say for instance a manifold) decomposes M into *strata* which are themselves union of *orbits* of the same type; i.e. they correspond to the different type of "local" symmetry. In all examples we study, the number of strata is finite, so it is so natural to list them.[2] For instance the action of the two-dimensional Euclidean group Eu_2 on the plane defines an action of Eu_2 on the triangles (= triples of distinct points) in this plane; there are three strata: the equilateral, the isosceles and the other triangles. There is only one stratum for the action of Eu_2 on the segments (= pair of distinct points) of the plane and this stratum contains a continuous set of orbits (labeled by the length of the segment), while for the action of the Poincaré group (= Lorentz inhomogeneous group) on the segments of the flat space-time there are three strata: space like, time like, and light like. Indeed the word "stratum" was coined by Thom (1954, 1962, 1969) 50 years ago, in a more general situation of differential topology and seems to have been first applied to group actions by one of us (Michel 1971), thirty years ago. More examples of strata will be discussed in Sections 3 and 7.

In Section 4 we study the G-invariant functions (e.g. Hamiltonian or Lagrangian); they play a great role. At each point of M, their gradient is tangent to the stratum; so the study of stratification of the orbits determines the "critical orbits" which are orbits of extrema for *all* G-invariant functions. One can also determine for any G-invariant function the minimum number of orbits of extrema on each stratum.

In Section 5 we review what is presently known on the nature of the ring of G-invariant functions on the space of a finite-dimensional linear representations and how to find their generators. We give tables of examples which will be used in the later chapters. In some chapters we shall show how to extend the techniques of Section 5 for describing the ring of functions invariant under some non linear group actions. All these examples also yield illustrations of the predictions of the theorems of Section 4.

In Section 6 we explain how one can apply Morse theory to G-invariant functions; this leads to the complete information on the minimal number of their extrema and on the nature of these extrema.

In Section 7 we shall sketch some physical applications of this general approach not studied in the other chapters.

Appendix A summarizes several important group-theoretical definitions which can be found in classical textbooks on group theory. We give them here to make this issue more self-contained. Appendix B includes some introduction into more complicated mathematical subject related with generalization of Morse theory to the case of function with continuous symmetry.

[2] That is done in the different domains of physics under different names!

2. Group actions and their strata

Definition (*Group action*). An *action of a group* G on a mathematical structure M is defined by a homomorphism $G \xrightarrow{\rho} \mathrm{Aut}\, M$ into the group of automorphisms of M.

For instance if M is a vector space V, then $\mathrm{Aut}\, M = GL(V)$, the linear group on V, and ρ is a linear representation. In the more particular case of a Hilbert space $\mathscr{H}$, the $\mathrm{Aut}\, \mathscr{H}$ is the unitary group $U(\mathscr{H})$ and ρ is a (linear) unitary representation of G.

We generally assume that $\mathrm{Ker}\, \rho$ is trivial: i.e. any element $g \in G$, except the identity ($g \neq 1$), moves at least one point of M. In that case the action is called *effective*. Otherwise we will specify the kernel $\mathrm{Ker}\, \rho$ and remark that this non-effective G action defines an effective action of the quotient $G/\mathrm{Ker}\, \rho$ on M. (See Section 3.5 for examples of non-effective actions.)

Next comes naturally the

Definition (*Equivalence of group actions*). The two actions $G \xrightarrow{\rho_i} \mathrm{Aut}\, M_i$, $i = 1, 2$ are equivalent if there exists an isomorphism: $M_1 \xrightarrow{\theta} M_2$ which is *equivariant*, i.e. it commutes with the two actions:

$$\forall g \in G: \quad \theta \circ \rho_1(g) = \rho_2(g) \circ \theta \;\Leftrightarrow\; \rho_2(g) = \theta \circ \rho_1(g) \circ \theta^{-1} \,. \tag{1}$$

The usual equivalence of group linear representations is a particular case of the equivalence of group actions.

When we consider a unique action of G on M we generally shorten the notation $\rho(g)(m)$, the transform of $m \in M$ by $g \in G$, into $g \cdot m$.

Definition (*Group orbit*). The set of transforms of m, that we denote by $G \cdot m$, is the *orbit* of m.

An orbit may have a unique element! this is a "fixed point". More generally, to be on the same orbit is an equivalence relation for the elements of M. So M is a disjoint union of its orbits. The set of orbits is called the *orbit space* and we denote it by $M \,|\, G$. In our applications the orbit space can be a manifold; more generally it is an *orbifold*, i.e. a manifold with singular points or sub-manifolds.

Definition (*Stabilizer*). The set $G_m = \{g \in G,\ g \cdot m = m\}$ of elements of G which leave m fixed, is the *stabilizer* of m; it is a subgroup of G. In physical applications a stabilizer is sometimes called a local symmetry group or a little group.

For a fixed point o, $G_o = G$. In the general case, it is easy to prove that $G_{g \cdot m} = g G_m g^{-1}$; so *the set of stabilizers of the elements of an orbit is a conjugacy class* $[H]_G$ *of subgroups of* G (H is one of the stabilizers).

A very simple, but important remark, is that the action $G \xrightarrow{\rho} M$ defines implicitly an action of any strict subgroup[3] $H < G$, by restricting ρ to H (the restriction is denoted by $\rho|_H$). When the action $G \xrightarrow{\rho} M$ is restricted to that of a subgroup H the stabilizer H_m of the H-action follows immediately from G-action

$$H < G \xrightarrow{\rho} \mathrm{Aut}\, M: \quad H_m = H \cap G_m \ . \tag{2}$$

In general the G-orbits split into a disjoint union of H-orbits and there is a natural (surjective) map

$$M|H \to M|G \ . \tag{3}$$

When H is an invariant subgroup of G (we write here $H \lhd G$, as usual in the mathematical literature on groups) there is a natural action of the quotient group G/H on the orbit space $M|H$. This general theorem is very intuitive when H is a G-subgroup of index 2, i.e. $G/H \sim Z_2$: then there are two types of Z_2 orbits on $M|H$, those of one point and those of two points. We shall use several times this theorem, most often in the simplest case.

Definition (*Orbit type*). Orbits with the same conjugacy class of stabilizers are of the same type.

One such type with G as stabilizer is the set of fixed points. Similarly the orbits with a trivial stabilizer 1 (then all stabilizers of the orbit are 1), are called *principal orbits*. The action of the group G on M is *free* if all orbits have trivial stabilizers (i.e. all orbits are principal).

We shall often use the notation $G:H$ for the type of a G-orbit whose stabilizers are the G-subgroups conjugate to H. For instance a principal orbit can be noted G:1.

For a finite set F we denote by $|F|$ its number of elements. When G is finite, the number of elements of an orbit of type G:H is

$$|G{:}H| = \frac{|G|}{|H|} \ . \tag{4}$$

For the smooth actions (= infinitely differentiable) of Lie groups, the orbit G:H is a manifold of dimension:

$$\dim(G{:}H) = \dim(G) - \dim(H) \ . \tag{5}$$

If $\dim(G{:}H) = 0$, i.e. the orbit has a finite number of points, this number is the quotient of the number of connected components of G and H.

[3] The traditional notation for subset is $X \subseteq M$ and, for strict subset, $X \subset M$. For subgroups of groups we find it convenient to use the less traditional notation $H \leq G$ (or for strict subgroups: $H < G$). This notation recalls also the fact that to be a subgroup of a group is a partial order relation (by inclusion) among the subgroups of G.

Group G acts on the space M *transitively* if there exists only one orbit, the space M itself. That is for instance the case of the action of an Euclidean group on its space.

Definition (*Stratum*). In a group action, a stratum is the union of orbits of the same type. Equivalently, *two points belong to the same stratum iff* (= *if and only if*) *their stabilizers are conjugate*.

When they exist, the fixed points form one stratum and the principal orbits form another one.

The set of strata is called the *stratum space* and is denoted by $M||G$. To belong to the same stratum is an equivalence relation for the elements of M or for those of the orbit space $M|G$. The set of strata $M||G$ is a (rather small in our applications) subset of the set of conjugacy classes of subgroups of G. Notice that there exists a natural partial order between these conjugacy classes of subgroups: one is smaller than the other if it contains a group which is a strict subgroup of a group of the other. That gives to the set of strata $M||G$ a structure of partially ordered set: $S_i \in M||G$, $S_1 < S_2$ means that the local symmetry of S_1 is smaller than that of[4] S_2; i.e. the stabilizers of the points of S_1 are, up to a conjugation, subgroups of those of S_2.

Remark that relation (3) between the orbit spaces of G and of the subgroup H obtained by restriction cannot be extended to the stratum spaces: indeed there is no natural map between them and often the set of strata is larger for the larger group.

2.1. Constructing more group actions from given ones

Given one or several G actions, one can consider other actions which are automatically defined from the given ones. For instance the action $G \xrightarrow{\rho} \mathrm{Aut}\, M$ defines automatically the action of G on the subsets of M or, in particular, on families of these subsets.[5] Similarly, from the actions $G \xrightarrow{\rho_i} M_i$ on different spaces M_i one defines "natural" actions on the structures built from the M_i, e.g. their topological product. An important example is the action on $\mathscr{F}(M_1, M_2)$, the space of function from M_1 to M_2. Denoting by $g \cdot f$ the transformed by $g \in G$ of the function $f \in \mathscr{F}(M_1, M_2)$ one has the definition

$$\forall g \in G, \quad \forall m \in M_1, \ (g \cdot f) \circ \rho_1(g)(m) = \rho_2(g) \circ f(m)$$

$$\Leftrightarrow (g \cdot f)(m) = \rho_2(g) \cdot f(\rho_1(g^{-1}) \cdot m) \ . \tag{6}$$

The function f is G-invariant when $g \cdot f = f$ for all $g \in G$. We will meet often the simpler case when G acts trivially on M_2; then the G-invariant functions satisfy $\forall g \in G$, $\forall m \in M_1$, $f(m) = f(g \cdot m)$.

[4] Beware that the less symmetric stratum might have a larger dimension than the more symmetric ones. So we emphasize that the partial order on the set of strata deals with their local symmetry and *not* with their size.

[5] In the introduction we gave the example of the Euclidean group acting on the triangles and of the Lorentz group acting on the segments of space time.

3. Examples of groups and group actions

We have first to recall the two standard notations used for subgroups of $O(d)$ ($d = 2, 3$) in molecular physics and chemistry and in solid state physics and crystallography. These are Schönflies notation (Landau and Lifshitz, 1965; Hamermesh, 1964) and International Tables of Crystallography (ITC, 1996) notations. (In what follows we will use the abbreviation ITC for International Tables of Crystallography (ITC, 1996).) In contrast to the abstract mathematical definition of groups (up to an *isomorphism*) the natural physical classification of point groups (finite or continuous subgroups of $O(3)$ group) is done up to conjugation in $O(3)$. We call them *geometric classes*. In crystallography one also needs to consider *arithmetic classes*, i.e. the classes of subgroups conjugated in $GL(3, Z)$, the group of 3×3 matrices with integer elements. More generally one may have to consider the classification of subgroups H of G up to conjugation in G. To see better the correspondence between different classifications of subgroups let us start with subgroups of $O(2)$, the group of orthogonal transformations of two-dimensional space.

The matrices of $O(2)$ of determinant 1 (respectively, -1) are the rotations $r(\theta)$ by an angle θ around the origin (respectively, the reflections $s(\phi)$ through the axis of azimuth ϕ):

$$r(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \quad \theta(\mathrm{mod}\, 2\pi)\,, \tag{7}$$

$$s(\phi) = \begin{pmatrix} \cos(2\phi) & \sin(2\phi) \\ \sin(2\phi) & -\cos(2\phi) \end{pmatrix}, \quad \phi(\mathrm{mod}\, \pi)\,.$$

They satisfy the following relations:

$$r(\theta)r(\theta') = r(\theta + \theta'), \quad s(\phi)s(\phi') = r(2(\phi - \phi'))\,,$$
$$r(\theta)s(\phi) = s(\theta + \phi) = s(\phi)r(-\theta)\,. \tag{8}$$

In particular

$$r(\theta)r(-\theta) = I, \quad s(\phi)^2 = I, \quad s(\phi)r(\theta)s(\phi) = r(-\theta)\,,$$
$$r(\theta)s(\phi)r(\theta)^{-1} = s(\phi + 2\theta)\,. \tag{9}$$

We denote by c_n the n-element group formed by the rotations $r(2\pi k/n), 0 \le k \le n-1$; it is isomorphic to Z_n, cyclic group of order n, and $c_n \lhd O_2$. We denote by c_s the conjugation class of subgroups $c_{s(\phi)} \sim Z_2$ generated by the reflection $s(\phi)$. The two reflections $s(\phi)$ and $s(\phi + \pi/n)$ generate a $2n$ element group that we denote[6] by $c_{nv(\phi)}$, with the simple notation c_{nv} for the conjugacy class $[c_{nv(\phi)}]_{O_2}$. These groups are isomorphic to the "dihedral" groups, defined by the generators and relations $s_1^2 = s_2^2 = 1 = (s_1 s_2)^n$; we denote them by d_n (Coxeter and Moser, 1972); they are non-Abelian for $n > 2$. The group c_{nv} is the symmetry group of a regular polygon of n vertices and edges.

[6] The notations c_n, c_s, c_{nv} are those of Schönflies. We use small letters for 2-D groups and capital letters for 3-D groups.

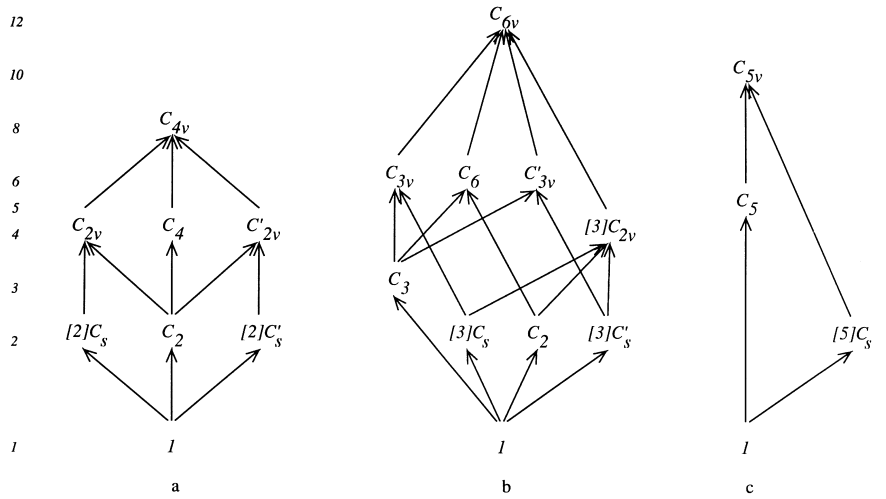


Fig. 1. The partially ordered sets of conjucacy classes of the subgroups of C_{4v}, C_{6v}, C_{5v}. When a subgroup is not invariant we indicate before its name, between [ ], the number of subgroups in its conjugacy classes. The order of subgroups is indicated at the left.

The set c_n, $n \geq 1$ and c_{nv}, $n \geq 1$ give the complete list of finite subgroups of $O(2)$. Remark that c_1 is a trivial "no symmetry" group, c_{1v} is the c_s group. To exhaust all subgroups of $O(2)$ we need to add c_∞ which is the $SO(2)$ and $c_{\infty v}$ which is the complete $O(2)$ group.

In Fig. 1 we give the partially ordered set of the conjugacy classes of subgroups of c_{4v}, c_{6v}, c_{5v} which are the symmetry groups of the square, the regular hexagon, and the regular pentagon, respectively. When n is prime, c_{nv} has only four conjugacy classes (including 1 and the whole group).

When n is even there are pairs of conjugacy classes which belong to the same geometric classes. To distinguish them, we have added prime " $'$ " at a member of each pair. However we do not need to invent a new notation since one already exists and is known by some of the readers. The symmetry point group of crystals are finite subgroups of $O(d)$, (here $d = 2, 3$). Their conjugation class in $O(d)$ is called the "geometry class". For $d = 2, 3$ there are 10, 32 geometric classes. This classification is generally sufficient for describing the symmetry of the macroscopic physical properties of crystals. It is not sufficient for the symmetry classification of microscopic properties. The action of a point group P on L, the lattice of translations of the crystals is given by the injective homomorphism (see the first definition of Section 2) $P \to \mathrm{Aut}\, L = GL(d, Z)$. Here we label the image of P by P^z, it defines a conjugacy class in $GL(d, Z)$. These classes are called *arithmetic classes*. For $d = 2, 3$ there are 13, 73 of them.

There are two maximal conjugacy classes of finite subgroups of $GL(2, Z)$. Their geometric classes are c_{4v} and c_{6v} and they coincide with the arithmetic classes which are denoted by *p*4*mm*, *p*6*mm*.

The symmetry group of the square $c_{4v} \sim O(2, Z)$ contains four reflections; they are represented by the two pairs of matrices:

$$\pm\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \pm\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

which are denoted, respectively, by $\pm pm$, $\pm cm$ in crystallography since they are not conjugate in $GL(2,Z)$. The same symbols are also used for the two-element groups they generate. More generally, for the eight conjugacy classes of subgroups of the symmetry group of the square, we give here the dictionary between the Schönflies notations used in Fig. 1 and the ITC, (1996) ones:

$$1\leftrightarrow p1,\ c_2\leftrightarrow p2,\ c_s\leftrightarrow pm,\ c'_s\leftrightarrow cm,\ c_4\leftrightarrow p4\ ,$$

$$c_{2v}\leftrightarrow p2mm, c'_{2v}\leftrightarrow c2mm,\ c_{4v}\leftrightarrow p4mm\ . \tag{10}$$

As we will show in Chapter IV, the first letters p, c distinguish between two Bravais classes of lattices.

The dictionary between the notations for the conjugacy classes of subgroups of c_{6v} is

$$c_{2v} = cmm,\ c_3\leftrightarrow p3,\ c_{3v} = p3m1,\ c'_{3v} = p31m\ , \tag{11}$$

$$c_6 = p_6,\ c_{6v} = p6mm\ . \tag{12}$$

The conjugacy classes cm and cm' of c_{6v} are conjugated in $GL(2,Z)$ and not distinguished by the ITC notation. The ITC notation will be partly defined below for $d = 3$ and fully explained in Chapter IV. Remark that for $d = 2, 3$ the orders of the elements of the finite groups of $GL(d,Z)$ are 1, 2, 3, 4, 6. We have decided to use both notations: that of Schönflies used by molecular physicists and chemists and that of ITC, so well adapted to crystallography and solid state physicist need. That will help each tribe of scientists to read the literature of another tribe. In this chapter, to help the reader, when we use a group we use both symbols.

The description of three-dimensional symmetry groups can be naturally based on the above established list of 2-D symmetry groups.

The two-dimensional subgroups, c_n, c_s, c_{nv} which act trivially in the perpendicular direction of their plane, are denoted in three-dimensions by C_n, C_s, C_{nv}. One adds C_i, the two-element group generated by $-I_3$, the symmetry through the origin, which can be equivalently described as S_2 group with the S_2 element being the rotation–reflection of order two, i.e. the product of C_2 rotation and the reflection in the perpendicular plane. Generalizing C_2 to C_n with n even leads to S_{2n} groups isomorphic to Z_{2n}, where we use again the notation Z_m for the m-element cyclic group.

Historically, the index v is for *vertical*; it is the direction of the rotation axis of C_n, C_{nv}. If one adds to C_n the symmetry through the horizontal plane, one obtains the group C_{nh}. Remark the isomorphisms: $C_{nh} \sim Z_n \times Z_2$; but when n is odd that is also $C_{nh} \sim Z_{2n}$. If one adds to C_n a rotation by π around a horizontal axis (containing the origin), one obtains the group $D_n < SO_3$; note that it is isomorphic to C_{nv}. Adding the symmetry through the horizontal plane to D_n or C_{nv} one obtains the same group which is denoted by D_{nh}. When one adds to D_n the vertical symmetry planes bisectors of neighbor axes of rotation by π, one obtains D_{nd}.

We have still to explain the irreducible subgroups of O_3:

The symmetry groups of the regular tetrahedron is denoted by T_d, of the cube (or regular octahedron) by O_h, of the regular icosahedron (or dodecahedron) by Y_h. Then we define $T = T_d \cap SO_3$, $O = O_h \cap SO_3$, $Y = Y_h \cap SO_3$; note that $T \times C_i = T_h$ (also $O \times C_i = O_h$, $Y \times C_i = Y_h$).[7]

[7] It would have been better to use the notation T_i, O_i, Y_i instead of T_h, O_h, Y_h but we follow the tradition.

Thus the complete list of finite 3-D geometrical classes includes the following groups given here in Schönflies notation. There are seven infinite sequences $C_n, C_{nh}, S_{2n}, C_{nv}, D_n, D_{nd}, D_{nh}$, and seven "exceptional" groups T, T_d, T_h, O, O_h, Y, Y_h. There are also five one-dimensional Lie subgroups C_∞, $C_{\infty h}$, $C_{\infty v}$, D_∞, $D_{\infty h}$, and $SO(3)$, and $O(3)$ itself. C_∞ is another notation for $SO(2)$, the group of rotations around the "vertical" axis and $C_{\infty v}$ is $O(2)$, i.e. it is generated by C_∞ and a reflection through any vertical plane containing the vertical rotation axis. Similarly $C_{\infty h}$ is generated by C_∞ and a reflection through the horizontal plane; it would be noted $C_{\infty i}$, indeed it contains the reflection through the origin $-I_3$ (notice that $C_{\infty h}$ is Abelian). D_∞ is generated by C_∞ and a rotation by π around an azimuthal axis passing through the origin. Finally, $D_{\infty h} = D_\infty \times C_i$.

The other standard notation, used in ITC (1996), is necessary for the study of crystals (Chapters IV–VI). It is based on the description of groups in terms of generators. In $O(3)$ there are two conjugacy classes of elements of finite order n. If its determinant is 1, it is a rotation by $2\pi/n$ which is denoted by n; if its determinant is -1 (n has to be even), then it is the product of a rotation by the matrix $-I_3$ and it is denoted by $\bar{n}$ with the exception that $\bar{2}$ is replaced by m, for *mirror* (indeed it is a reflection through a plane). The cyclic groups generated by these finite-order elements are denoted by the same symbol: hence the translation ITC $\leftrightarrow$ Schönflies:

$$n \leftrightarrow C_n,\ \bar{1} \leftrightarrow C_i,\ m \leftrightarrow C_s\ , \tag{13}$$

$$n \equiv 0 \bmod 4\text{: } \bar{n} \leftrightarrow S_n, \quad 6 \leq n \equiv 2 \bmod 4\text{: } \bar{n} \leftrightarrow C_{n/2h}\ , \tag{14}$$

$$n \text{ odd: } \bar{n} \leftrightarrow C_{ni} \sim S_{2n}\ . \tag{15}$$

For the finite subgroups of $O(3)$ with two or three generators one writes these generators together; for example: $nm \leftrightarrow C_{nv}$, $n2 \leftrightarrow D_n$. Beware that, to distinguish different groups with the same generators, a convention is made for the order of generators, e.g. $32 \leftrightarrow D_3$, $23 \leftrightarrow T$, $\bar{3}m \leftrightarrow D_{3d}$, $m\bar{3} = T_h$. The ITC notation can be used as well for one-dimensional Lie subgroups of $O(3)$: $C_\infty = \infty$, $C_{\infty v} = \infty m$, $C_{\infty h} = \infty/m$, $D_\infty = \infty 2$, $D_{\infty h} = \infty mm$ (see ITC, 1996, p. 783).

The full list of the 32 geometric classes was established (independently) by Frankenheim (1826) and Hessel (1830) before the word group was created by Galois in 1830 (Galois' work was published only in 1846 (Galois, 1846)). Table 1 gives the list of these 32 geometric classes in the two notations and classes them among the 18 isomorphy classes they form; note that half of them are isomorphy classes of Abelian groups.

Among all crystallographic 3-D-geometrical classes there are two maximal ones: $O_h = m\bar{3}m$ and $D_{6h} = 6/mmm$.

In particular the symmetry group O_h of the three-cube has 48 elements. It is generated by nine reflections forming two conjugacy classes. In the coordinate system we defined above (in dimension d), O_h is represented by $O(3, Z)$ and the matrices representing its reflections are the three (Pm_i) and the six (Cm_i) and (Cm_i'):

$$(Pm_3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (Pm_1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (Pm_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{16}$$

Table 1
The 32 crystallographic geometric classes and their 18 isomorphy classes. The isomorphy classes are listed in columns 1, 3 and are defined as direct products of cyclic groups Z_n, dihedral groups c_{nv}, permutation group of four objects $\mathscr{S}_4$, and its subgroup of even permutations $\mathscr{A}_4$. In column 2, 4 the geometric classes are listed in ITC and Schönflies notations

Isom.	Geometric	Isomorphic	Geometric
1	$1 = 1$	Z_2	$\bar{1} = C_i$, $m = C_s$, $2 = C_2$
Z_2^2	$2/m = C_{2h}$, $mm2 = C_{2v}$, $222 = D_2$	Z_2^3	$mmm = D_{2h}$
Z_3	$3 = C_3$	$Z_2 \times Z_3$	$6 = C_6$, $\bar{3} = C_{3i}$, $\bar{6} = C_{3h}$
Z_4	$4 = C_4$, $\bar{4} = S_4$	$Z_2 \times Z_4$	$4/m = C_{4h}$
c_{3v}	$3m = C_{3v}$, $32 = D_3$	$Z_2^2 \times Z_3$	$6/m = C_{6h}$
c_{4v}	$4mm = C_{4v}$, $422 = D_4$, $\bar{4}m2 = D_{2d}$	$c_{4v} \times Z_2$	$4/mmm = D_{4h}$
$c_{3v} \times Z_2$	$6mm = C_{6v}$, $622 = D_6$, $\bar{3}m = D_{3d}$, $\bar{6}m2 = D_{3h}$	$c_{3v} \times Z_2^3$	$6/mmm = D_{6h}$
$\mathscr{A}_4$	$23 = T$	$\mathscr{A}_4 \times Z_2$	$m\bar{3} = T_h$
$\mathscr{S}_4$	$\bar{4}3m = T_d$, $432 = O$	$\mathscr{S}_4 \times Z_2$	$m\bar{3}m = O_h$

$$(Cm_3) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (Cm_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad (Cm_2) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{17}$$

$$(Cm'_i) = -(Pm_i)(Cm_i)\,. \tag{18}$$

We also introduce the orthogonal matrices:

$$(P4) = (Pm_1)(Cm_3) = -(P\bar{4})\,,$$

$$(R3) = (Cm_1)(Cm_2) = (Cm_2)(Cm_3) = (Cm_3)(Cm_1) = -(R\bar{3})\,. \tag{19}$$

$O(3,Z)$ is generated by the three matrices Pm_3, $(R\bar{3})$, (Cm_3); that explains the ITC notation $Pm\bar{3}m$ for $O(3,Z)$. Let us recall that the symmetry group of the three-cube corresponds to a unique geometry class (conjugacy class in O_3 or $GL(3,R)$) which is denoted by $O_h = m\bar{3}m$, but it is isomorphic to three arithmetic classes in $GL(3,Z)$ which are denoted in ITC $Pm\bar{3}m$, $Fm\bar{3}m$, $Im\bar{3}m$; the first one will be studied here and the last two in Chapter IV.

The group $O_h = m\bar{3}m$ has 98 subgroups including $c_1 = 1$ and O_h itself falling into 33 conjugacy classes. For $O(3,Z) = Pm\bar{3}m$ these classes coincide with the conjugacy classes in the larger group $GL(3,Z)$, so they are arithmetic classes. We shall denote them by their ITC labels. These 33 arithmetic classes form only 25 crystallographic geometric classes, so their Schönflies notation is ambiguous. For each arithmetic class $\leq O(3,Z)$ we choose a representative subgroup and give in Table 2 a set of matrices which generate it.

In Fig. 2 we give the partial ordered set of the 33 conjugacy classes of subgroups of $O(3,Z) = Pm\bar{3}m$ in Schönflies and ITC notation. These classes are arithmetic classes; each one is explicitly defined by matrices generating its subgroups. Of course the notation used for arithmetic classes is that of ITC. Explicitly, when more than one arithmetic class correspond to a geometric class $\leq O_h$, we list them in Table 3 with gc for geometric class, ac for arithmetic class:

Table 2
Set of generators for arithmetic classes. For each arithmetic class $\leq O(3,Z)$ we choose a representative subgroup and give a set of matrices which generate it. The matrices are $-I$ and those defined in Eqs. (16)–(19)

$P\bar{1}$: $(-I)$	$P2$: $-(Pm_3)$	Pm: (Pm_3)	P/m: $\pm(Pm_3)$
$C2$: $-(Cm_3)$	Cm: (Cm_3)	$C2/m$: $\pm(Cm_3)$	$P222$: $-(Pm_3), -(Pm_1)$
$Pmm2$: $-(Pm_3), (Pm_1)$	$Pmmm$: (Pm_i)	$C222$: $-(Cm_3), -(Pm_3)$	$Cmm2$: $(Cm_3), -(Pm_3)$
$Amm2$: $-(Cm_3), (Pm_3)$	$Cmmm$: $\pm(Cm_3), (Pm_3)$	$P4$: $(P4)$	$P\bar{4}$: $-(P4)$
$P4/m$: $(P4), (Pm_3)$	$P422$: $(P4), -(Pm_1)$	$P4mm$: $(P4), (Pm_1)$	$P\bar{4}2m$: $-(P4), -(Pm_1)$
$P\bar{4}m2$: $-(P4), (Pm_1)$	$P4/mmm$: $(P4), (Pm_i)$	$R3$: $(R3)$	$R\bar{3}$: $-(R3)$
$R32$: $(R3), -(Cm_i)$	$R3m$: $(R3), (Cm_i)$	$R\bar{3}m$: $-(R3), \pm(Cm_i)$	$P23$: $-(Pm_i), (R3)$
$Pm\bar{3}$: $(Pm_i), (R3)$	$P432$: $-(Pm_i), -(Cm_i)$	$P\bar{4}3m$: $-(Pm_i), (Cm_i)$	$Pm\bar{3}m$: $(Pm_i), (Cm_i)$

Table 3
Correspondence between geometric and arithmetic classes for subgroups of $O_h \sim Pm\bar{3}m$

gc:	C_2	C_s	C_{2h}	C_{2v}
ac:	$P2, C2$	Pm, Cm	$P2/m, C2/m$	$Pmm2, Cmm2, Amm2$
gc:	D_2	D_{2h}	D_{2d}	
ac:	$P222, C222$	$Pmmm, Cmmm$	$P\bar{4}2m, P\bar{4}m2$	

To distinguish between $P\bar{4}m2$ and $P\bar{4}2m$ we note that the first symbol after $\bar{4}$ indicates the symmetry element in the coordinate planes: they are the reflections through the planes for $\bar{4}m2$ and the axes of rotation of order 2 in $\bar{4}2m$. It is this last group which is a subgroup of the tetrahedron group $\bar{4}3m$.

Similar analysis can be done for another maximal finite subgroup of $O(3)$, namely $D_{6h} = P6/mmm$. The diagram of the partially ordered conjugacy classes of subgroups of $P6/mmm = D_{6h}$ is given in Fig. 3. The 32 conjugacy classes of subgroups correspond to 28 conjugacy classes in $GL(3,Z)$; for them we use the names of ICT. Only 16 of them are not orthogonal arithmetic classes $< O(3,Z)$. They all contain $3 = C_3$ which is the derived group. There are three conjugate subgroups $Cmmm$; this arithmetic class is the largest of all arithmetic classes contained also in $Pm\bar{3}m = O(3,Z)$.

Remark that there are four pairs of isomorphic hexagonal arithmetic classes:

$$D_3 = P321, P312, \quad C_{3v} = P3m1, P31m\,, \tag{20}$$

$$D_{3d} = P\bar{3}m1, P\bar{3}1m, \quad D_{3h} = P\bar{6}m2, P\bar{6}2m \tag{21}$$

among the subgroups of $P6/mmm$.

3.1. Action of the group G on itself or on the lattice of its subgroups

The homomorphism $G \to \mathrm{Aut}\, G$ has for kernel $C(G)$, the center of G and for image the group In Aut G of inner automorphisms, i.e. G acts on itself by conjugation: $g \cdot x = gxg^{-1}$. The stabilizer

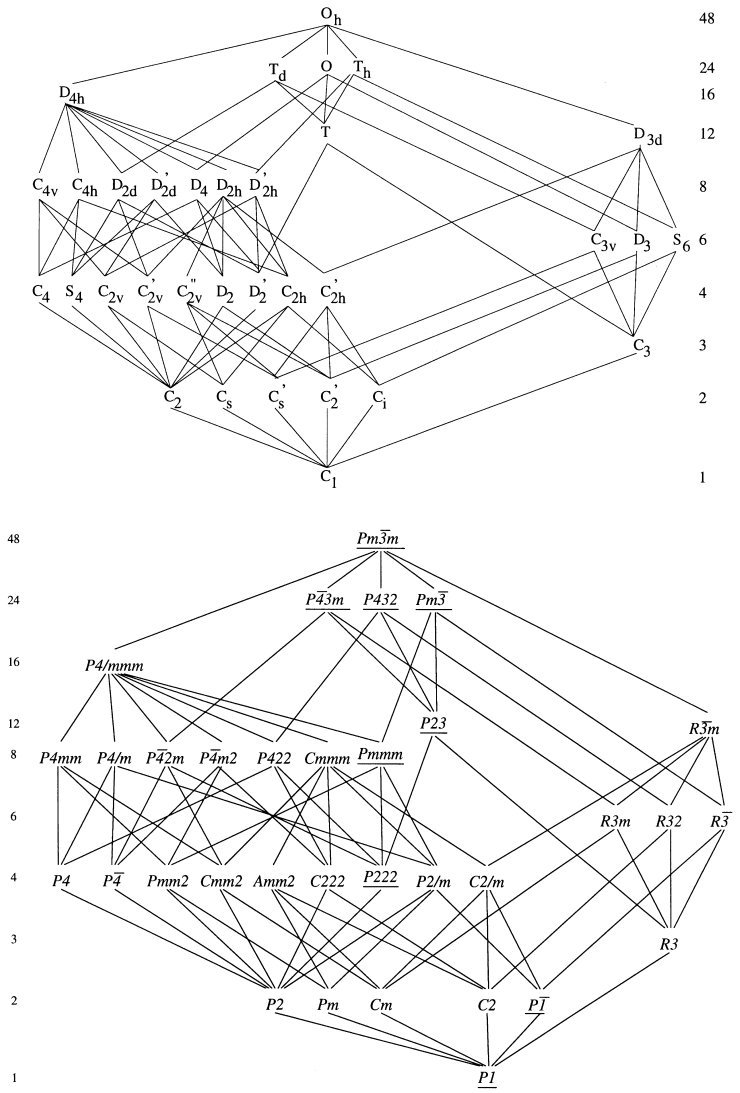


Fig. 2. Lattice of conjugated subgroups of $O_h = Pm\bar{3}m$. Two parts of the figure are identical except for the notation. Schönflies notation is used in the upper part of the figure and the ITC notation in the lower part. The 33 conjugacy classes of subgroups of $Pm\bar{3}m = O(3,Z) \sim O_h$ correspond to 33 arithmetic classes $\leq O(3,Z)$. Invariant subgroups are underlined.

G_x is the set of group elements commuting with x; it is a subgroup (the whole group for Abelien group) called the centralizer of x and denoted by $C_G(x)$. The orbit $G \cdot x$ is the conjugacy class of x. For finite groups $|C_G(x)||G \cdot x| = |G|$. We will often use the corresponding action of G on the set of its subgroups. The centralizer of the subgroup H is the set $\{g \in G, gHg^{-1} = H\}$. It is a subgroup called the normalizer of H in G and denoted by $N_G(H)$; it is the largest subgroup of G which contains H as an invariant subgroup. The orbit is the conjugacy class $[H]_G$ of H in G. The orbit

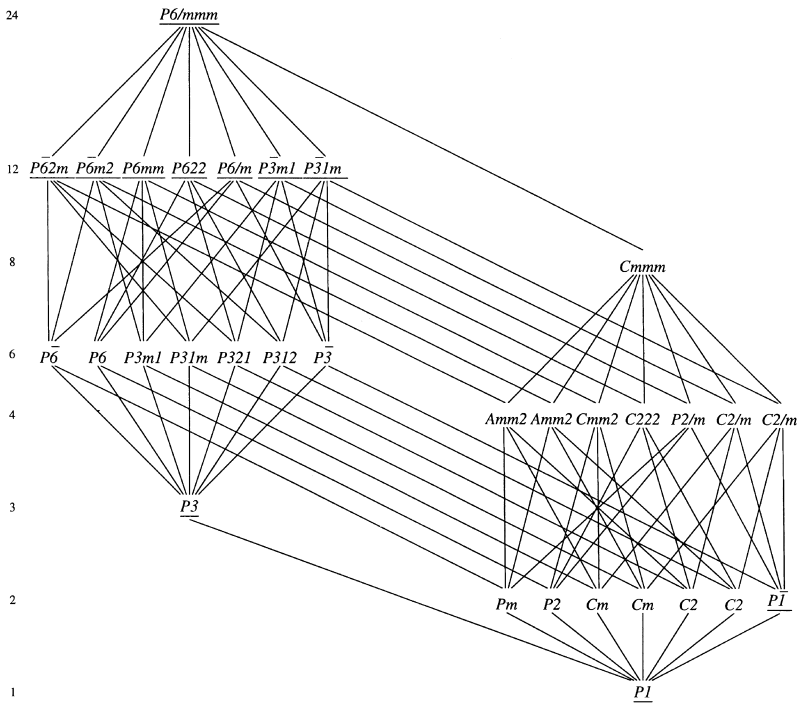


Fig. 3. Lattice of conjugated subgroups of $P6/mmm$.

space is the set of conjugacy classes of subgroups; it is a partially ordered set. Such partially ordered sets are shown in Fig. 1 for the subgroups of c_{4v}, c_{5v}, c_{6v}.

Classes of conjugated subgroups of the O_h group are given in Fig. 2 for the convenience of reader using both Schönflies (Hamermesh, 1964; Landau and Lifshitz, 1965; Lyubarskii, 1957; ITC, 1996) and international crystallographic notation (ITC, 1996). There are several invariant subgroups $T_d = P\bar{4}3m$, $O = P432$, $T_h = Pm\bar{3}$, $T = P23$, $D_{2h} = Pmmm$, $D_2 = P222$, $C_i = P\bar{1}$, $C_1 = P1$, i.e. corresponding classes of conjugated subgroups include only one subgroup. We remark the existence of three non-conjugated C_{2v} subgroups ($Pmm2$, $Cmm2$, $Amm2$) and six pairs of non-conjugated subgroups D_{2d}, $(P\bar{4}2m, P\bar{4}m2)$; D_{2h}, $(Cmmm, Pmmm)$; D_2, $(C222, P222)$; C_{2h}, $(P2/m, C2/m)$; C_2, $(P2, C2)$; C_s, (Pm, Cm). Fifteen classes of conjugated subgroups include each three subgroups ($P2$, Pm, $P4$, $P\bar{4}$, $Pmm2$, $Cmm2$, $C222$, $P2/m$, $P4mm$, $P4/m$, $P\bar{4}2m$, $P\bar{4}m2$, $P422$, $Cmmm$, $P4/mmm$). All five R classes include each four conjugated subgroups and four classes ($C222$, $C2/m$, Cm, $C2$) consist of six subgroups.

All 33 classes of conjugated subgroups (we count the $O_h = Pm\bar{3}m$ group itself and the trivial $C_1 = P1$ subgroup as well) remain inequivalent (non-conjugated) even if we consider them as subgroups of the larger group $GL(3, Z)$. This means that all these subgroups correspond to different arithmetic classes of 3D-crystals. (Arithmetic classes will be more fully discussed in Chapter IV.) At the same time three non-conjugated C_{2v} ($Pmm2, Cmm2, Amm2$) subgroups as well as all mentioned above pairs of non-conjugated subgroups become conjugated as subgroups of $O(3)$. Non-conjugated in $O(3)$ classes of subgroups correspond to geometrical classes of crystals. There

are 25 different geometrical classes which are the subgroups of $O_h = Pm\bar{3}m$. Remind that there are 32 different geometric classes. At the same time only two isomorphy classes ($6/m \sim C_{6h}$ and $6/mmm \sim D_{6h}$) are absent among subgroups of $O_h = Pm\bar{3}m$.

Another maximal subgroup $P6/mmm \sim D_{6h}$ and its classes of conjugated subgroups are given in Fig. 3. The complete list of arithmetic classes will be constructed in Chapter IV.

3.2. Action of the group G on another group K

A group homomorphism $G \xrightarrow{\rho} \mathrm{Aut}\, K$ gives an action of G on K respecting its group structure. We will meet many examples of this construction. Given such an action we can build a new group on the Cartesian product (K, G) of the sets of elements of K and G. This group is called the semi-direct product of K by G and is usually denoted by $K \rtimes G$; its group law is

$$(k_i, g_\alpha) \in (K, G), \quad (k_1, g_1) \cdot (k_2, g_2) = (k_1(g_1 \cdot k_2), g_1 g_2)\ . \tag{22}$$

The d-dimensional Euclidean group Eu_d and the Poincaré group P_0 are the semi-direct products

$$Eu_d = R^d \rtimes O(d), \qquad P_0 = R^4 \rtimes O(3,1) \tag{23}$$

where $O(3,1) \sim O(1,3)$ is the Lorentz group, i.e. the group which leaves invariant the quadratic form $(x_0^2 - x_1^2 - x_2^2 - x_3^2)$. It is useful to know a linearization of the Euclidean group (and of the Poincaré group), but for this we have to use $(d+1) \times (d+1)$ matrices

$$(\boldsymbol{t}, A) \in R^d \rtimes O(d) \mapsto \begin{pmatrix} A & \boldsymbol{t} \\ 0 & 1 \end{pmatrix}, \tag{24}$$

acting on the $(d+1)$ variables[8] $(x_1, \ldots, x_d, 1)$.

Using Fourier transform one can also work in the space of momenta (or energy momenta in special relativity). We remind the reader that this space is a vector space (containing a null vector $p = 0$). So the action of Eu_d on the momentum space is linear; indeed it is not faithful: the translations act trivially.

In crystallography each arithmetic class (= conjugacy classes of finite subgroups of $GL(3, Z)$) defines an action of a finite subgroup (the point group) on a lattice (isomorphic to the Abelian group Z^3), so 73 of the crystallographic space groups in dimension 3 are semi-direct products.

The direct product $K \times G$ is the particular case of semi-direct product when the action of G on K is trivial.

3.3. Action of G on its set of elements $\mathscr{G}$

Beware that $\mathscr{G}$ is only a set (the corresponding automorphism group is the permutation group of its elements). The natural action of $g \in G$ is by multiplication on the left $g \cdot x = gx$ (or on the right

[8] These inhomogeneous groups are written as subgroups of the affine group $R^d \rtimes GL(d, R) = Aff_d < GL(d+1, R)$. Beware that for $n > 2$ the adjoint representation $GL(n, R) \ni g \mapsto \tilde{g} \equiv (g^{-1})^\top = (g^\top)^{-1}$ is not equivalent to the natural one. So one can extend Eu_2 to two Aff_2 non-conjugate in $GL(3, R)$.

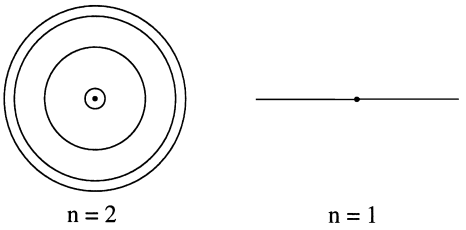


Fig. 4. Action of the $O(n)$ group on n-dimensional space defined by its natural (vector) representation. $n = 1, 2$ are shown. For each n there are two types of orbits: one point orbit with the $O(n)$ stabilizer (the origin) and a continuous family of orbits with the $O(n-1)$ stabilizer.

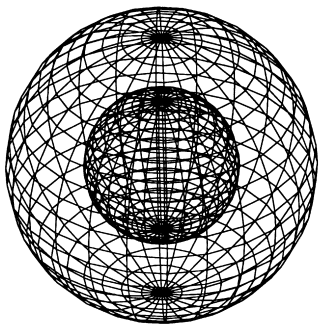


Fig. 5. Action of the $O(3)$ group on three-dimensional space defined by its natural (vector) representation. Two orbits with the $O(2)$ stabilizer are shown.

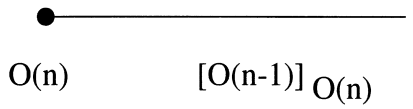


Fig. 6. Space of orbits for the natural action of the $O(n)$ group on n-dimensional space. Two different strata are indicated by their stabilizers $O(n)$ and $[O(n-1)]_{O(n)}$.

$g \cdot x = xg^{-1}$). The orbit is $\mathcal{G}$ itself: it is a principal orbit. For the corresponding action of G on its subgroups, $g \cdot H = gH$, the left coset of H by g; so the stabilizer is H itself. The orbit is the set of H left cosets and is often denoted by $G:H$; this orbit is often considered as the prototype of the orbits of type $[H]_G$.

3.4. Action of the group G on a manifold

1. The natural (also called *vector*) representation of $O(n)$ on the orthogonal space V_n has two strata: the origin, a fixed point and a one parameter family of $(n-1)$-dimensional spheres S_{n-1} with stabilizers $[O(n-1)]_{O(n)}$. Examples of orbits are shown in Figs. 4 and 5 for $n = 1, 2$, and 3. Corresponding spaces of orbits are given in Fig. 6. For every n the space of orbits is one-dimensional. If we restrict the action of $O(n)$ to its strict subgroup $SO(n)$ the system of orbits does not change but their stabilizers do. (Stabilizers become $SO(n)$ and $SO(n-1)$.)

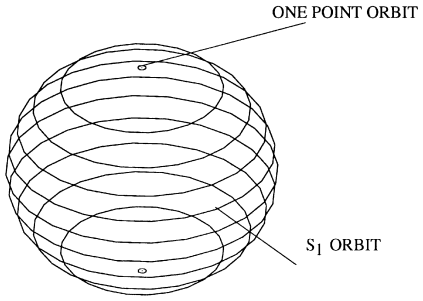


Fig. 7. Action of $C_\infty = \infty$ and $C_{\infty v} = \infty m$ on S_2 induced by natural action of $O(3)$. There are two one-point orbits (north and south poles of the sphere) and a one-parameter family of circle orbits (each one being a parallel).

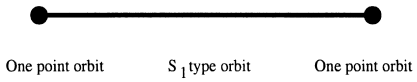


Fig. 8. Orbifold for $C_\infty = \infty$ and $C_{\infty v} = \infty m$ group action on S_2 induced by natural action of $O(3)$. The stabilizer for one-point orbits is C_∞ ($C_{\infty v}$) and for generic S_1 orbits is C_1 (C_s) for the symmetry groups C_∞ ($C_{\infty v}$), respectively.

2. The vector representation of $O(3)$ defines an action of its one-dimensional subgroups on S_2, with S_2 being one orbit of the natural $O(3)$ action. For the action of $C_\infty = \infty$ and $C_{\infty v} = \infty m$ subgroups there are two strata: one consists of two fixed points (= the two poles), the other includes a one-parameter family of circles (the "parallels") with stabilizers 1 and C_s for C_∞ and $C_{\infty v}$ subgroups, respectively. A coordinate of the one-dimensional orbit space is called the latitude λ with $-90^\circ \leq \lambda \leq 90^\circ$. See Fig. 7 for the representation of orbits and Fig. 8 for the space of orbits (orbifold).

For the action of $C_{\infty h} = \infty/m$, $D_\infty = \infty 2$, $D_{\infty h} = \infty mm$ subgroups, there are three strata. Two strata consist of one orbit: one contains the two poles (stabilizers C_∞, C_∞, $C_{\infty v}$, respectively), the other, the equator (stabilizers C_s, C_2, C_{2v}). The third stratum is the generic one, containing a one-parameter family of pairs of parallels with the same absolute value λ of latitude, i.e. $0 < \lambda < 90^\circ$. Fig. 9 gives orbits for these groups. Notice that for these five groups, the orbit space is a closed line segment. (See Figs. 8 and 10.)

3a. Vector representation of $O_h = Pm\bar{3}m$, the symmetry group of the cube; see e.g. Jaric et al. (1984), and Michel and Mozrzymas (1978). This group contains the reflections through nine symmetry planes intersecting at the cube symmetry center. These planes fall into two O_h-orbits (for the O_h-induced action on the set of two-dimensional subspaces = planes of the representation space V_3): one orbit contains the three planes P_i, parallel to the faces, the other orbit contains the six planes P'_j, each one containing two opposite edges. Each reflection generates a two-element group conjugate in $O(3)$ to C_s. We denote, respectively, by $[C_s]_{O_h} = Pm$ and $[C'_s]_{O_h} = Cm$ the two corresponding conjugacy classes of, respectively, 3, 6 two-element subgroups. The group O_h contains three families of rotation axes which are, respectively, made up of three axes of rotations by $\pi/2$ (they contain the center of opposite faces), four axes of rotations by $2\pi/3$ (they contain opposite

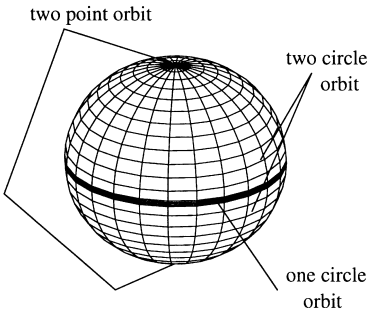


Fig. 9. Action of $C_{\infty h} = \infty/m$, ($D_\infty = \infty 2$, and $D_{\infty h} = \infty mm$) on S_2 induced by natural action of $O(3)$. There are one two-point-orbit (north and south poles of the sphere) with the stabilizer $C_\infty, (C_\infty, C_{\infty v})$, one S_1 circle orbit with the stabilizer C_s, (C_2, C_{2v}), and a one-parameter family of orbits (each one being a pair of circles) with the stabilizer $C_1, (C_1, C_s)$.

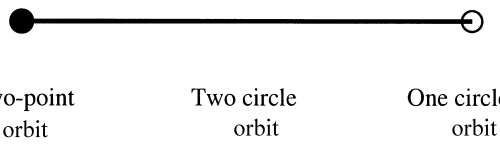


Fig. 10. Orbifold for $C_{\infty h} = \infty/m$, $D_\infty = \infty 2$, and $D_{\infty h} = \infty mm$ group action on S_2 induced by natural action of $O(3)$. The stabilizer for two-point-orbit is, respectively, C_∞, C_∞, and $C_{\infty v}$. The stabilizer for one circle orbit is C_s, C_2, and C_{2v}. The stabilizer for two-circle-orbit is C_1, C_1, and C_s.

vertices), six axes of rotations by π (they contain the middle of opposite edges). Hence the existence of seven strata:

- the generic three-dimensional stratum contains all points which do not belong to a symmetry plane: stabilizer $C_1 = 1$; each orbit includes 48 points;
- the two-dimensional strata whose stabilizers are $[C_s]_{O_h} = Pm$ and $[C'_s]_{O_h} = Cm$, respectively: they contain all points belonging to a unique symmetry plane: P_i and P'_j, respectively; each orbit consists of 24 points;
- the stratum of stabilizers $[C_{3v}]_{O_h} = R3m$, it contains all points which are at the intersection of only three symmetry planes of type P'_j and it has an alternative description as the union of four three-fold rotation axes minus the origin; each orbit includes eight points;
- the stratum of stabilizers $[C_{2v}]_{O_h} = Amm2$, it contains all points which are at the intersection of only two symmetry planes, one of type P_i the other of type P'_j and it is the union of six two-fold rotation axes minus the origin; each orbit includes 12 points;
- the stratum of stabilizers $[C_{4v}]_{O_h} = P4mm$, it contains all points which are at the intersection of only four symmetry planes, two of type P_i and the other two of type P'_j, that stratum is the union of three four-fold rotation axes minus the origin; each orbit consists of six points;
- the maximal stratum contains only one point, fixed by $O_h = Pm\bar{3}m$: the origin.

The nine symmetry planes partition the space V_3 into 48 convex cones; any one closed cone can be identified with an orbit space. The corresponding space of orbits is given in Fig. 11.

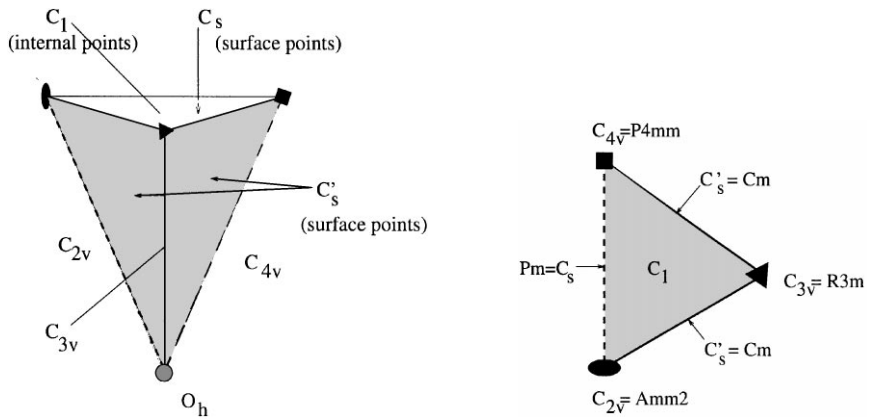


Fig. 11. Orbifold for $O_h = Pm\bar{3}m$ group action on 3-D-space induced by natural action of $O(3)$. Seven different strata are given by their stabilizers.

Fig. 12. Orbifold for O_h group action on S_2 deduced from its action on 3-D-space. Six different strata are given by their stabilizers.

3b. The non-linear action of $O_h = Pm\bar{3}m$ on S_2 is deduced from the previous action. There are no fixed point. The three maximal strata have for stabilizers: $[C_{4v}]_{O_h} = P4mm$, $[C_{3v}]_{O_h} = R3m$, $[C_{2v}]_{O_h} = Amm2$ and each contains a unique orbit of 6, 8, 12 points, respectively. The orbit space is a two-dimensional orbifold schematically represented in Fig. 12 as a filled triangle. Each of its three vertices represents the orbit of a maximal stratum; the open edge between the vertices $[C_{4v}]_{O_h} = P4mm$ and $[C_{2v}]_{O_h} = Amm2$ represents the one-parameter family of 24-point orbits with stabilizers forming $[C_s]_{O_h} = Pm$. The other two open edges represent the stratum whose 24-point orbits have $[C'_s]_{O_h} = Cm$ as stabilizers. The inside of the triangle represents the $|O_h| = 48$ point orbits of the generic stratum.

3c. The action of two-element inversion group $C_i = P\bar{1}$ on two-dimensional sphere S_2 induced by its natural action on three-dimensional space. This action is free. All orbits formed by two opposite points on the sphere are principal and there is only one stratum. The space of orbits is a manifold, namely the real projective space RP_2.

4. The action of $SO(2)$ group on the direct product of two-dimensional spheres $S_2 \times S_2$. To define such an action we introduce explicitly spheres in three-dimensional space as $\sum x_i^2 = R_1^2$ and $\sum y_i^2 = R_2^2$ and consider the diagonal action of the $SO(2)$ group as a simultaneous rotation around x_3 and y_3 axes of two spheres. It is clear that this action creates two kind of orbits. There are four exceptional one-point orbits with the stabilizer $SO(2)$. These four orbits correspond to the choice of north or south pole on each of two spheres.

All other orbits are circles which have a trivial stabilizer and can be characterized by specifying the relative orientation of two vectors defined on two spheres. We can specify each orbit by two projections of corresponding vectors on axes x_3 and y_3, by scalar product of these vectors, and by additional parameter which distinguishes the orientation of the triple formed by two vectors and the axis of rotation. This construction arises quite naturally in the classical analysis of the Rybderg

atoms and molecules (see Chapter III) and in the problem of coupling of two angular momenta (Sadovskii and Zhilinskii, 1999).

5. Action of the $SO(2)$ group on the N-dimensional complex space C_N. Let us define the action of $SO(2)$ group on N complex variables through

$$(z_1, z_2, \ldots, z_N) \to (z_1 e^{i\phi}, z_2 e^{i\phi}, \ldots, z_N e^{i\phi}) . \tag{25}$$

This action leaves invariant the norm $\sum_i |z_i|^2$. For each non-zero norm the space of orbits gives the complex projective space CP_{N-1} (Cox et al., 1992; Mumford, 1976).

The construction of the complex projective space as a space of orbits of the $SO(2)$ group acting on N complex variables will be studied in more details in Chapter II devoted to molecular models because this construction is naturally related to the reduction of the dynamic symmetry in the study of the internal structure of the so-called vibrational polyads (Zhilinskii, 1989a).

One sees immediately that the restriction of the action of the $SO(2)$ group defined on C_N to $2N-1$ real-dimensional sphere possesses N exceptional one point orbits whose homogeneous coordinates are

$$(z_1, 0, \ldots, 0), \quad (0, z_2, 0, \ldots, 0), \quad \ldots, \quad (0, \ldots, 0, z_N) . \tag{26}$$

6. Action of a finite group on complex projective space CP_2. The action of a finite group on the complex projective space can be naturally induced from its action on initial complex variables (Zhilinskii, 1989a) after constructing the complex projective space as a space of orbits of $SO(2)$ action on C_N given by Eq. (25). As the simplest example here we define the action of the two-elements group $C_2 = \{E, C_2\}$ on three complex variables (z_1, z_2, z_3) as

$$E(z_1, z_2, z_3) \to (z_1, z_2, z_3) , \tag{27}$$

$$C_2(z_1, z_2, z_3) \to (-z_1, z_2, z_3) . \tag{28}$$

This action induces the action on the points of CP_2 space given by their homogeneous coordinates (z_1, z_2, z_3). There is one isolated orbit with the stabilizer C_2, namely the point $(1, 0, 0)$ of C_2 (having the homogeneous coordinates $(z_1, 0, 0)$), and a continuous set of orbits with the stabilizer C_2 (having the homogeneous coordinates $(0, z_2, z_3)$). All these C_2 invariant points form $CP_1 \sim S_2$ invariant two-dimensional sub-manifold of the four-dimensional CP_2 space. This example of the group action is in some sense trivial but it is interesting because the C_2 stratum is the union of a two-dimensional manifold and an isolated point (Fig. 13).

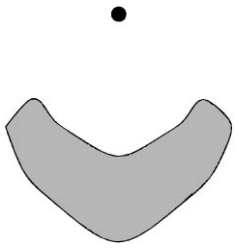


Fig. 13. Schematic representation of the stratification of CP_2 space under the action of C_2 group. Isolated point and S_2 surface formed by points with C_2 local symmetry. All other orbits are generic two-point orbits with trivial stabilizer.

Another interesting and important example of the action of two-element group on CP_2 space is the action through complex conjugation. Set of CP_2 space points invariant with respect to complex conjugation form two-dimensional invariant sub-manifold which is a real projective space RP_2 from the topological point of view. All other points form generic two-point orbits. The space of orbits is the S_4 space from the topological point of view (Kuiper, 1974; Massey, 1973; Arnol'd, 1988).

3.5. Representations. Non-effective actions. Kernels and images of the irreducible representations of 3-D-point groups

Very often in physics under the presence of a symmetry group G we analyze properties of functions constructed from variables which span themselves some representation Γ (we can limit ourselves with the study of irreducible representations) of the symmetry group G (the model space V of the representation Γ). In such a case the action of the symmetry group G of the initial physical problem on V depends on the representation and can be described as the natural vector representation of another group $\mathrm{Im}_\Gamma(G)$ acting in the space V. The group $\mathrm{Im}_G(\Gamma)$ is the image of the group G in the representation Γ. From the mathematical point of view it is the quotient group $G/\mathrm{Ker}\,\Gamma$ of the initial group G over the kernel of the representation Γ ($\mathrm{Ker}\,\Gamma$ is an invariant subgroup of G represented in Γ by identity). In many cases it is sufficient to study only different images. The model is independent of the initial group and representation if their images are the same (Michel and Mozrzymas, 1978; Michel, 1980; Zhilinskii, 1989b; Izyumov and Syromyatnikov, 1984). The extreme case is the trivial representation of any group G; its image is $C_1 = 1$ and the kernel is the group itself. Image of group G in any of its one-dimensional real (but not trivial) representation is always a group z_2 of order 2 and the kernel enables us to distinguish different representations. In particular, Table 2 defines the vector representation which is also a faithful representation for $O_h = Pm\bar{3}m$ group. This representation is used further in Table 4 below (Section 5.4) to give the system of invariants for all subgroups of $O_h = Pm\bar{3}m$.

More generally one needs to know both the image and the kernel of the representation but this information is not sufficient to completely describe different irreducible representations.

From Table 1 we can immediately define the unitary irreducible representations (unirreps for short) of the 32 crystallographic geometric classes of point groups. First we recall that geometric classes form only 18 isomorphic classes; nine of them are Abelian. The others are the direct product of one of the four groups D_3, D_4, T, O with Abelian groups. We recall that the images of unirreps of finite groups are cyclic (i.e. $1, Z_n$) and that the unirreps of a direct product of two groups is the tensor product of their unirreps.

Many books list these unirreps with their characters. It is unnecessary to reproduce them here. But it is very useful to characterize these unirreps by their kernel and their image. These 163 unirreps of crystallographic point groups have only 13 distinct images: $1, z_2, z_3, z_4, z_6, c_{3v}, c_{4v}, c_{6v}$, T, T_h, T_d, O, O_h. Remark that among these images there are five one-dimensional, three two-dimensional, and five three-dimensional.

For 32 crystallographic groups, the couple Ker, Im characterizes all their unirreps except those of images z_3, z_4, z_6, O_h which correspond to pairs of unirreps obtained from each others through an involutive outer automorphism of the image which does not correspond to equivalent representations with the same kernel. For the three cyclic images z_3, z_4, z_6 it corresponds to their complex

conjugation. For $O_h = Pm\bar{3}m$ it is the automorphism which exchanges the following conjugacy classes of its subgroups: $P\bar{4}3m \leftrightarrow P432$, $P\bar{4}2m \leftrightarrow P422$, $P\bar{4}m2 \leftrightarrow P4mm$, $P\bar{4} \leftrightarrow P4$, $R3m \leftrightarrow R32$, $Cmm2 \leftrightarrow C222$, $Cm \leftrightarrow C2$. We distinguish these two representations of $O_h = Pm\bar{3}m$ with the same image by using notation O_h for the vector representation and O_h' for the other one.

The unirreps of the 32 geometric point groups are characterized below by their images and kernels. (We omit the trivial group $C_1 = 1$ which has the only trivial representation.) 15 non-trivial Abelian geometrical classes forming eight isomorphy classes give

Ker	$\bar{1} = C_i$	1	Ker	$2/m = C_{2h}$	$\bar{1}$	2	m
Ker	$2 = C_2$	1	Ker	$mm2 = C_{2v}$	m_x	$m_y 2$	2_z
Ker	$m = C_s$	1	Ker	$222 = D_2$	2_x	2_y	2_z
Im	1	z_2	Im	1	z_2	z_2	z_2

Ker	$mmm = D_{2h}$	$mm2_x$	$mm2_y$	$mm2_z$	222	$(2/m)_x$	$(2/m)_y$	$(2/m)_z$
Im	1	z_2	z_2	z_2	z_2	z_2	z_2	z_2

Ker	$4 = C_4$	2	1	Ker	$4/m = C_{4h}$	$(2/m)$	4	$\bar{4}$	m	$\bar{1}$
Ker	$\bar{4} = S_4$	2	1	Im	1	z_2	z_2	z_2	$z_4, \bar{z}_4$	$z_4, \bar{z}_4$
Im	1	z_2	$z_4, \bar{z}_4$							

Ker	$3 = C_3$	1	Ker	$6 = C_6$	3	2	1
Im	1	$z_3, \bar{z}_3$	Ker	$\bar{3} = C_{3i}$	3	$\bar{1}$	1
			Ker	$\bar{6} = C_{3h}$	3	m	1
			Im	1	z_2	$z_3, \bar{z}_3$	$z_6, \bar{z}_6$

Ker	$6/m = C_{6h}$	$\bar{3}$	$\bar{6}$	6	$2/m$	m	2	$\bar{1}$
Im	1	z_2	z_2	z_2	$z_3, \bar{z}_3$	$z_6, \bar{z}_6$	$z_6, \bar{z}_6$	$z_6, \bar{z}_6$

For 16 non-Abelian geometrical classes forming nine isomorphy classes we have the following description of unirreps by their images and Kernels:

Ker	$4mm = C_{4v}$	4	$mm2$	$mm2'$	1
Ker	$422 = D_4$	4	222	$222'$	1
Ker	$\bar{4}m2 = D_{2d}$	$\bar{4}$	222	$mm2$	1
Im	1	z_2	z_2	z_2	c_{4v}

Ker	$4/mmm = D_{4h}$	$4/m$	mmm	mmm'	422	$4mm$	$\bar{4}m2$	$\bar{4}m2'$	$\bar{1}$	m
Im	1	z_2	z_2	z_2	z_2	z_2	z_2	z_2	c_{4v}	c_{4v}

Ker	$6mm = D_{6v}$	6	$3m$	$3m'$	2	1
Ker	$622 = D_6$	6	32	32′	2	1
Ker	$\bar{3}m = D_{3d}$	$\bar{3}$	32	$3m$	$\bar{1}$	1
Ker	$\bar{6}m2 = D_{3h}$	$\bar{6}$	32	$3m$	2	1
Im	1	z_2	z_2	z_2	c_{3v}	c_{6v}

Ker	$6/mmm = D_{6h}$	$\bar{6}$	$\bar{3}m$	$\bar{3}m'$	622	$6mm$	$\bar{6}m2$	$\bar{6}2m$	$2/m$	$\bar{1}$	$2\ m$
Im	1	z_2	z_2	z_2	z_2	z_2	z_2	z_2	c_{3v}	c_{6v}	$c_{6v}c_{6v}$

Ker	$23 = T$	222	1	Ker	$m\bar{3} = T_h$	23	mmm	222	$\bar{1}$	1
Im	1	$z_3, \bar{z}_3$	T	Im	1	z_2	$z_3, \bar{z}_3$	$z_6, \bar{z}_6$	T	T_h

Ker	$\bar{4}3m = T_d$	23	222	1	1
Ker	$432 = O$	23	222	1	1
Im	1	z_2	c_{3v}	O	T_d

Ker	$m\bar{3}m = O_h$	$m\bar{3}$	432	$\bar{4}3m$	mmm	222	$\bar{1}$	$\bar{1}$	1	1
Im	1	z_2	z_2	z_2	c_{3v}	c_{6v}	O	T_d	O_h	O'_h

4. Compact group smooth actions; their critical orbits; their linearization

One can say more on the strata in the cases of our applications; indeed we shall deal most often with smooth actions of compact Lie groups or finite groups (which are the particular cases of Lie groups of dimension zero) on finite-dimensional manifolds M. We quote here some theorems that we shall need in our applications:

Theorem 4a (Montgomery and Yang, 1957). *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional manifold, the set of strata is finite. There exists a unique stratum with minimal symmetry; it is open dense in M. The maximal strata are closed; more generally the union of a stratum S and of all the strata* $> S$ *is a closed set.*

The open dense stratum is often called *the generic stratum*. From this theorem we can prove (see also, (Michel, 1971) for a direct proof) the

Corollary 4a.[9] *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional manifold M, at each point* $m \in M$ *one can define a neighborhood* $\mathscr{V}_m$ *such that* $x \in \mathscr{V}_m \Rightarrow G_x \leq G_m$ *up to a conjugation.*

Given a smooth action of G on the manifold M, at $m \in M$, the stabilizer G_m acts linearly on the tangent hyper-plane $T_m(M)$ of M at m. A G-invariant vector field $\boldsymbol{v}(m)$ on M has to be a fixed vector of G_m, which leads to

Lemma. *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional manifold M, a G-invariant vector field on M must at each point* $m \in M$ *be tangent to the closure of the stratum of m; i.e.* $v(m) \in T_m(S(m))$:

This lemma imposes no condition for the gradient at points of the generic stratum. In many examples we have seen, the closure of strata are symmetry axes, symmetry planes, etc.; it is obvious from symmetry that at points of a symmetry axis, of a symmetry plane, etc., an invariant vector field must be along the symmetry axis, inside the symmetry plane, etc.

Let f be a function on M; if G is finite, $|G|^{-1}\sum_{g\in G} f(g^{-1}\cdot m)$ is the average of f on G; it is easy to verify that it is a G-invariant function. This average can be generalized to a compact Lie group; indeed on such a group there exists, up to a factor an invariant measure $\mu(g)$ which can be normalized by $\int_G \mu(g) = 1$. Then the average of f on G is $\int_G f(g^{-1}\cdot m)\mu(g)$. By taking the average on G of an arbitrary Riemann metric we obtain a G-invariant Riemann metric on M. Since a G-invariant function f is constant on each orbit, at each point m of the orbit, the gradient of f has to be in the normal plane $N_m(G\cdot m)$ to the orbit. This condition is trivial for finite groups.

We can always take a local system of geodesic coordinates. In this system we can identify $T_m(M)$ with M and $N_m(G\cdot m) = T_m(G\cdot m)^{\perp}$ is called the *slice* in the mathematical literature. Indeed every orbit in a neighborhood of $G\cdot m$ cuts the slice transversally. Moreover the linear representation of G_m on $T_m(M)$ is orthogonal. Combining the condition $\nabla f(m)$ (= the gradient of f at m) with that imposed by Lemma 4a we obtain

$$\nabla f(m) \in F(m) = T_m(S(m)) \cap N_m(G\cdot m)\ . \tag{29}$$

Equivalently, the orthogonal representation of G_m at m can be decomposed into the direct sum of three representations and that on $F(m)$ is a trivial representation. It is of dimension zero ($F(m) = m$) if the tangent plane to the stratum, $T_m(S(m))$ coincides with the tangent plane to the orbit. That means that the orbit is *isolated in its stratum* (= there are no other orbits of the same stratum in a neighborhood of m). In that case $\nabla f(m) = 0$ and this is independent of the function:

Theorem 4b (Michel, 1971). *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional manifold M, the gradient of every G-invariant functions vanishes on the orbits which are isolated in their strata. These orbits are called* critical.

[9] A corollary is labeled by the number of the theorem to which it relates.

That is the case when a stratum contains a finite number of orbits. Then it is closed, since the orbits are closed. The converse of that theorem was also proven by Michel (1971) as well as the next theorem. As we saw (Theorem 4a), it is equivalent for a stratum to be of maximum symmetry or to be closed; if moreover M is compact, then the closed strata are compact. The first proof of the theorem was given in Michel (1970) (Theorem 2, p.133).

Theorem 4c (Michel, 1970). *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional compact manifold M*, *on a closed stratum containing an infinity of orbits*, *the gradient of each G-invariant function vanishes at least on two orbits of the stratum.*

These orbits might be different for different functions. The proof can be sketched as follows: every continuous function on a compact has at least one maximum and one minimum; that occurs for the restriction to the stratum of every G-invariant function on M. Since the gradient of the whole function is tangent to the stratum, on it the zeroes of the gradients of the restriction and of the whole function coincide.

We can reformulate part of the last two theorem into

Corollary 4c. *In the smooth action of a compact* (*or finite*) *group G on a finite-dimensional compact manifold M*, *every G-invariant smooth function has orbits of extrema on* every *stratum with maximal symmetry. When such a stratum has a finite number of orbits all its orbits are critical*; *on the other maximal symmetry strata*, *every G-invariant function has at least two orbits of extrema on each connected component.*

In Section 6 we will recall all information we can obtain on the nature of each extremum.

When a physicist, interested for instance by spontaneous symmetry breaking, makes a model whose Lagrangian or any other function to be varied has an extremum on a maximal symmetry stratum, he verifies this corollary, but cannot claim that it is a specific success of his model!

An excellent monograph on the compact group smooth actions is that of Palais (1960) (see also, Bredon, 1972). In it he proves that the continuous map $M \xrightarrow{\pi} M|G$ of M on the orbit space is open and closed,[10] so the Montgomery Theorem 2a (Montgomery and Yang, 1957) applies also to the images of the strata in the orbit space. Palais (1961) has also shown that all the properties given here for compact groups are also true in the more general case of the action of a non compact Lie group (or countable discrete group) when *all* stabilizers are compact (or finite). We shall make two applications of this result in Chapter IV. One is for the action of a crystallographic space group on our space, the other for its action on the corresponding momentum space, called the Brillouin zone; instead to be described by a real vector space, it is a U_1^d group.

There are remarkable theorems on the compact group actions on compact manifolds; Palais (1970) proved that such a differentiable (in short C^1) action is equivalent to an infinitely differentiable (in short C^∞ or "smooth") action. In that case Mostow (Mostow, 1957a, b) proved that the number of strata ($= |(M||G)|$) is finite and that there exists an orthogonal representation of G on

[10] That is: the images of open sets are open sets, the image of closed sets are closed sets.

a finite-dimensional orthogonal space[11] V containing M in such a way that the action of G on M can be obtained as a restriction of the orthogonal representation of G on V.

In physical applications studied below the group actions are either linear representations on a real (orthogonal) vector space V or can be considered as their restriction to an invariant manifold contained in V. For example, in Chapter V we transform the non-linear action of an arithmetic class on the Brillouin zone to the orthogonal representation on higher-dimensional space.

So in all our applications the study of the group action on M can be obtained by the restriction of the action of an orthogonal linear representation to an invariant manifold $M \subset V$, the carrier space of the representation. That explains our interest in the next section.

4.1. Examples of critical orbits for group actions

Let us now return to examples of group actions on manifold cited in 3.4 from the point of view of critical orbits.

1. There is one critical orbit for the action of $O(n)$ group on orthogonal space V_n. It is the origin which is a fixed point (a one-point orbit with the stabilizer $O(n)$).

2. Action of $C_\infty = \infty$ and $C_{\infty v} = \infty m$ subgroups of the $O(3)$ group on a two-dimensional sphere induced by the natural action of $O(3)$ group on 3-D space leads to two one-point critical orbits with the same stabilizer (two poles of the sphere). At the same time action of $C_{\infty h} = \infty/m$ and $D_{\infty h}\ \infty/mm$ subgroups induces appearance of one two-point critical orbit with the stabilizer C_∞ or $C_{\infty v}$ (two poles) and one critical manifold (the equator, having S_1 topology).

3. Action of the point group $O_h = Pm\bar{3}m$ on the 3-D space gives only one critical orbit, namely the origin with the stabilizer O_h. At the same time the restriction of this action on the two-dimensional sphere leads to several critical orbits: one six-point orbit with stabilizer $C_{4v} = P4mm$, one eight-point orbit with stabilizer $C_{3v} = R3m$, and one 12-point orbit with stabilizer $C_{2v} = Amm2$.

4. Action of the point group $C_i = \bar{1}$ on the 3-D space gives only one critical orbit, namely the origin with the stabilizer $C_i = \bar{1}$. At the same time the restriction of this action on the two-dimensional sphere possesses no critical orbits.

5. Natural diagonal action of the $SO(2)$ group on the direct product of two two-dimensional spheres $S_2 \times S_2$ possesses four critical orbits which are stationary points for any smooth $SO(2)$ invariant function defined over $S_2 \times S_2$.

6. Natural diagonal action of the $SO(2)$ group on the space of N complex variables restricted to the sphere $\sum_i |z_i|^2 = \text{const}$ (see Eq. (25)) possesses N isolated critical points.

5. Rings of *G*-invariant functions

Given an n-dimensional linear orthogonal representation on V_n of a compact (or finite) group G, all C^∞ (i.e. infinitely differentiable) G-invariant functions are C^∞ functions of invariant polynomials

[11] Unfortunately the proof does not give an upper bound on $\dim(V)$.

(this is the statement of the Schwarz theorem (Schwarz, 1975)). So we can restrict our study to the ring $\mathscr{P}_n^G$ of invariant polynomials on V_n ($\mathscr{P}_n^G$ is a ring since the sum and the product of invariant polynomials are invariant polynomials). For more details on the structure of $\mathscr{P}_n^G$ see the reviews (Stanley, 1979; Jaric et al., 1984).

We must first recall some results on the action of G on $\mathscr{P}_n$, the ring of polynomials on V_n (they depend on n variables). $\mathscr{P}_n$ is also an infinite-dimensional vector space of functions. We denote by $\mathscr{P}_n^{(m)}$ the subspace of homogeneous polynomials of degree m. That is a finite-dimensional subspace of $\mathscr{P}_n$:

$$\mathscr{P}_n = \bigoplus_{m=0}^{\infty} \mathscr{P}_n^{(m)}, \quad \dim(\mathscr{P}_n^{(m)}) = \binom{m+n-1}{m}. \tag{30}$$

Let $\boldsymbol{v} \in V_n$ and $p \in \mathscr{P}_n$. The action of G on $\mathscr{P}_n$ is defined by

$$g \cdot p(\boldsymbol{v}) = p(g^{-1} \cdot \boldsymbol{v}). \tag{31}$$

This equation shows in particular that if the representation of G on V_n contains the matrix $-I_n$, every invariant polynomial must contain only monomials of even degree. It is easy to obtain an invariant polynomial starting from an arbitrary polynomial. One simply sums all polynomials of a G-orbit: $q = \sum_{g \in G} g \cdot p(\boldsymbol{v})$. This construction is well known in physical and chemical applications as a projection operator (Hamermesh, 1964) whereas in mathematics it is often referred as Reynolds operator (Sturmfels, 1993). Another systematic procedure for the invariant construction (especially for high-order invariants) is based on the coupling of irreducible tensors using vector coupling coefficients (mainly known to physicists and chemists as Clebsch–Gordan or Wigner coefficients (Wigner, 1959; Hamermesh, 1964; Biedenharn and Louck, 1981a, b)).

Let us consider before going to a generalization a simple example of the construction of the system of invariants for an Abelian group c_n acting in the natural way on the two-dimensional vector representation x, y. Changing the variable x, y into the complex linear combinations $x \pm \mathrm{i}y$ we diagonalize the two-dimensional representation. Now the construction of invariants is straightforward. We can construct one invariant of degree 2, namely $(x + \mathrm{i}y)(x - \mathrm{i}y) = x^2 + y^2$ and two linearly independent invariants of degree n, which can be chosen as $\mathfrak{Re}(x + \mathrm{i}y)^n$ and $\mathfrak{Im}(x + \mathrm{i}y)^n$. It is important to note that the three invariants are not algebraically independent. There is an algebraic relation between them

$$(x^2 + y^2)^n = (\mathfrak{Re}(x + \mathrm{i}y)^n)^2 + (\mathfrak{Im}(x + \mathrm{i}y)^n)^2 . \tag{32}$$

The existence of this relation (in theory of invariants, this type of relations is named *syzygy*) means that to construct all linearly independent invariants we can take all polynomials in two algebraically independent invariants (say $x^2 + y^2$ and $\mathfrak{Re}(x + \mathrm{i}y)^n$, we will name them basic invariants) and form arbitrary polynomials $\mathscr{P}(x^2 + y^2, \mathfrak{Re}(x + \mathrm{i}y)^n)$ and similar arbitrary polynomial multiplied by the third invariant (we will name it auxiliary invariant) $\mathscr{P}(x^2 + y^2, \mathfrak{Re}(x + \mathrm{i}y)^n)\mathfrak{Im}(x + \mathrm{i}y)^n$. This means that all c_n invariants form the module[12] of dimension two over the ring formed by two basic invariants.

[12] A module is similar to a vector space except that its scalars do not form a field, but only a ring (not every scalar is divisible by another one $\neq 0$). The property that every vector space has bases extends only to free modules. For a very simple counter-example see Eq. (27) in Ref. (Jaric et al., 1984).

As soon as we have the system of c_n invariants we can immediately construct the system of c_{nv} invariants using the fact that c_n is an invariant subgroup of c_{nv} (see Section 3). The action of the quotient group $z_2 = c_{nv}$: c_n on c_n invariants shows that the basic invariants of c_n remain invariants of the larger group c_{nv}. At the same time the auxiliary invariant of c_n becomes the pseudoinvariant of c_{nv} because it changes the sign under the z_2 action. Consequently to construct all invariants of c_{nv} it is sufficient to take an arbitrary polynomial in two basic invariants $\mathscr{P}(x^2 + y^2, \Re e(x + iy)^n)$. We see that the module of invariants of the higher group c_{nv} is a submodule of the module of invariants of a smaller group c_n. We give here this simple example because many more complicated examples treated further in this and following chapters are based essentially on the same construction.

Now we want to proceed to a systematic knowledge of $\mathscr{P}^G$ in all orders. To perform such an analysis we remark that the action defined in Eq. (31) transforms the $\mathscr{P}_n^{(m)}$ into themselves. The character $\chi^{(m)}(g)$ of the linear representation of G on $\mathscr{P}_n^{(m)}$ was first given by Molien (1897) more than one hundred years ago through the generating function

$$\sum_{m=0}^{\infty} \chi^{(m)}(g)\lambda^m = \det(I_n - \lambda g)^{-1} , \tag{33}$$

where λ is a dummy variable. We label by an index α the different equivalent classes of irreducible representations of the compact or finite group G (with $\alpha = 0$ for the trivial representation) and we denote by $\chi_\alpha(g)$ the corresponding character. Let $c_\alpha^{(m)}$ be the multiplicity of the irreducible representation α which appears in the G representation on $\mathscr{P}_n^{(m)}$; when G is finite, its value can be computed from the Molien generating functions (Burnside, 1911; Weyl, 1939):

$$M_\alpha(\lambda) \equiv \sum_{m=0}^{\infty} c_\alpha^{(m)}\lambda^m = |G|^{-1}\sum_{g\in G} \bar{\chi}_\alpha(g)\det(I_n - \lambda g)^{-1} . \tag{34}$$

To extend this formula to Lie groups, one must replace the group average $|G|^{-1}\sum_{g\in G}$ by the integral on the group $\int_G d\mu(g)$ where $\mu(g)$ is an invariant measure on G whose integral is normalized to 1. The Molien functions are rational fractions (i.e. ratios of polynomials) in λ. It is quite important that these rational functions give symbolic information about the structure of the ring of invariant polynomials rather than the numbers of invariants in every degree.

To explain the symbolic meaning of Molien generating functions we start with an example of one specific class of groups. Chevalley (1955) proved that for finite groups generated by reflections the following theorem takes place.

Theorem Chevalley 1. *The ring $\mathscr{P}^G$ of invariant polynomials of a finite reflection group G acting on the orthogonal space V_n, is an n-variable polynomial ring.*

In the same paper Chevalley (1955) proved the second theorem:

Theorem Chevalley 2. *For a finite reflection group G, the ring $\mathscr{P}$ of the polynomials on V_n is a free module on the ring $\mathscr{P}^G$ of invariant polynomials; its dimension is $|G|$ and it carries the regular representation of G.*

More explicitly, $\mathscr{P}^G$ is the ring of all n variable polynomials whose variables are n algebraically independent polynomials θ_k, $1 \leq k \leq n$. The degrees d_k of the θ_k are obtained from the Molien function which has the form

$$M(\lambda) = \frac{N(\lambda)}{D(\lambda)} \quad \text{with } N = 1, \quad D = \prod_{k=0}^{n} (1-\lambda)^{d_k} \,. \tag{35}$$

Parameters d_k are related with the structure of the group G itself, namely,

$$\prod_k d_k = |G|, \quad \sum_k (d_k - 1) = b_1 \,, \tag{36}$$

where $|G|$ is the order of group G and b_1 is a number of reflections in G. More generally (as was found empirically by Shephard, 1956 and proved by Solomon, 1963)

$$\prod_k^n (1 + (d_k - 1)t) = \sum_j^n b_j t^j \,, \tag{37}$$

where b_j is the number of elements of G whose space of invariant vectors has dimension $n - j$.

For finite groups which are not generated by reflections, the Molien function M has still a denominator of the form (35). The numerator $N(\lambda)$ is a polynomial with positive coefficients

$$N(\lambda) = \sum_\delta v_\delta \lambda^\delta, \quad v_\delta > 0 \,. \tag{38}$$

In the case of a Molien function for invariants we always have $N(0) = v_0 = 1$. In contrast, the Molien function for covariants does not have a constant term in the numerator.

For each power δ which appears in the numerator polynomial (38), there exist v_δ G-invariant linearly independent homogeneous polynomials φ_α of degree δ; of course these polynomials have to be algebraic functions of the n "denominator invariants" θ_k (see below). The ring $\mathscr{P}^G$ is a free module and the $N(1)$ polynomials φ_α's form a basis of it. That is, there is a unique way to write any G-invariant polynomial as a linear combination of the φ_α's:

$$p = \sum_{\alpha=0}^{|N(1)|-1} p_\alpha(\theta_k(x_j))\varphi_\alpha(x_j) \quad \text{with } \varphi_0 = 1 \,, \tag{39}$$

where the coefficients p_α's are n variable polynomials. Moreover every n-variable polynomial (with the θ_i's as variable) can appear in such a decomposition. A similar decomposition is valid for covariants but now there is no $\varphi_0 = 1$ term.

For any finite group G there exists a general relation between numbers and degrees of denominator and numerator invariants and the structure of group G, namely with its order $|G|$ and the number of reflections r contained in G (see p. 487 of Stanley, 1979).[13] Let $d_1, d_2, \ldots, d_n$ be the degrees of denominator invariants and $e_1, e_2, \ldots, e_t$ the degrees of numerator invariants

[13] This formula was proved by Stanley (1979) in the more general case of complex groups with reflexions replaced by pseudoreflexions, i.e. symmetry operations with one eigenvalue $s \neq 1$, $|s| = 1$ different from 1.

(The number t of numerator invariants includes unity as a numerator invariant of degree 0). Then the following relation generalizes relation (36)

$$t|G| = d_1 d_2 \cdots d_n \,, \tag{40}$$

$$rt + 2(e_1 + \cdots + e_t) = t(d_1 + \cdots + d_n - n) \,. \tag{41}$$

5.1. Molien function manipulations

We want in this section to give some useful formula for Molien function calculations which will be used later in this issue. Some of them are well known, others are less frequently used, especially in physical applications. Much more still can be found in mathematical literature.

We start with rewriting the Molien generating function (34) using more detailed notation which specifies explicitly the group G and the initial Γ_i and final Γ_f representations.

$$M^G(\Gamma_f;\Gamma_i;\lambda) = |G|^{-1}\sum_{g\in G}\bar{\chi}^{\Gamma_f}(g)\det(I_n - \lambda\Gamma_i(g))^{-1} \,. \tag{42}$$

In fact the Molien function depends only on the image of the group G in the representation Γ_i, but for physical applications often it is useful to construct the Molien functions for all different irreducible representations of the same group.

Moreover very often the space of variables span the reducible representation. In such a case, if the Γ_i is reducible and decomposes as $\Gamma_i = \Gamma_{i_1}\oplus\Gamma_{i_2}$ we have

$$M^G(\Gamma_f;\Gamma_{i_1}\oplus\Gamma_{i_2};\lambda) = \sum_{\Gamma_{f_1},\Gamma_{f_2}} n^{\Gamma_f}_{\Gamma_{f_1}\Gamma_{f_2}} M^G(\Gamma_{f_1};\Gamma_{i_1};\lambda)M^G(\Gamma_{f_2};\Gamma_{i_2};\lambda) \,, \tag{43}$$

where $n^{\Gamma_f}_{\Gamma_{f_1}\Gamma_{f_2}}$ are the multiplicities of Γ_f in the decomposition of the product $\Gamma_{f_1}\otimes\Gamma_{f_2}$ into irreducible representations (Hamermesh, 1964)

$$\Gamma_{f_1}\otimes\Gamma_{f_2} = \sum_{\Gamma_f} n^{\Gamma_f}_{\Gamma_{f_1}\Gamma_{f_2}}\Gamma_f \,. \tag{44}$$

In the particular case of invariants (we put $\Gamma_f = \Gamma_0$ for invariants) formula (43) simplifies into

$$M^G(\Gamma_0;\Gamma_{i_1}\oplus\Gamma_{i_2};\lambda) = \sum_{\text{all }\Gamma} M^G(\Gamma;\Gamma_{i_1};\lambda)M^G(\Gamma^*;\Gamma_{i_2};\lambda) \,. \tag{45}$$

If the initial representation is a direct sum of two representations we can distinguish Γ_{i_1} and Γ_{i_2} by different auxiliary variables thus constructing the Molien function with two parameters. For example, instead of (43) we can write

$$M^G(\Gamma_f;\Gamma_{i_1}\oplus\Gamma_{i_2};\lambda,\mu) = \sum_{\Gamma_{f_1},\Gamma_{f_2}} n^{\Gamma_f}_{\Gamma_{f_1}\Gamma_{f_2}} M^G(\Gamma_{f_1},\Gamma_{i_1};\lambda)M^G(\Gamma_{f_2},\Gamma_{i_2};\mu) \,. \tag{46}$$

This formula will be quite useful for the construction of the integrity basis for reducible representations from known integrity bases for irreducible components.

In some cases one needs to calculate the total number of terms of several different symmetry types. In such a case one is interested in generating functions for final representations

Γ_f being the direct sum of representations $\Gamma_f = \Gamma_1 \oplus \Gamma_2$, the corresponding generating function has the form

$$M^G(\Gamma_1 \oplus \Gamma_2; \Gamma_i; \lambda) = M^G(\Gamma_1; \Gamma_i; \lambda) + M^G(\Gamma_2; \Gamma_i; \lambda) \,. \tag{47}$$

In particular if the final representation is the regular representation $\Gamma_{\text{reg}} = \oplus_k |\Gamma_k| \Gamma_k$, we simply count the total sum of polynomials which can be constructed from initial variables (see Theorem Chevalley 2), this means

$$M^G(\Gamma_f = \Gamma_{\text{reg}}; \Gamma_i; \lambda) = \frac{1}{(1-\lambda)^{|\Gamma_i|}} \,. \tag{48}$$

Generating functions for the number of invariants and all possible covariants for all finite groups can be found in Ref. (Patera et al., 1978; Desmier and Sharp, 1979) Below, we give several simple examples.

The generating function for the initial trivial representation Γ_0 ($\text{Im}\,\Gamma_0 = C_1 = 1$) of any group G is trivial

$$M^G(\Gamma_0; \Gamma_0; \lambda) = \frac{1}{1-\lambda} \,. \tag{49}$$

In the case of real one-dimensional but not totally symmetric representation Γ_1 ($\text{Im}\,\Gamma_1 = z_2$) the generating function for invariants has the form

$$M^G(\Gamma_0; \Gamma_1; \lambda) = \frac{1}{1-\lambda^2} \,, \tag{50}$$

whereas the generating function for the covariants of type Γ_1 is

$$M^G(\Gamma_1; \Gamma_1; \lambda) = \frac{\lambda}{1-\lambda^2} \,. \tag{51}$$

Generating functions for the invariants and the two types of covariants constructed from two-dimensional representations Γ_2 with $\text{Im}\,G = c_{3v}$ have the form

$$M^{c_{3v}}(\Gamma_0; \Gamma_2; \lambda) = \frac{1}{(1-\lambda^2)(1-\lambda^3)} \,, \tag{52}$$

$$M^{c_{3v}}(\Gamma_1; \Gamma_2; \lambda) = \frac{\lambda^3}{(1-\lambda^2)(1-\lambda^3)} \,, \tag{53}$$

$$M^{c_{3v}}(\Gamma_2; \Gamma_2; \lambda) = \frac{\lambda + \lambda^2}{(1-\lambda^2)(1-\lambda^3)} \,. \tag{54}$$

We can immediately verify relation (48) for this simple example.

$$M^{c_{3v}}(\Gamma_0; \Gamma_2; \lambda) + M^{c_{3v}}(\Gamma_1; \Gamma_2; \lambda) + 2M^{c_{3v}}(\Gamma_2; \Gamma_2; \lambda) = (1-\lambda)^{-3} \,. \tag{55}$$

Let us now consider the situation where the initial representation Γ_i is reducible. We take as an example the six-dimensional representation of the Abelian group C_4 which will be used later in Chapter V for the description of the ring of invariant functions on the Brillouin zone for the

tetragonal 3-D arithmetic classes. This particular representation Γ_6 has the following decomposition into irreducible representations of C_4 group.

$$\Gamma_6 = \gamma \oplus \sigma; \quad \gamma = [(1) \oplus (1) \oplus (-1)] , \quad \sigma = [(1) \oplus (-i) \oplus (i)] . \tag{56}$$

We use for the four complex irreducible representations of the group C_4 the following notation (1), $(i), (-1), (-i)$. From the physical reason (see Chapter V, Section 5.3) it is useful to treat separately two three-dimensional reducible representations σ and γ. To do that we use Molien function with two parameters and first remark the identity

$$\begin{aligned} M^{C_4}(\Gamma_f = 1; \Gamma_i = \gamma \oplus \sigma; \lambda, \mu) \\ = M^{C_4}(\Gamma_f = (1); \Gamma_i = \gamma; \lambda) M^{C_4}(\Gamma_f = 1; \Gamma_i = \sigma; \mu) \\ + M^{C_4}(\Gamma_f = (-1); \Gamma_i = \gamma; \lambda) M^{C_4}(\Gamma_f = (-1); \Gamma_i = \sigma; \mu) \end{aligned} \tag{57}$$

which follows from (46). Remark that only $\Gamma_f = 1, (-1)$ give non-zero contributions. Intermediate Molien functions can be easily calculated:

$$M^{C_4}(\Gamma_f = (1); \Gamma_i = \gamma; \lambda) = \frac{1}{(1-\lambda)^2 (1-\lambda^2)} , \tag{58}$$

$$M^{C_4}(\Gamma_f = (-1); \Gamma_i = \gamma; \lambda) = \frac{\lambda}{(1-\lambda)^2 (1-\lambda^2)} , \tag{59}$$

$$M^{C_4}(\Gamma_f = (1); \Gamma_i = \sigma; \mu) = \frac{1 + 2\mu^3 + \mu^4}{(1-\mu^2)^2 (1-\mu^4)} , \tag{60}$$

$$M^{C_4}(\Gamma_f = (-1); \Gamma_i = \sigma; \mu) = \frac{\mu + 2\mu^2 + \mu^5}{(1-\mu^2)^2 (1-\mu^4)} . \tag{61}$$

Thus, for the Molien function (57) we get the expression

$$M^{C_4}(\Gamma_f = 1; \Gamma_i = \gamma \oplus \sigma; \lambda, \mu) = \frac{1 + \lambda\mu + 2\lambda\mu^2 + 2\mu^3 + \mu^4 + \lambda\mu^5}{(1-\lambda)^2 (1-\lambda^2)(1-\mu^2)^2 (1-\mu^4)} . \tag{62}$$

Somewhat different interpretation of the information encoded in Molien function turns out to be quite useful if in physical applications we are interested in number of tensors of different symmetry types of various degrees. We remind that the power series expansion of the Molien function gives these numbers

$$M^G(\lambda) = \sum_N C_N \lambda^N . \tag{63}$$

Direct calculation of the formal series expansion gives these numbers numerically but in fact it is possible to give the function $C(N)$ which equals C_N for integer values of N. Moreover this function turns out to be relatively simple. For sufficiently high N it can be written in the form of a quasi-polynomial as discussed, for example, by Stanley (1986, Chapter 4.4).

A quasi-polynomial of degree d is a function $f: N \to C$

$$f(n) = c_d(n) n^d + c_{d-1}(n) d^{n-1} + \cdots + c_0(n) \tag{64}$$

with each term $c_i(n)$ being a periodic function with integer period. To illustrate the construction of such quasi-polynomial let us consider the generating function of the form

$$g(\lambda) = \frac{1}{(1-\lambda^{n_1})\cdots(1-\lambda^{n_s})}\,, \tag{65}$$

which has in the denominator the product of s terms $(1-\lambda^{n_i})$, $i=1,\ldots,s$ with positive integers $n_1,\ldots,n_s$. The formal expansion of $g(\lambda)$ gives the series

$$g(\lambda) = \sum_{N=0}^{\infty} C_N \lambda^N \tag{66}$$

and coefficients C_N can be considered as values of the function $C(N)$ defined for arbitrary N but taken for integer N.

$C(N)$ is a quasi-polynomial (64) of degree $s-1$ with oscillating coefficients. The period of oscillations equals the least common multiple, Δ, of all n_i. In fact the period can be different for different terms C_k

$$C_k(N) = C_k(N+\Delta_k)\,, \tag{67}$$

but all Δ_k divide Δ. The regular part of the quasi-polynomial can be unambiguously defined after averaging over the period Δ:

$$d_k^{\mathrm{reg}}(N) = \frac{1}{\Delta}\sum_{k=a+1}^{a+\Delta} C_k(N)\,. \tag{68}$$

The coefficients of the regular part of the quasi-polynomial

$$C^{\mathrm{reg}}(N) = \sum_{k=0}^{s-1} d_k^{\mathrm{reg}} N^k \tag{69}$$

can be related explicitly with the n_i numbers of the initial generating function. Several initial terms look like

$$d_{s-1}(n_1,\ldots,n_s) = \frac{1}{(s-1)!\prod n_i}\,, \tag{70}$$

$$d_{s-2}(n_1,\ldots,n_s) = \frac{\sum n_i}{2(s-2)!\prod n_i}\,, \tag{71}$$

$$d_{s-3}(n_1,\ldots,n_s) = \frac{3(\sum n_i)^2 - \sum n_i^2}{24(s-3)!\prod n_i}\,, \tag{72}$$

$$d_{s-4}(n_1,\ldots,n_s) = \frac{(\sum n_i)^3 - \sum n_i \sum n_i^2}{48(s-4)!\prod n_i}\,, \tag{73}$$

$$d_{s-5}(n_1,\ldots,n_s) = \frac{15(\sum n_i)^4 + 5(\sum n_i^2)^2 - 30(\sum n_i)^2\sum n_i^2 + 2\sum n_i^4}{8\cdot 6!(s-5)!\prod n_i}\,, \tag{74}$$

$$d_{s-6}(n_1,\ldots,n_s) = \frac{3(\sum n_i)^5 - 10(\sum n_i)^3\sum n_i^2 + 5\sum n_i(\sum n_i^2)^2 + 2\sum n_i\sum n_i^4}{16\cdot 6!(s-6)!\prod n_i}\,. \tag{75}$$

Let us remark that these coefficients are proportional to Todd polynomials, Td_i defined through the generating function as given, for example by Griffiths and Harris (1978, Section 3.4)

$$\frac{\det A}{\det(I - e^{-tA})} = (-1)^n t^{-n}\left\{\sum_i Td_i(P^1(a), \ldots, P^i(a))t^i\right\}, \tag{76}$$

where P^i are symmetric functions over eigenvalues of the matrix A. This means that in a formal way expressions (70)–(75) can be obtained from the generating function (65) by replacing $\lambda \to \exp(-w)$ and taking initial coefficients of the Laurent series (see Chapter II for some examples). This procedure can be generalized to calculate the oscillatory part.

5.2. *Integrity basis, syzygies, and other related notions*

We will use the name integrity basis for the basis formed by "denominator" and "numerator" invariants in order to follow notation used initially by Weyl (1939) and accepted in considerable part of physical literature (Gilmore and Draayer, 1985; Bickerstuff and Wyborne, 1976; Jaric and Birman, 1977; Judd et al., 1974; Schmelzer and Muller, 1985; Izyumov and Syromyatnikov, 1984). The same polynomial basis is referred in mathematical literature as homogeneous system of parameters (Stanley, 1979, 1996) or as Hironaka decomposition (Sturmfels, 1993).

From now on we shall write this structure of module as

$$\mathscr{P}^G = P[\theta_1, \theta_2, \ldots, \theta_n]\bullet(1, \varphi_1, \ldots, \varphi_k)\,. \tag{77}$$

We have to emphasize that this notation represents a ring and a module structure. Indeed any polynomial in the φ_α's is an invariant polynomial and should be written in a unique way as a linear combination of the φ's with coefficients in $P[\theta_1,\theta_2,\ldots,\theta_n]$. So Eq. (77) describes a structure of module algebra, i.e. an algebra whose vector space formed by its elements is replaced by a module of ring of scalars $P[\theta_1,\theta_2,\ldots,\theta_n]$ and of basis $\{\varphi_\alpha\}$. In the computation of the algebra module it might be useful to check its structure by computing its structure "constants"; they are polynomials in the θ_i's:

$$\varphi_\alpha\varphi_\beta = \sum_\gamma p^\gamma_{\alpha\beta}\varphi_\gamma, \quad p^\gamma_{\alpha\beta} = p^\gamma_{\beta\alpha} \quad \text{with } \varphi_0 = 1\,. \tag{78}$$

Throughout this issue we shall use the notation of Eq. (77); the θ_i, $(i = 1, \ldots, n)$ within the brackets are n algebraically independent ("denominator") invariants and φ_α, $(\alpha = 0, \ldots, k)$ with $\varphi_0 = 1$ are algebraically dependent ("numerator" or auxiliary) invariants which form the basis of the module of invariant polynomials. Given a ring $\mathscr{P}^G$, it can be represented by different modules. For example the obvious equivalence

$$\begin{aligned}\mathscr{P}^G &= P[\theta_1, \theta_2, \ldots, \theta_n]\bullet(1, \varphi_1, \ldots, \varphi_k)\\ &= P[\theta_1, \theta_2, \ldots, \theta_n^2]\bullet(1, \varphi_1, \ldots, \varphi_k)(1, \theta_n)\,.\end{aligned} \tag{79}$$

enables one to change the system of denominator invariants (to go from θ_n to θ_n^2) with simultaneous doubling of the number of numerator invariants. The Molien functions in both cases are the same, but to pass from the first form to the second form, the numerator and denominator of the first one are both multiplied by $(1 + \lambda^d)$, where d is the degree of θ_n. That possibility is quite useful when one wants to impose constraints on θ_n^2 rather than on θ_n, for example.

A similar, but more sophisticated equivalence appears in our discussion of Rydberg problems (see Chapter III). One should also note that there is a difficulty: it may happen that the generating function $M(\lambda)$ (35) could not be used under its most reduced form with positive coefficients in the numerator. Such a possibility is given by Sloane (1977, Eq. (47)), the reduced form cannot represent a module.

The symbolic interpretation of the Molien function introduced above is related with the structure of the integrity basis. There is another possibility of the symbolic interpretation (Hilbert, 1890, 1893). One can use all generators of the ring of invariants as denominator invariants. The number of generators is finite but it is larger than the number of algebraically independent polynomials. In such a case the numerator of the generating function has both positive and negative integer coefficients. The symbolic meaning of the numerator in this case is the relations (syzygies) between generators of the ring. For example the representation of the generating function for invariant polynomials in the form

$$M(\lambda) = \frac{1 - \sum \lambda^{f_i} + \sum \lambda^{g_i} - \cdots \pm \sum \lambda^{k_i}}{\prod (1 - \lambda^{d_i})} , \tag{80}$$

can be interpreted in the following way (see example in Section 5.4 below). There are s generators having the degree $d_1, d_2, \ldots, d_s$. The generators are algebraically dependent and there are t polynomial relations between these generators which are, respectively, of degree $f_1, f_2, \ldots, f_t$ with respect to initial variables (these relations are called syzygies of the first kind). Further, the set of syzygies of the first kind is not generically independent. There possibly exist some relations between syzygies of the first kind (syzygies of the second kind) characterized by degrees $g_1, g_2, \ldots, g_u$, etc. This approach introduced in invariant theory by Hilbert (Hilbert, 1890, 1893) enabled him to prove many important theorems, in particular to show that the number of generators and syzygies is finite. Description of the ring of invariant polynomials in terms of generators and syzygies is in some aspects complementary to the analysis based on the integrity basis construction. We will mainly use the explicit description of the system of invariants and the form of generating functions giving information about the integrity basis. The non-trivial example of the set of syzygies arising in very simple group action (spatial inversion in three-dimensional space) will be discussed in the example below.

One of the goals is to use the integrity basis to describe the space of orbits (the idea is to use invariant polynomials as coordinates on the space of orbits, see Section 5.6). By definition an invariant polynomial is constant along an orbit. Given two orbits, there is at least one polynomial of $\mathscr{P}^G$ (the ring of G-invariant polynomials whose variables are the coordinates of the vector space of the linear representation of G) which takes different values on them (see e.g. Michel, 1979). Then that has also to be true for the finite set of polynomials $\{\theta_i, \varphi_\alpha\}$, forming an integrity basis. So one can label the points of the orbit space $V|G$ by the set of values of these polynomials. The number n of different θ_i is equal to the dimension of the orbit space and these n θ's form a global system of coordinates of $V|G$ when there are no numerator invariants. The latter, when they exist, resolve the ambiguities left by the value of the θ's. As values of $n + k$ real polynomials of n real variables, the coordinates of the orbit space must satisfy polynomial equalities and inequalities; this is summarized by "the orbit space $V|G$ is semi-algebric". Moreover as image of polynomials on the (connected) orthogonal vector space V, the orbit space $V|G$ is connected.

In the case that G is an invariant subgroup of a reflection group G_r and G_r/G is Abelian,[14] Stanley (1977) has given a systematic way[15] for building the module of invariant polynomials for such a subgroup of reflection unitary groups. In the case of orthogonal groups which interest us here, the method is obvious. By the second theorem of Chevalley (see the paragraph preceding Eq. (35) each non-trivial one-dimensional representation of G_r appears once in $\mathscr{P}$. We call them the pseudo invariants of G_r. We keep among them only those which are invariant for G. They are products of the linear forms whose zeros define the symmetry planes of G_r. For instance for the unimodular subgroup of G_r (i.e. the subgroup of elements of determinant 1), there is only one non-trivial numerator invariant: the product of the equations of all symmetry planes; it was known that it is, up to a factor, the Jacobian of the G_r invariants.

Instead of smooth invariant functions it might also be useful to consider the field $\mathscr{F}^G$ of invariant rational fractions over V_n. In Chapter XVII of his famous book Burnside (1911) proved that the number of generators of $\mathscr{F}^G$ is either n or $n+1$. Notice that the numerator and the denominator of an invariant rational function are not necessarily invariant. However we should also point out, as a general theorem, that an invariant rational fraction can always be written as a quotient of invariant polynomials.

For reflection groups this number is n since $\mathscr{F}^G = F[\theta_1, \ldots, \theta_n]$. For some groups in 3D-space which are not generated by reflections (for example the group O) we can prove that it is 4. At the same time even for some groups which are not generated by reflections the number of generators is only 3. The group C_i gives such an example

$$\mathscr{F}_3^{C_i} = F\left[x_1^2, \frac{x_2}{x_1}, \frac{x_3}{x_1}\right]. \tag{81}$$

It can be easily verified that all generators for $\mathscr{F}_3^{C_i}$ may always be rewritten as a quotient of invariant polynomials: $x_2/x_1 = x_1x_2/x_1^2$ and $x_3/x_1 = x_1x_3/x_1^2$.

The group of linear transformations of coordinates of a space V_n, i.e. $GL(n,R)$, transforms polynomials into polynomials. Notice that the Laplacian (which appears in the Schrödinger equation) commutes with all matrices of the orthogonal representation of a group G. So

$$\Delta\mathscr{P}^{(m)G} \subset \mathscr{P}^{(m-2)G}, \tag{82}$$

remember that $\mathscr{P}^{(0)}$ is the one-dimensional space of constants; it carries the trivial representation of G.

General coordinate transformations of a smooth manifold M preserve only properties of smooth functions (they do not generally transform polynomials into polynomials). But the Schwarz theorem (Schwarz, 1975) shows the interest to consider G-invariant polynomials of the coordinates on M. When the action of G on M has been embedded in an orthogonal representation of G on V_n, it is not difficult to compute, from the module $\mathscr{P}_n^G$ of invariant polynomials on V_n, the module of their restriction on M. Let M, of dimension $n-d$, be defined by d algebraic equations[16] $q_\rho = 0$.

[14] That is equivalent to $G'_r \leq G < G_r$ where the "derived group" group G'_r is the group generated by the commutators of G_r.

[15] Very natural to physicists, that method was immediately applied to all finite subgroups of $O(3)$ by Michel (1977). Unfortunately the last table of this paper is marred by many misprints; they are corrected in Jaric et al. (1984).

[16] In the general case some inequalities might also be necessary, but that will not be needed in this paper.

Since M is transformed into itself by G, the q_ρ must be (pseudo)invariant polynomials. Note that the equation can be replaced by $q_\rho^m = 0$ where m is the smallest integer ≥ 2 such that q_ρ^m is invariant. The simplest situation corresponds to the case when these polynomials q_ρ belong to the ring of scalars of the module, they define an ideal of it; let $\mathcal{Q}$ be the corresponding quotient. Then $\mathscr{P}^G|_M$ is a module on $\mathcal{Q}$, either with the same basis as the module $\mathscr{P}^G$ or smaller if some φ become proportional. The denominator of M_0 of $\mathscr{P}^G|_M$ has only $n-d$ factors which is the maximal number of polynomials on V_n which are algebraically independent on M.

5.3. Extension to continuous groups

The theory of invariants of finite groups can be extended to continuous groups with serious caution. We give in this section several applications in the case of the $SO(2)$ symmetry group and show that the module of covariants is not free even in rather simple cases.

Let us consider the four-dimensional space with the action of $SO(2)$ group on it which is equivalent to twice the natural vector representation. More formally the initial representation is

$$\Gamma_{\text{in}} = (m = +1) + (m = -1) + (m = +1) + (m = -1)\,. \tag{83}$$

Molien function for invariants and covariants of $SO(2)$ reads

$$M[(m) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{1}{2\pi}\int_0^{2\pi} \frac{[\chi^{(m)}(\phi)]^*\,\mathrm{d}\phi}{(1-\lambda\exp(\mathrm{i}\phi))^2(1-\lambda\exp(-\mathrm{i}\phi))^2} \tag{84}$$

with

$$\chi^{(m)}(\phi) = \exp(\mathrm{i}m\phi)\,. \tag{85}$$

An explicit calculation gives for invariants and covariants the following generating functions:

$$M[(0) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{1+\lambda^2}{(1-\lambda^2)^3}, \qquad M[(1) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{2\lambda}{(1-\lambda^2)^3}\,, \tag{86}$$

$$M[(2) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{3\lambda^2-\lambda^4}{(1-\lambda^2)^3}, \qquad M[(3) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{4\lambda^3-2\lambda^5}{(1-\lambda^2)^3}\,, \tag{87}$$

with the general expression for $|m| \geq 2$

$$M[(m) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{(|m|+1)\lambda^{|m|} - (|m|-1)\lambda^{|m|+2}}{(1-\lambda^2)^3}\,. \tag{88}$$

We see that for $|m| \geq 2$ the numerator includes negative terms. One can easily verify that the sum over all covariants gives the generating function for polynomials in four independent variables.

$$M[(0) \leftarrow (\Gamma_{\text{in}}); \lambda] + 2\sum_{m=1}^{\infty} M[(m) \leftarrow (\Gamma_{\text{in}}); \lambda] = \frac{1}{(1-\lambda)^4}\,. \tag{89}$$

Remark that the substitution $\lambda = 1$ into the numerators of all generating functions for invariants and covariants gives always 2. This fact shows that all unirreps are one-dimensional.

Numbers of invariants and covariants can be calculated for any form of Molien functions (irrespective of positive or negative terms in the numerator). They are, respectively,

$$M[(0) \leftarrow (\Gamma_{\text{in}}); \lambda] = 1 + 4\lambda^2 + 9\lambda^4 + 16\lambda^6 + \cdots , \tag{90}$$

$$M[(1) \leftarrow (\Gamma_{\text{in}}); \lambda] = 2\lambda + 6\lambda^3 + 12\lambda^5 + 20\lambda^7 + \cdots , \tag{91}$$

$$M[(2) \leftarrow (\Gamma_{\text{in}}); \lambda] = 3\lambda^2 + 8\lambda^4 + 15\lambda^6 + \cdots . \tag{92}$$

Let us now introduce four dynamical variables x_1, y_1 and x_2, y_2 in such a way that $\{x_1, y_1\}$ span the two-dimensional vector representation $(m = -1) + (m = +1)$ of $SO(2)$ and $\{x_2, y_2\}$ span the same representation.

Integrity basis for invariants can be easily written explicitly. It includes three quadratic denominator polynomials $\theta_a, \theta_b, \theta_c$ and one numerator (auxiliary) polynomial φ_0 (with φ_0^2 expressible in terms of denominator invariants).

$$\theta_a = x_1^2 + y_1^2, \quad \theta_b = x_2^2 + y_2^2, \quad \theta_c = x_1 x_2 + y_1 y_2 , \tag{93}$$

$$\varphi_0 = x_1 y_2 - x_2 y_1, \quad \varphi_0^2 = \theta_a \theta_b - \theta_c^2 . \tag{94}$$

All invariant polynomials can be unambiguously represented in the form

$$\mathscr{P}(\theta_a, \theta_b, \theta_c) + \varphi_0 \mathscr{R}(\theta_a, \theta_b, \theta_c) , \tag{95}$$

where $\mathscr{P}(\theta_a, \theta_b, \theta_c)$ and $\mathscr{R}(\theta_a, \theta_b, \theta_c)$ are arbitrary polynomials. This means that invariant polynomials form a free module

$$\mathscr{P}(\theta_a, \theta_b, \theta_c)\bullet(1, \varphi_0) . \tag{96}$$

Covariants of type $m = 1$ also form a free module with two generators

$$\varphi_{1a} = x_1 + \mathrm{i}y_1, \quad \varphi_{1b} = x_2 + \mathrm{i}y_2 , \tag{97}$$

$$\mathscr{P}(\theta_a, \theta_b, \theta_c)\bullet(\varphi_{1a}, \varphi_{1b}) . \tag{98}$$

The situation becomes more complicated in the case of covariants with $m = 2$. We have now three linearly independent quadratic covariants

$$\varphi_{2a} = (x_1 + \mathrm{i}y_1)^2, \quad \varphi_{2b} = (x_2 + \mathrm{i}y_2)^2, \quad \varphi_{2c} = (x_1 + \mathrm{i}y_1)(x_2 + \mathrm{i}y_2) . \tag{99}$$

At the same time these three quadratic covariants are algebraically dependent. There exists one quartic relation between quadratic covariants and quadratic basic invariants

$$2\varphi_{2c}\theta_c = \varphi_{2a}\theta_a + \varphi_{2b}\theta_b . \tag{100}$$

This means that the module of $m = 2$ covariants is not free. To keep only uncorrelated terms we should write the general polynomial expansion for $m = 2$ covariants, for example, in the following form:

$$\varphi_{2a}\mathscr{P}_a(\theta_a, \theta_b, \theta_c) + \varphi_{2b}\mathscr{P}_b(\theta_a, \theta_b, \theta_c) + \varphi_{2c}\mathscr{P}_c(\theta_a, \theta_b) . \tag{101}$$

Remark that $\mathscr{P}_a$ and $\mathscr{P}_b$ are arbitrary polynomials in three variables while $\mathscr{P}_c$ is a polynomial in two variables only.

This particular form is specific to the problem considered. But the general recipe seems to be the same. In the case of presence of negative terms in numerator for covariants the general polynomial expansion of covariants will not include all polynomials in denominator invariants.

5.4. Invariant polynomials and integrity bases for 3-D crystallographic point groups

Invariant polynomials for finite groups and the integrity bases for different irreducible and certain reducible representations were calculated by many authors (see Patera et al., 1978; Gaskel et al., 1979; Michel, 1977; Jaric et al., 1984; Sturmfels, 1993; Worfolk, 1994, and references therein). The explicit form of the invariant polynomials depends on the choice of coordinate system and it remains ambiguous even in an unambiguously chosen coordinate system because an arbitrary linear transformation within the space of basic polynomials of the same degree is possible. The choice of a coordinate frame is of particular importance when the geometric symmetry is analyzed together with periodic symmetry imposed by crystal lattice. This choice is essentially done when the arithmetic class is specified.

In Table 4 we give the module of invariant polynomials for the 33 arithmetic classes $\leq O(3,Z) = Pm\bar{3}m$. To help the reader we give the translation of the ITC notation of these arithmetic classes into the ambiguous Schönflies notation (which is valid only for geometrical classes). In all cases we use the orthonormal system of coordinates defined by three C_4 axes of the O_h group. When the center of a cube is at the origin, the coordinate axes are orthogonal to the faces of the cube and pass through the symmetry centers. The orientation of the coordinate system with respect to symmetry elements for each arithmetic class can be reconstructed by using Table 2 for a list of generators and expressions (16)–(19) for the matrix representation of these generators.

We will make for $D_{6h} = P6/mmm$ the same study we have done for $O(3,Z) = Pm\bar{3}m$. The 32 conjugacy classes of subgroups correspond to 28 conjugacy classes in $GL(3,Z)$; for them we use the names of ICT. Only 16 of them are not orthogonal arithmetic classes $< O(3,Z)$. All these contain $3 = C_3$ which is the derived group. There are three conjugate subgroups $Cmmm$; this arithmetic class is the largest of all arithmetic classes contained also in $Pm\bar{3}m = O(3,Z)$. The system of invariant polynomials for 16 hexagonal arithmetic classes is given in Table 5 using an orthonormal coordinate system $\{x,y,z\}$ with axes z aligned along the C_3 or C_6 symmetry axes. We can rewrite invariant polynomials in the non-orthogonal coordinate system associated with the non-orthogonal lattice. Such transformation will be discussed and used in Chapter IV. Let us give two examples for the two other cubic arithmetic classes.

For F and I arithmetic classes (see Chapters IV, V for details) it could be interesting to use non-orthogonal coordinate system to give the invariant polynomials. We can easily transform the invariant polynomials forming integrity basis from an orthogonal system to a non-orthogonal one. For example, in the non-orthogonal system with $\{x,y,z\}$ axes coinciding with three C_2 axes of O_h (F arithmetic class) the basic invariants of O_h can be chosen as[17]

$$\theta_1^F = x^2 + y^2 + z^2 + xy + yz + zx\,, \tag{102}$$

$$\theta_2^F = xyz(x + y + z)\,, \tag{103}$$

$$\theta_3^F = (x + y)^2(y + z)^2(z + x)^2\,. \tag{104}$$

[17] In fact, the analytical form given in Eqs. (102) and (105) for θ_2^F and θ_2^I differs from the straightforward transformation of the θ_2 invariant given in Table 4. We give the simplified form by substracting the θ_1^2 invariant with an appropriate coefficient.

Table 4
Invariant polynomials for the 33 conjugacy classes of subgroups of $O_h = O(3, Z)$. Column 1 gives the Schönflies notations (they are ambiguous); column 2 gives the eventual arithmetic class with the same matrices. Column 3 give the number of groups in each conjugacy class of subgroups. In the three cases $C_i = P\bar{1}$, $S_4 = P\bar{4}$, $C_{3i} = R\bar{3}$ there are three non-trivial numerator invariants

Geom.	Arithm.	#	θ_1	θ_2	θ_3	φ
C_1	$P1$	1	x	y	z	
C_i	$P\bar{1}$	1	x^2	y^2	z^2	$xy\|yz\|zx$
C_2	$P2$	3	x^2	y^2	z	xy
C_s	Pm	3	x	y	z^2	
C_{2h}	$P2/m$	3	x^2	y^2	z^2	xy
C_2	$C2$	6	$x-y$	xy	z^2	$(x+y)z$
C_s	Cm	6	$x+y$	xy	z	
C_{2h}	$C2/m$	6	x^2+y^2	xy	z^2	$(x+y)z$
C_{2v}	$Pmm2$	3	x^2	y^2	z	
D_2	$P222$	1	x^2	y^2	z^2	xyz
D_{2h}	$Pmmm$	1	x^2	y^2	z^2	
C_{2v}	$Cmm2$	3	x^2+y^2	xy	z	
C_{2v}	$Amm2$	6	$x-y$	xy	z^2	
D_2	$C222$	3	x^2+y^2	xy	z^2	$(x^2-y^2)z$
D_{2h}	$Cmmm$	3	x^2+y^2	xy	z^2	
C_4	$P4$	3	x^2+y^2	x^2y^2	z	$xy(x^2-y^2)$
C_{4v}	$P4mm$	3	x^2+y^2	x^2y^2	z	
S_4	$P\bar{4}$	3	x^2+y^2	x^2y^2	z^2	$xyz\|z(x^2-y^2)\|xy(x^2-y^2)$
C_{4h}	$P4/m$	3	x^2+y^2	x^2y^2	z^2	$xy(x^2-y^2)$
D_{2d}	$P\bar{4}2m$	3	x^2+y^2	x^2y^2	z^2	xyz
D_{2d}	$P\bar{4}m2$	3	x^2+y^2	x^2y^2	z^2	$z(x^2-y^2)$
D_4	$P422$	3	x^2+y^2	x^2y^2	z^2	$xyz(x^2-y^2)$
D_{4h}	$P4/mmm$	3	x^2+y^2	x^2y^2	z^2	
C_3	$R3$	4	$x+y+z$	$x^2+y^2+z^2$	xyz	$\phi=(x-y)(y-z)(z-x)$
C_{3v}	$R3m$	4	$x+y+z$	$x^2+y^2+z^2$	xyz	
D_3	$R32$	4	$(x+y+z)^2$	$x^2+y^2+z^2$	ϕ	$(x+y+z)xyz$
C_{3i}	$R\bar{3}$	4	$(x+y+z)^2$	$x^2+y^2+z^2$	$x^2y^2z^2$	$(x+y+z)xyz\|(x+y+z)\phi\|xyz\phi$
D_{3d}	$R\bar{3}m$	4	$(x+y+z)^2$	$x^2+y^2+z^2$	$x^2y^2z^2$	$(x+y+z)xyz$
T	$P23$	1	$x^2+y^2+z^2$	$x^4+y^4+z^4$	xyz	$(x^2-y^2)(y^2-z^2)(z^2-x^2)$
T_d	$P\bar{4}3m$	1	$x^2+y^2+z^2$	$x^4+y^4+z^4$	xyz	
T_h	$Pm\bar{3}$	1	$x^2+y^2+z^2$	$x^4+y^4+z^4$	$x^2y^2z^2$	$(x^2-y^2)(y^2-z^2)(z^2-x^2)$
O	$P432$	1	$x^2+y^2+z^2$	$x^4+y^4+z^4$	$x^2y^2z^2$	$xyz(x^2-y^2)(y^2-z^2)(z^2-x^2)$
O_h	$Pm\bar{3}m$	1	$x^2+y^2+z^2$	$x^4+y^4+z^4$	$x^2y^2z^2$	

Table 5
Module of invariant polynomials for the 16 hexagonal arithmetic classes. Column 1 gives the Schönflies notation of the geometric class; column 2 gives the arithmetic classes. The three θ_i generate the module ring, and 1 and the φ's form the bases of the modules. Six groups are generated by reflections (one-dimensional module), the other modules are of dimension 2 except that of $P\bar{3} = C_{3i}$ which is of dimension 4

Geom.	Arithm.	θ_1	θ_2	θ_3	φ
C_3	$P3$	x^2+y^2	$x(x^2-3y^2)$	z	$y(3x^2-y^2)$
C_{3v}	$P3m1$	x^2+y^2	$x(x^2-3y^2)$	z	
C_{3v}	$P31m$	x^2+y^2	$y(3x^2-y^2)$	z	
D_3	$P321$	x^2+y^2	$y(3x^2-y^2)$	z^2	$zx(x^2-3y^2)$
D_3	$P312$	x^2+y^2	$x(x^2-3y^2)$	z^2	$zy(3x^2-y^2)$
C_{3i}	$P\bar{3}$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	$xz(x^2-3y^2)$ $yz(3x^2-y^2)$ $xy(3x^2-y^2)(x^2-3y^2)$
D_{3d}	$P\bar{3}m1$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	$zx(x^2-3y^2)$
D_{3d}	$P\bar{3}1m$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	$zy(3x^2-y^2)$
C_{3h}	$P\bar{6}$	x^2+y^2	$x(x^2-3y^2)$	z^2	$y(3x^2-y^2)$
D_{3h}	$P\bar{6}m2$	x^2+y^2	$x(x^2-3y^2)$	z^2	
D_{3h}	$P\bar{6}2m$	x^2+y^2	$y(3x^2-y^2)$	z^2	
C_6	$P6$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z	$xy(3x^2-y^2)(x^2-3y^2)$
C_{6h}	$P6/m$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	$xy(3x^2-y^2)(x^2-3y^2)$
C_{6v}	$P6mm$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z	
D_6	$P622$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	$xyz(3x^2-y^2)(x^2-3y^2)$
D_{6h}	$P6/mmm$	x^2+y^2	$\mathfrak{Re}(x+iy)^6$	z^2	

In another non-orthogonal system with $\{x, y, z\}$ axes coinciding with three C_3 axes of O_h (I arithmetic class) the basic invariants are

$$\theta_1^I = 3(x^2+y^2+z^2) - 2(xy+yz+zx)\,, \tag{105}$$

$$\theta_2^I = x^2y^2 + y^2z^2 + z^2x^2 - xyz(x+y+z)\,, \tag{106}$$

$$\theta_3^I = (x+y-z)^2(y+z-x)^2(z+x-y)^2. \tag{107}$$

5.5. *Ring of C_i invariant polynomials. Description in terms of generators and syzygies*

Let us now analyze the description of the ring of invariant function in terms of generators and syzygies (as it was generally outlined earlier, see Eq. (80)) using as example the C_i natural action on 3-D-space and its induced action on the two-dimensional sphere. $C_i = \bar{1}$[18] is the two-element group generated by $-I_3$, the symmetry through the origin. The smallest reflection group which contains it is the eight element group $D_{2h} = mmm$ whose three symmetry planes are the planes of

[18] In molecular physics and chemistry the group C_i is often denoted as S_2. We prefer to avoid this notation because it can be easily confused with the S_2 notation for two-dimensional sphere frequently used in this paper.

coordinates. The group D_{2h} has eight one-dimensional inequivalent representations. Only four of them have character 1 for $-I_3$. They yield the four numerator invariant of C_i. With the convention that the indices i,j,k form a permutation of $1,2,3$, the Molien function, the denominator and numerator invariant polynomials of C_i are

$$M_{C_i}(\lambda) = \frac{1+3\lambda^2}{(1-\lambda^2)^3}, \quad \theta_k = x_k^2,\ \varphi_0 = 1,\ \varphi_i = x_j x_k\ . \tag{108}$$

The structure of the module of the C_i invariant functions on the 3-D-space corresponding to the Molien function in Eq. (108) may be written as

$$\mathscr{P}^{C_i} = P[x_1^2, x_2^2, x_3^2]\bullet(1, x_1x_2, x_1x_3, x_2x_3)\ . \tag{109}$$

From Eq. (109) we deduce immediately the module structure for the ring of invariant polynomials after restriction of the 3-D action on the two-dimensional subspace given by equation $x_1^2 + x_2^2 + x_3^2 = r^2$.

$$\mathscr{P}_3^{C_i}|_{S_2} = P[x_1^2, x_2^2]\bullet(1, x_1x_2, x_1x_3, x_2x_3)\ . \tag{110}$$

The corresponding Molien function for the C_i invariant polynomials on the sphere S_2 is $(1+3\lambda^2)(1-\lambda^2)^{-2}$.

The natural action of C_i on 3-D-space gives us the possibility to illustrate the non-trivial character of syzygies even for very small groups (see Example 6.6 in Stanley, 1979). The minimal set of generators of the ring of C_i invariants includes six generators of degree 2 each (including all denominator and numerator invariants corresponding to the most reduced form of the Molien function (108)). To get the symbolic information about the set of syzygies we can multiply both numerator and denominator of the Molien function (108) by $(1-\lambda^2)^3$ to get the expression with six denominator invariants of degree two. Such a transformation gives

$$M_{C_i} = \frac{1 - 6\lambda^4 + 8\lambda^6 - 3\lambda^8}{(1-\lambda^2)^6}\ . \tag{111}$$

Naturally, the numbers of invariant polynomials in each degree do not alter upon such a transformation but we have new symbolic information. There are six syzygies of the first kind, eight syzygies of the second kind and three syzygies of the third kind. One should not think that it is always easy to interpret the numerator of a Molien function in terms of numbers of syzygies of different kinds (sometimes this is even impossible without independent explicit calculation of syzygies as shown for example by Stanley (1996, Chapter I-11)). At the same time the symbolic interpretation is quite useful to see the complexity of the invariant ring and to verify the system of relations. We end this example with the complete list of all syzygies between generators of the ring of invariants for the C_i action of 3-D space.

Let us denote the generators by $g_1 = x_1^2$, $g_2 = x_2^2$, $g_3 = x_3^2$, $g_4 = x_1x_2$, $g_5 = x_1x_3$, $g_6 = x_2x_3$. Six syzygies of the first kind can be written as

$$s_a^1 = g_1g_2 - g_4^2, \quad s_b^1 = g_1g_3 - g_5^2, \quad s_c^1 = g_2g_3 - g_6^2\ ,$$

$$s_d^1 = g_4g_5 - g_1g_6, \quad s_e^1 = g_4g_6 - g_2g_5, \quad s_f^1 = g_5g_6 - g_3g_4\ .$$

All these relations are of degree 4 in x_i variables. These six relations are not independent. Eight relations between them (syzygies of second kind) can be given as

$$
\begin{aligned}
&s_a^2 = g_5 s_a^1 + g_4 s_d^1 + g_1 s_e^1, \quad s_b^2 = g_6 s_a^1 + g_2 s_d^1 + g_4 s_e^1 \,, \\
&s_c^2 = g_4 s_b^1 + g_5 s_d^1 + g_1 s_f^1, \quad s_d^2 = g_6 s_b^1 + g_3 s_d^1 + g_5 s_f^1 \,, \\
&s_e^2 = g_4 s_c^1 + g_6 s_e^1 + g_2 s_f^1, \quad s_f^2 = g_5 s_c^1 + g_3 s_e^1 + g_6 s_f^1 \,, \\
&s_g^2 = g_3 s_a^1 - g_2 s_b^1 + g_5 s_e^1 - g_4 s_f^1, \quad s_h^2 = g_3 s_a^1 - g_1 s_c^1 + g_6 s_d^1 - g_4 s_f^1 \,. \qquad (112)
\end{aligned}
$$

These eight syzygies of second type are of degree 6 in x_i variables. They are dependent as well. Three syzygies of the third kind have the form

$$
\begin{aligned}
&s_a^3 = g_6 s_a^2 - g_5 s_b^2 + g_2 s_c^2 - g_1 s_e^2 + g_4 s_g^2 - g_4 s_h^2 \,, \\
&s_b^3 = g_3 s_a^2 - g_6 s_c^2 - g_4 s_d^2 - g_1 s_f^2 + g_5 s_h^2 \,, \\
&s_b^3 = g_3 s_b^2 - g_2 s_d^2 + g_5 s_e^2 - g_4 s_f^2 + g_6 s_g^2 \,.
\end{aligned}
$$

These three syzygies of third type are of degree 8 in x_i variables. We remark at the end of this example that the construction we have realized above is well known in commutative algebra construction of a finite free resolution (Cox et al., 1998; Stanley, 1996).

5.6. *Representation of the orbit space in terms of invariant polynomials*

We have defined the orbit space for the G-action on M in Section 2 and denoted it by $M|G$. Invariant functions on M have constant values on an orbit. For the linear orthogonal representations of a compact group from Schawrz theorem (Schwarz, 1975) (see the beginning of Section 5) we need only to consider the invariant polynomials. Another theorem says that invariant polynomials separate the orbits, i.e. given two different orbits, there is an invariant polynomial taking different values on them. This implies that any system of generators of the ring of invariant polynomials must separate the orbits. This fact enables one to use invariant polynomials to represent orbit spaces geometrically (Kim, 1984; Sartori, 1991).

Let us consider the system of generators containing the d basic invariants θ_i of the denominator and n' generators ϕ_i of the numerator $n' \leq N(t=1)$. Every orbit can be defined by the values of these generators and represented by a point in a $R^{d+n'}$ space. The orbit space is a semi-algebraic set of points, i.e. it is defined by algebraic equations (the algebraic relations between the ϕ_i and θ_j) and inequalities, since we work on the real. The largest dimension of connected components is d (the number of algebraically independent polynomials). In all examples, we give here, the orbit space is connected. Then it is an orbifold.

In Chapter V, for the non-linear action of space groups on the Brillouin zone (BZ), we show that for a natural global coordinate system on BZ we have a module structure for all arithmetic classes. So all we said extends to this non-linear action.

The description of the ring of invariant polynomials in terms of integrity bases is advantageous because typically the invariant functions are given in terms of the same invariant polynomials and thus we can easily study functions geometrically on the orbit space through their level sets. The role of basic and auxiliary polynomials is quite different. We illustrate the geometrical construction in several simple examples.

5.6.1. O_h and O natural action on 3-D-space

The space of orbits for the O_h or O natural group action on the 3-D-space arises in many different physical problems. We can just cite the triply degenerate molecular vibrations of octahedral molecules described by irreducible representation with Ker 1 and Im O_h (F_{1u} irreducible representation as listed in most tables of characters used by physicists and chemists (Landau and Lifshitz, 1965)) or rotation of spherical top molecules described by three rotational angular momentum (F_{1g} representation of O_h with Ker $\bar{1}$ and Im O).

It is well known (e.g., Michel, 1977) that the $O_h = m\bar{3}m$ group is generated by reflections and the values of the three d_k (degrees of denominator invariants) are $2, 4, 6$. The corresponding Molien function has the form

$$M_{O_h}(\lambda) = \frac{1}{(1-\lambda^2)(1-\lambda^4)(1-\lambda^6)} \,. \tag{113}$$

The explicit form of the invariants depends on the choice of basis in V_n. We choose an orthonormal basis whose coordinates axes are identical to the four-fold rotation axes (orthogonal to the cube faces). Then we can choose

$$k = 1, 2, 3, \quad \theta_k = \sum_{i=1}^{3} x_i^{2k} \,. \tag{114}$$

The polynomial θ_1 is invariant for every orthogonal group representation. The choice of the other θ's is not unique. For instance we could choose instead of θ_2 any linear combination $\theta'_2 = \theta_2 + \alpha\theta_1^2$, α real; e.g. for $\alpha = -1$, $\theta'_2 = \sum_{i\neq j} x_i^2 x_j^2$. Often instead of $x^6 + y^6 + z^6$ one uses $x^2y^2z^2$ as one of basic invariant polynomials of degree six. (See expression in Eq. (117) below for the relation between these two choices.)

It is easy now to restrict the above-defined action of O_h group on 3-D-space to the sphere S_2 of equation $\theta_1 \equiv x_1^2 + x_2^2 + x_3^2 = r^2$ and to characterize the polynomial ring of invariants on this sub-manifold. Let us denote by θ'_2, θ'_3 the polynomials in x_1, x_2 obtained from θ_k, $k = 2, 3$, defined in Eq. (114), by replacing their monomial x_3^{2k} by $(r^2 - x_1^2 - x_2^2)^k$. Then $\mathscr{P}_3^{O_h}|_{S_2} = P[\theta'_2, \theta'_3]$, the polynomial ring of all the polynomials in these two variables. The transformation of the Molien function corresponding to this restriction consists in simple elimination from the denominator of (113) the factor $(1 - \lambda^2)$.

The group $O = 432$ is the rotational (unimodular) subgroup of the group $O_h = m\bar{3}m$. It possesses the only non-trivial numerator polynomial φ

$$\frac{1}{24}\frac{D(\theta_1, \theta_2, \theta_3)}{D(x_1, x_2, x_3)} = \varphi = x_1x_2x_3(x_1^2 - x_2^2)(x_2^2 - x_3^2)(x_3^2 - x_1^2) \,. \tag{115}$$

The polynomial φ is a *pseudoinvariant*[19] of O_h; it is the (non-trivial) numerator invariant of O, the unimodular subgroup of O_h. This means that the φ^2 is a polynomial in basic invariants, namely if we take as basic invariants $\theta_1 = x^2 + y^2 + z^2$,

$$\varphi^2 = \theta_3(\tfrac{1}{2}\theta_2^3 - 27\theta_3^2 - 9\theta_2\theta_3\theta_1 - \tfrac{5}{4}\theta_2^2\theta_1^2 + 5\theta_3\theta_1^3 + \theta_2\theta_1^4 - \tfrac{1}{4}\theta_1^6) \,. \tag{116}$$

[19] We call pseudoinvariant of a group G, every quantity transforming as a non-trivial one-dimensional representation of G.

Table 6
Strata equations for the O_h group action on S_2. Basic invariant polynomials $\theta_1 = x^4 + y^4 + z^4$ and $\theta_2 = x^2y^2z^2$ are used as coordinates for the orbifold representation

Stabilizer	Equations and/or inequalities
$C_{4v} = P4mm$	$\theta_1 = 1,\ \theta_2 = 0$
$C_{3v} = R3m$	$\theta_1 = 1/3,\ \theta_2 = 1/27$
$C_{2v} = Amm2$	$\theta_1 = 1/2,\ \theta_2 = 0$
$C_s = Pm$	$1/2 < \theta_1 < 1,\ \theta_2 = 0$
$C_s' = Cm$	$\theta_1 = 1 - 2s + 3s^2/2,$
	$\theta_2 = s^2(1 - s)/4,$
	$0 < s < 1,\ s \neq 2/3$
$C_1 = 1$	Internal points

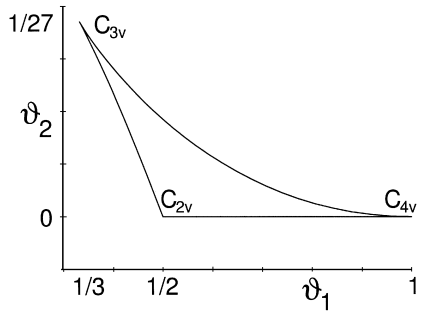


Fig. 14. Orbifold for the natural action of the O_h group on the two-dimensional sphere S_2. Invariant polynomials are specified in Table 6. Singular points C_{4v}, C_{3v}, C_{2v} correspond, respectively, to six-point, eight-point, and 12-point orbits on S_2. Notice that cusp points C_{4v}, C_{3v} persist under the change of the form in invariant polynomials whereas the geometrical form itself varies.

This relation should be simplified in the case of the O_h action on the S_2 subspace by imposing $\theta_1 = 1$. The resulting relation for φ^2 becomes inhomogeneous in two basic invariants. Remark, that in Table 6 and Fig. 14 which describe the action of the O_h group on the S_2 sphere we use only two basic invariants specified in the caption to Table 6.

Schematic representation of the orbifold of the O_h action on 3-D space and on two-dimensional S_2 subspace was given in a previous section (see Fig. 12). Here we represent the same space of orbits using invariant polynomials as coordinates. The polynomial ring of O_h invariants is generated by two basic polynomials (one of fourth and another of sixth degree) which can be chosen as $\theta_1 = x^4 + y^4 + z^4$ and $\theta_2 = x^2y^2z^2$. These two invariant polynomials can be used to label orbits. Fig. 14 shows the geometrical form of the orbifold in the space of invariant polynomials. Different strata are defined by equalities and inequalities summarized in Table 6. The boundary of the orbifold in the space of invariant polynomials shown in Fig. 14 is defined by the relation in Eq. (116) after imposing $\varphi^2 = 0$, $\theta_1 = 1$ and changing the notation for invariant polynomials $\theta_2 \to \theta_1$ and $\theta_3 \to \theta_2$ because on the S_3 subspace we have only two basic invariants. One could use instead

of the $x^2y^2z^2$ invariant polynomial another polynomial of degree 6, namely $x^6 + y^6 + z^6$. In fact, on the S_2 surface the linear relation exist between these two polynomials:

$$x^6 + y^6 + z^6 = 3x^2y^2z^2 + \tfrac{3}{2}(x^4 + y^4 + z^4) - \tfrac{1}{2}\,. \tag{117}$$

Consequently, an alternative choice of basic invariants corresponds to linear transformation in the space of basic invariants.

The geometrical form of the orbifold in the invariant polynomial variables reflects certain important aspects of the behavior of invariant functions. Two vertexes of the orbifold (C_{3v} and C_{4v}) are formed by two boundary lines with the same slope at singular cusp point. This means that the corresponding critical orbit (C_{3v} and C_{4v}) should be always maximum or minimum for any generic function possessing only non-degenerate stationary points. (This is the Morse-type function, see next section for definitions). At the same time the critical orbit C_{2v} which lies at the intersection of two boundary lines with different slopes can be a saddle point as well.

Using the orbifold representation in the invariant polynomials we can use simple geometrical analysis to judge the existence of stationary points of a function defined over the manifold. In order to do that it is sufficient to plot the contour lines of a function (level set of a function) directly on the orbifold and to analyze the topology of different level sets. Stationary points may exist only for level sets with exceptional topological structure.

Let us consider, for example, an O_h invariant function written in the form of a linear combination of two basic polynomials

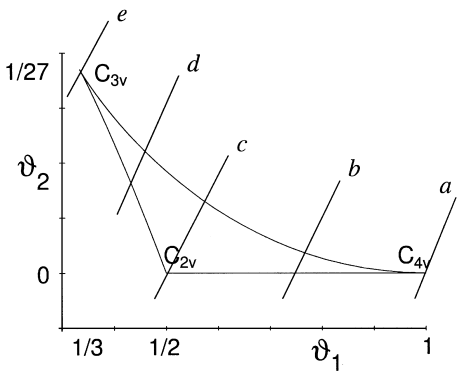
$$\alpha\theta_1 + \beta\theta_2\,. \tag{118}$$

Apart from a trivial scalar factor this is the most general O_h invariant function up to the sixth degree in initial variables. At the same time this is just a linear function in terms of invariant polynomials and its level set on the orbifold is the set of straight lines.

Figs. 15 and 16 show examples of contour plots (levels of constant value of functions) for two qualitatively different types of invariant functions. Function plotted in Fig. 15 has three orbits of stationary points. These orbits are critical and consequently this function has a minimal possible number (namely 26) of stationary points. Three level sets (a, c, e) of this function have exceptional topology. The topological structure of level sets (b) and (d) does not vary if the value of the function varies slightly, i.e. these sets are regular.

The function plotted in Fig. 16 has four exceptional level sets (a, c, e, g). The level sets (a, e, g) include critical orbits. The level set (e) is exceptional because it touches the boundary and the touching point is a stationary non-critical point. Its position is not fixed but this point persists on the boundary even after a small perturbation of the function. We should remark that among different functions of the form (118) there are functions with the minimal possible number of stationary points (only critical orbits), functions with one additional orbit of non-critical stationary points, and exceptional type functions corresponding to the qualitative phenomenon known as bifurcation of stationary points. More exact terminology for these different types of functions based on the Morse theory will be introduced in the next section.

The space of orbits for the O group action follows immediately from the analysis made above for the O_h group action. The system of denominator invariants are the same for two groups. To completely characterize orbits for O group we should add the value of auxiliary invariant polynomial. All principal orbits of O_h (internal points of the orbifold) are split into two orbits of the



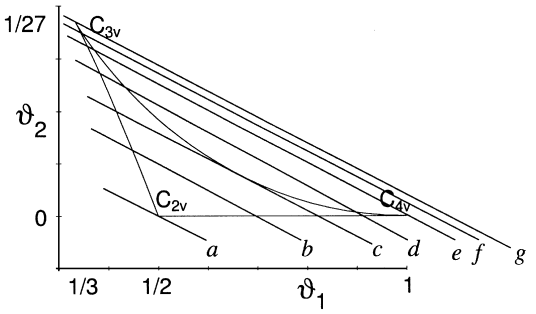


Fig. 15. Contour plot of the level set of the invariant function in Eq. (118) on the orbifold. The function corresponds to $\alpha/\beta \sim -1/10$. It has only three critical levels (a, c, e) and two different types of regular levels (b, d).

Fig. 16. Contour plot of the level set of the invariant function in Eq. (118) with $\alpha/\beta \sim \frac{1}{20}$ on the orbifold. The function possesses stationary points outside of critical orbits. There are four critical levels (a, c, e, g) and three different types of regular levels (b, d, f). The non-critical stationary point located at the touching point of level c and the boundary.

O group which have the opposite values of the numerator invariant φ. All O_h orbits lying on the boundary of the orbifold correspond to the zero value of auxiliary O invariant φ. This means that the auxiliary O invariant φ defines the form of the O_h orbifold and the complete representation of the O orbifold consists of two parts (two O_h orbifolds with identification of corresponding points on the orbifold boundary).

5.6.2. Orbifold for the C_i natural action on 3-D-space

Integrity basis includes in this case three basic polynomial invariants and three auxiliary invariants (see Eq. (108)). Basic polynomial invariants can be used to label unambiguously the orbits within any region where all auxiliary polynomials keep their sign. The boundary of those regions is defined as a set of points where at least one of the auxiliary polynomials equals zero. Consequently, the space of orbits can be represented by a set of smaller orbifolds that have to be glued together by identification of some boundaries. Each part corresponds to one region where all auxiliary polynomials have the constant sign (with the boundary of the region corresponding to zero value of some of the auxiliary polynomials). Boundary points of different parts should be identified to represent properly the topology of the whole space of orbits. Fig. 17 shows the representation of the orbifold as a four-part decomposition with identification of side-planes labeled by identical letters. It is a connected orbifold.

5.6.3. Finite group action on 2-D-torus

Let us start with a trivial example of the C_1 group action on a torus. We treat this case in order to demonstrate the representation of a manifold with non-trivial topology in terms of polynomial functions defined on it.

2-D-torus can be represented in (k_1, k_2) variables restricted, for example as $0 \leq k_1, k_2 < 2\pi$ and taken modulo 2π. This is a standard representation of a torus as a square with identification of

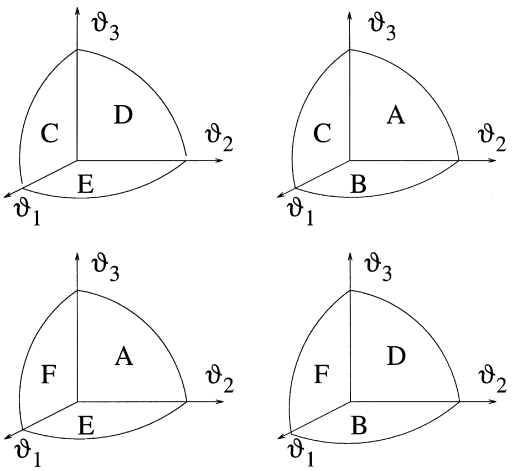


Fig. 17. Orbifold for the natural action of the C_i group on three-dimensional Euclidean space. To understand the topology of the orbifold four 3-D-parts should be glued together through identification of coordinate planes marked by the same letters.

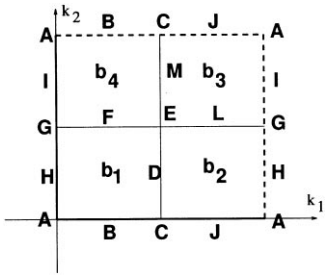


Fig. 18. Tore without symmetry in k_1, k_2 variables. Opposite sides should be glued together respecting the letters on the boundary to get the torus. Internal letters and auxiliary decomposition will be useful to make the comparison with the representation of torus in terms of invariant polynomials constructed from $\cos(k_i)$ and $\sin(k_i)$ functions. See Fig. 19.

opposite sides (see Fig. 18) To introduce an alternative representation of the same torus let us introduce the ring of smooth functions defined on it and the associated integrity basis. It is clear that any smooth function on the torus can be expresses as formal series in 2π periodic functions

$$c_1 = \cos(k_1), \quad c_2 = \cos(k_2), \quad s_1 = \sin(k_1), \quad s_2 = \sin(k_2)\,. \tag{119}$$

Naturally these four functions are algebraically dependent and the generating function for the number of linearly independent homogeneous polynomials in c_1, c_2, s_1, s_2 has the form

$$\frac{1 + 2t + t^2}{(1 - t)^2}\,. \tag{120}$$

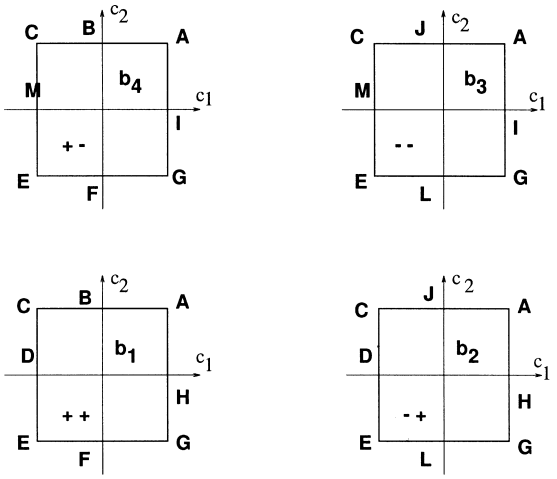


Fig. 19. Tore without symmetry in c_1, c_2 variables. The space of trivial orbits is represented in terms of integrity basis polynomials. Four parts correspond to different signs of auxiliary invariants s_1, s_2 which are marked inside each part. To construct the whole orbifold (the torus) four parts should be glued together through identification of their boundaries. Partial identification of boundaries *EFG*, *ELG*, *CME*, and *CDE* leads to the representation of the torus as a square with identified opposite sides as in Fig. 18.

It reflects the structure of integrity basis of invariant polynomials depending on four variables c_1, c_2, s_1, s_2 and defined on the two-torus. The two basic (denominator) invariants can be taken as $c_1 = \cos(k_1)$, $c_2 = \cos(k_2)$, while three auxiliary (numerator) invariants can be chosen as $s_1 = \sin(k_1)$, $s_2 = \sin(k_2)$, and $s_1 s_2$.

The module of polynomials which can be considered as invariant polynomials with respect to the trivial C_1 symmetry group acting on the torus can be written as

$$\mathscr{P}^{P_1} = P[c_1, c_2] \bullet (1, s_1, s_2, s_1 s_2) \,. \tag{121}$$

Now we can use the denominator basic polynomials as continuous variables to represent the trivial orbits of the C_1 group action on the torus. To represent completely the orbifold we need to add auxiliary invariant polynomials. This leads us to representation of the orbifold as four body decomposition with the each body being the same square in c_1, c_2 variables but characterized by different sets of signs of auxiliary polynomials. In fact, it is sufficient to use only signs of two numerator invariants because the third invariant is simply the product of the two first. The geometrical representation of orbifold in terms of c_i which shows explicit correspondence with the representation of the same orbifold in k_1, k_2 variables is given in Fig. 19.

Remark that if we consider the finite group *p2mm* action on the torus its ring of invariant polynomials includes only basic invariants c_1 and c_2. This means that the orbifold for the *p2mm* action on the torus coincides with one sub-orbifold drawn in Fig. 19. This situation is quite general. It was illustrated in previous example of O_h and O group actions on S_2 and still will be discussed in Chapters II and V.

To describe the ring of functions on the torus we could use instead of the integrity basis construction the alternative approach based on the system of generators and syzygies and leading to the so-called finite free resolution widely used in mathematical literature (Stanley, 1979; Cox et al., 1992, 1998). To construct the minimal free resolution we take first four generators c_1, c_2, s_1, s_2 and form polynomial ring with four variables. Next step is to introduce relations (syzygies of the first kind)

$$s_i^2 = 1 - c_i^2, \quad (i = 1, 2), \quad s_1 s_2 = z \ . \tag{122}$$

This gives us two restrictions but the third relation gives new variables and we can further consider the polynomial ring with three variables c_1, c_2, z. Again these three variables are not independent. There exist syzygies of the second kind

$$z^2 = (1 - c_1)^2 (1 - c_2)^2 \ , \tag{123}$$

which is in fact of the fourth degree in initial generators.

To see the presence of syzygies in the symbolic representation we can rewrite the generating function (120) as

$$\frac{1 + 2t + t^2}{(1 - t)^2} = \frac{(1 + 2t + t^2)(1 - t)^2}{(1 - t)^4} = \frac{(1 - t^2)^2}{(1 - t)^4} = \frac{1 - 2t^2 + t^4}{(1 - t)^4} \ . \tag{124}$$

This form shows that there are two quadratic syzygies of the first kind and one quartic syzygies of the second kind.

This example illustrates once more the relation between the description of the ring of invariant functions in terms of integrity basis and in terms of generators and syzygies. While generators–syzygies construction is more appropriate for abstract mathematical study and theorem proving, the integrity basis approach is more suited for detailed analysis of concrete examples.

6. Morse theory

In this work we also need to apply some results of Morse theory (Morse, 1925; Seifert and Threlfall, 1938; Milnor, 1963; Poènaru, 1976; Palais and Terng, 1980; Bott, 1982; Dubrovin et al., 1990; Fomenko, 1983). Consider a smooth (= infinitely differentiable) real-valued function f on a real compact manifold M with a coordinate system[20] $\{x_k\}$, $1 \leq i \leq d = \dim M$. If at a point $m \in M$ of coordinates x_k the function satisfies the equations: vanishing gradient, i.e. $\partial f/\partial x_i = 0$, and non-vanishing determinant of the Hessian, i.e. $\det(\partial^2 f(x)/\partial x_i \partial x_j) \neq 0$, we say that it has a non-degenerate extremum. Then by a change of coordinates $\{x_i\} \mapsto \{y_i\}$, in a neighborhood of m the function can be transformed into $f = \sum_i \varepsilon_i y_i^2$ with $\varepsilon_i = \pm 1$. The number of minus signs is independent of the coordinate transformation 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

[20] In general a coordinate system cannot be defined on the whole manifold.

non-degenerate is called a Morse function. Let c_k be the number of its extrema of Morse index k; these numbers are finite[21] and may be used to construct the Morse polynomial $\mathscr{M}_f(t)$ for a Morse function which counts all stationary points of the function f with their indices

$$\mathscr{M}_f(t) = \sum_{k=0}^{d} c_k t^k \quad \text{with } d = \dim(M) . \tag{125}$$

More generally the Morse polynomial $\mathscr{M}_f(t)$ for a Morse function on M may be defined as

$$\mathscr{M}_f(t) = \sum_{p \in C(f)} t^{\mu(p)}, \quad \mathscr{M}_f(1) = |C(f)| , \tag{126}$$

where the sum is taken over the set $C(f)$ of extrema and $\mu(p)$ is the Morse index of the point p. The polynomial $\mathscr{M}_f(t)$ is a quantitative measure of the critical behavior of f.

The essence of the Morse theory is the relation between the numbers of extrema and the Betti numbers of the manifold M. The Betti number b_k is defined as the rank of the kth homology group of M. Intuitively b_k is the maximal number of k-dimensional sub-manifolds of M which cannot be transformed one into another or into a sub-manifold of a smaller dimension; for instance for the sphere S_d of dimension[22] d, $b_0 = b_d = 1$ and all the others b_k vanish.

To formulate Morse inequalities for a given d-dimensional manifold M we introduce the "Poincaré polynomial" $P_M(t)$ in which the coefficient of t^k is the Betti number b_k of M:

$$P_M(t) = \sum_{k=0}^{d} b_k t^k \quad \text{with } d = \dim(M) . \tag{127}$$

The *Euler–Poincaré characteristic* χ_M of the manifold M is defined by

$$\chi_M = P_M(t = -1) . \tag{128}$$

The Poincaré polynomial of a topological product $M = \times_i M_i$ is the product of the Poincaré polynomials:

$$M = \times_i M_i \Rightarrow P_M(t) = \prod_i P_{M_i}(t) \Rightarrow \chi_M = \prod_i \chi_{M_i} . \tag{129}$$

For instance the Poincaré polynomial of the manifold $\Sigma = S_2 \times S_2$ has the following explicit form:

$$P_\Sigma(t) = (1 + t^2)^2, \quad b_0 = b_4 = 1, \quad b_1 = b_3 = 0, \quad b_2 = 2, \quad \chi_\Sigma = 4 , \tag{130}$$

whereas for d-dimensional torus S_1^d we see immediately that the Betti numbers are binomial coefficients.

$$P_\Sigma(t) = (1 + t)^d = \sum_{k=0}^{d} \binom{d}{k} t^k . \tag{131}$$

[21] If there were an infinite number of extrema on the compact manifold $\mathscr{M}$ there would be an accumulation point which would be a degenerate extremum.

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

Using the Poincaré polynomial of the manifold, $P_M(t)$, and the Morse polynomial $\mathscr{M}_f(t)$ for a Morse function f we can formulate the relations between the Betti numbers and the numbers of stationary points of the function f. The precise statement is as follows.

Morse inequalities. For every Morse function f there exists a polynomial $Q_f(t) = q_0 + q_1 t + \cdots$ with *non-negative coefficients* such that

$$\mathscr{M}_f(t) - P_M(t) = (1 + t)Q_f(t) \,. \tag{132}$$

This statement may be rewritten in terms of d inequalities

$$0 \le \ell < d: \quad \sum_{k=0}^{\ell} (-1)^{\ell - k}(c_k - b_k) \ge 0 \tag{133}$$

$$\Rightarrow c_k \ge b_k \tag{134}$$

and one equality

$$\sum_{k=0}^{d} (-1)^k (c_k - b_k) = 0 \Leftrightarrow \sum_{k=0}^{d} (-1)^k c_k = \sum_{k=0}^{d} (-1)^k b_k \overset{\text{def}}{=} \chi_M \,, \tag{135}$$

where χ_M is the Euler–Poincaré characteristic of the manifold M. The inequalities (134) are *not* equivalent to Morse inequalities (133), but they give lower bounds to the number of extrema of a Morse function.

There exists another limit on the number of stationary points of any smooth function on the manifold which is valid for an arbitrary non-Morse function with degenerate stationary points. The number of stationary points cannot be larger than the Lusternik–Schnirelmann category of the manifold (initially introduced in Lusternik and Schnirelmann (1930), two chapters of which were translated into French (Lusternik and Schnirelmann, 1934). Lusternik–Schnirelmann category is the homotopy invariant which is not easy to calculate in general case. For n-dimensional sphere S_n this invariant is equal to 2 and for an n-dimensional torus it is equal $n + 1$ (Seifert and Threlfall, 1938; Fomenko and Fuks, 1989).

In the absence of any symmetry requirements many sufficiently good manifolds allow the existence of a so-called *perfect Morse function* which reduces all Morse inequalities into equalities. In other words for the perfect Morse function $Q_t(f) = 0$, i.e. $\mathscr{M}_f(t) = P_M(t) \sim c_k = b_k$. In particular, the number of stationary points $|C(f)|$ of a perfect Morse function f equals the sum of Betti numbers ($= P_M(1)$). When a finite symmetry group G acts on the manifold M, there are further requirements on the c_k's of G-invariant Morse function: all points of a G-orbit should be simultaneously either extrema with the same index or not be extrema. Some simple physical applications of the Morse theory under the presence of symmetry which are close in spirit to the present analysis were given by Michel and Mozrzymas (1978), Michel (1979) and Zhilinskii (1989a) (see also Zhilinskii, 1989b).

As we saw in Section 4, very often the group action itself insures (Corollary 4c) that several orbits (the critical orbits) should be stationary for any G-invariant function f. If apart from that there exist closed strata (those with maximal symmetry) and if the orbits they contain are not all critical, then Theorem 4c (see Section 4) applies and requires for any function at least two orbits of extrema in these strata. In any case, among all invariant Morse functions there exist some of them with the minimal possible number of extrema. We will call such functions *the simplest Morse-type functions*.

We can still introduce the natural measure of the complexity of a given Morse-type function just by counting the total number of stationary points.

In case of a symmetry realized by the effective action of a compact Lie group, orbits are themselves continuous compact manifolds (some of them might be of dimension zero = finite set of points). The situation becomes more complicated when some of these orbits are orbits of extrema of an invariant function f: indeed these extrema of f are degenerated along the directions tangent to the orbit. So the Morse theory in its original form is not applicable.

There exists an extension of Morse theory for G-invariant function with non-zero-dimensional orbits of extrema. Atiyah and Bott (1982), Bott (1982) and Fomenko (1983) give the basic mathematical facts with some ideas of physical applications. Analysis of one particular physical problem using this technique is made, for example, by Kirwan (1988). We give some hint of this theory in Appendix B.

We can define now the simplest Morse (Morse–Bott)-type functions as a class of functions possessing the minimal number of non-degenerate stationary points (or manifolds). This minimal number cannot be less than the number of critical orbits but it is allowed to be larger. To give the classification of Morse (Morse–Bott)-type functions due to complexity of the system of stationary points we introduce the measure of complexity to be the number of stationary points and the number of stationary manifolds excluding those associated with critical orbits.

Further classification of the Morse-type functions within one class of the same complexity (i.e. with the same number of stationary points (manifolds)), takes into account possible different distributions of stationary points (manifolds) over strata or within one stratum.

Now the general aim of the qualitative analysis may be formulated:

(i) To describe qualitatively different generic Hamiltonians invariant under given symmetry group.
(ii) To describe possible qualitative generic changes of Hamiltonians occurring under the variation of a given number of parameters.
(iii) To relate qualitative changes of classical functions with corresponding changes of quantum Hamiltonians.

6.1. Examples of Morse theory applications. Stationary points of the simplest Morse-type functions

Morse theory enables one to find restrictions on the numbers of stationary points of a generic function defined over compact manifolds. Table 7 shows examples of minimal sets of stationary points for several manifolds which are relevant for molecular and solid-state physical applications. Perfect Morse-type functions exist on all cited manifolds.

6.1.1. Function on the sphere in the presence of finite symmetry

Normally under the presence of symmetry the minimal possible number of stationary points of an invariant function is larger than that in the absence of symmetry. The simplest example is given by functions defined over S_2 in the presence of a point symmetry group with natural action induced by its linear action on three-dimensional ambient space (see Table 8). Remark that for some cases all stationary points of the simplest Morse-type function belong to critical orbits, sometimes they

Table 7
Stationary points of the simplest Morse functions defined on some manifolds

Manifold	Betti numbers	Stationary points[a]	Σ[b]	$\sum_i c_i$[c]
$S^2 \cong CP_1$	$b_0 = b_2 = 1, b_1 = 0$	$c_0 = c_2 = 1$	2	2
$T_2 = S_1 \times S_1$	$b_0 = b_2 = 1, b_1 = 2$	$c_0 = c_2 = 1, c_1 = 2$	0	4
$T_3 = S_1 \times S_1 \times S_1$	$b_0 = b_3 = 1, b_1 = b_2 = 3$	$c_0 = c_3 = 1, c_1 = c_2 = 3$	0	8
CP_2	$b_0 = b_2 = b_4 = 1$ $b_1 = b_3 = 0$	$c_0 = c_2 = c_4 = 1$	3	3
CP_N	$b_{2k} = 1$ $b_{2k+1} = 0$	$c_{2k} = 1$	$N + 1$	$N + 1$
$S_2 \times S_2$	$b_0 = b_4 = 1, b_2 = 2,$ $b_1 = b_3 = 0$	$c_0 = c_4 = 1, c_2 = 2$	4	4

[a] c_k is the number of stationary points of Morse index k.
[b] $\Sigma = \sum(-1)^k b_k$ is the Euler–Poincaré characteristics of the manifold (cf. Eq. (135)).
[c] Minimal number of stationary points.

Table 8
Simplest Morse functions defined on S^2 in the presence of symmetry

c_k[a]	Group					
	C_n, C_{nv}	C_i, C_{2h}, D_2, D_{2h}	D_n, D_{nd}, D_{nh}	T, T_d	O, O_h, T_h	I, I_h
c_0	1	2	2 or n	4	6 or 8	12 or 20
c_1	0	2	n	6	12	30
c_2	1	2	n or 2	4	8 or 6	20 or 12
$Q(t)$	0	$1 + t$	$(n-1)t + 1$ or $(n-1) + t$	$3 + 3t$	$7 + 5t$ or $5 + 7t$	$19 + 11t$ or $11 + 19t$

[a] c_k is the number of stationary points of Morse index k.

lie on the close strata as well, and for $C_i = S_2 = \bar{1}$ they are on the generic stratum. Table 8 gives examples of the simplest Morse-type functions defined over the S_2 sphere in the presence of symmetry. The polynomial $Q(t)$ (see Eq. (132)) is given to show that except for C_n, C_{nv} the simplest functions are not the perfect ones.

6.1.2. Functions on the d-torus in the presence of symmetry

Most physical properties of crystals are described by functions on the Brillouin zone invariant by the crystal symmetry and time reversal. Chapters IV–VI give detailed analysis of this symmetry.

Here we just note that the characterization of the system of stationary points of a function defined over the torus in the presence of the symmetry follows the same ideas based on the Morse theory as a simple example cited above for invariant functions over the two-dimensional sphere. The complete description of the system of stationary points for functions invariant under crystal arithmetic classes and time reversal was first given in Michel (1996) and reproduced in Chapter IV with the misprints corrected.

6.2. *Modifications of the system of stationary points. Bifurcations*

Very often in applications we work with families of functions depending on one or several control parameters rather than with a single specific function. In such a case instead of qualitative characterization of one chosen function we need to describe possible qualitative modifications occurring under the variation of the control parameters. One of the simplest cases to study is the possible modifications of the system of stationary points of a function under the variation of a control parameter. Morse theory naturally imposes severe restrictions on the type of possible modification of the system of stationary points. The simplest consequence is the impossibility to add just one stationary point (without removing the requirement for the function to be of Morse type).

The classification of possible modifications depends on the number of parameters and on the presence of symmetry. Bifurcations of the stationary points are responsible for the qualitative modifications of a function and to the appearance of new features for physical models. We will see in Chapter II many examples of the manifestation of the bifurcations of stationary points in molecular problems, in both classical and quantum pictures.

In order to supply here one simple example let us return to the analysis of O_h invariant functions defined over S_2 sphere (see Section 5.6.1). If we consider the one-parameter family of functions (similar to Eq. (118) but with slightly different parametrization)

$$H(\alpha) = \sin\alpha\theta_1 + \cos\alpha\theta_2 \ , \tag{136}$$

it is easy to verify that $H(\alpha)$ is a Morse-type function for $\tan\alpha \neq 0, -\frac{1}{4}, -\frac{1}{6}$. Moreover for $-\infty < \tan\alpha < -\frac{1}{4}$ we have the simplest Morse-type function. For $-\frac{1}{4} < \tan\alpha < \infty$ the function has the first level of complexity, i.e. the number of stationary points equals 50. One additional non-critical stationary orbit formed by 24 points exists on a one-dimensional stratum $C'_s = Cm$. It is possible even to precise the position of stationary orbit. For $-\frac{1}{4} < \tan\alpha < -\frac{1}{6}$ the stationary point lies between $C_{2v} = Amm2$ and $C_{3v} = R3m$, whereas for $-\frac{1}{6} < \tan\alpha < \infty$ the stationary point lies between $C_{3v} = R3m$ and $C_{4v} = P4mm$. Exceptional values $\tan\alpha = -\frac{1}{4} - \frac{1}{6}, \pm\infty$ correspond to functions which are not of the Morse type. $\tan\alpha = -\frac{1}{4}$ corresponds to the function with a degenerate stationary point at the $C_{2v} = Amm2$ critical orbit. In other words if we consider the family of functions $H(\alpha)$ and vary α from $(-\frac{1}{4} - \delta)$ to $(-\frac{1}{4} + \delta)$, the number of stationary orbits changes and the bifurcation of stationary points takes place at $\delta = 0$ (i.e. at $\alpha = -\frac{1}{4}$). $\delta = -\frac{1}{6}$ corresponds to another typical bifurcation for a one-parameter dependent family of functions. These two bifurcations can be easily characterized geometrically. At a bifurcation point the contour plot of the function on the orbifold becomes tangent to the boundary at C_{2v} or at C_{3v} critical orbit. The exceptional value $\tan\alpha = \pm\infty$ corresponds to the function which

possesses a continuum set of stationary points. Such behavior is not typical and slight perturbation by functions of higher degree removes this non-generic situation.

7. Physical applications

We conclude this chapter with general remarks about several physical applications which are not studied in details in the following chapters of this issue.

7.1. Action of the Lorentz group on the Minkowski space

The Minkowski space M is the space of energy $E = p_0$ and three-momentum $\boldsymbol{p}$ in the theory of special relativity. It is mathematically described by a four-dimensional real vector space carrying the invariant scalar product (in a unit system with $c = 1$) $s(p) = p_0^2 - \sum_i p_i^2$ invariant under the linear action of the Lorentz group [$\sim O(1,3)$]. The origin $p = 0$ is the unique fixed point; so it is its own stratum. The three other strata are the set of four-vectors p with, respectively,

$s > 0$, called time-like vectors; their stabilizers are conjugated to O_3,

$s < 0$, called space-like vectors; their stabilizers are conjugated to $O(1,2)$,

$s = 0, p \neq 0$, called light-like vectors (they form the light cone minus its vertex); their stabilizers are conjugated to a subgroup of $O(1,3)$ isomorphic to Eu_2.

7.2. Physical examples of systems and phenomena with continuous subgroups of $O(3) \times \mathscr{T}$ as symmetry groups

In 1894 P. Curie wrote the remarkable paper (Curie, 1894) which is concerned to the symmetry of physical phenomena and gives the realization of the one-dimensional Lie subgroups of the $O(3)$ group as symmetry groups of different physical phenomena. The study of $O(3)$ group is quite important for physical applications because it reflects the isotropy of our 3-D-physical space. We extend here the $O(3)$ group by adding the time reversal symmetry operation. The resulting group $O(3) \times \mathscr{T}$ has larger number of continuous symmetry subgroups and consequently we can give the more detailed description of physical systems and phenomena in the spirit of Curie analysis taking into account the presence or breaking of time reversal invariance.

The connected group $SO(3)$ is a "complete" group, i.e. it has no center and no outer automorphisms.[23] The following theorem for complete groups can be found in mathematical literature on group theory (Hall 1959, Section 6.4): if the complete group H is an invariant subgroup of group G, then $G \sim H \times Q$ with $Q = G/H$.[24] So the combined action of the geometric $O(3)$ and time reversal $\mathscr{T}$ symmetry on classical or quantum states with integral spin is that of the group

[23] The permutation groups S_n, for $n \neq 6$ give another example of "complete" groups.

[24] Probably the first application in physics of this theorem has been made with the group generated by $SO(3)$ of isospin and $Q = Z_2(C)$, where C is the charge conjugation; the two groups do not commute. Michel (1953) proved that their action on isospin states is that of a group isomorphic to $O(3)$ and called *isotopic parity* (now physicists say "isoparity") the corresponding new quantum number.

$G = O(3) \times Z_2(\mathscr{T}) = SO(3) \times Z_2(i) \times Z_2(\mathscr{T})$ where i is one of the traditional notations used in some domains of physics for the symmetry through the origin. We remind that we use the notation $H = K \wedge g$ to say that the group H is generated by the subgroup K and its element g.

In this section we will consider physical states whose symmetry is that of a Lie subgroup of G. To study their symmetry, we have to consider all conjugacy classes of Lie subgroups of G. The group $G \sim SO(3) \times Q$, with $Q \sim z_2^2$ has four connected components. The three-dimensional Lie subgroups of G are the counter image of the five subgroups of Q for the group homomorphism $G \to Q$. So the three Lie subgroups of G with two connected components are: $O(3)$, $SO(3) \wedge \mathscr{T}$, and $SO(3) \wedge \mathscr{T}_i = SO(3) \wedge \mathscr{T}_s$, where $\mathscr{T}_i = \mathscr{T} i$ and $\mathscr{T}_s = \mathscr{T} s$ where the s is any reflection through a plane.

In order to determine all one-dimensional Lie subgroups of $O(3) \times \mathscr{T}$ (up to a conjugation) we remark that the connected component of the identity for *all* one-dimensional Lie subgroups of $O(3) \times \mathscr{T}$ is C_∞ and it is an invariant subgroup of any of them. There is a partial ordering of their conjugacy classes.

The maximal one is $D_{\infty h} \times \mathscr{T}$. The quotient group $(D_{\infty h} \times \mathscr{T})/C_\infty = Z_2^3$ has 16 subgroups, seven of two elements, seven of four elements, itself Z_2^3 (eight elements), and the identity (trivial subgroup). The counter image of these 16 subgroups yields the 16 one-dimensional Lie subgroups of $O(3) \times \mathscr{T}$. Those which have two connected components are the union of two cosets of C_∞. The one different from C_∞ is of the form gC_∞. We can take for g the elements (the C_∞ axis will be considered as vertical and denoted by v)

$$v,\ h,\ vh = 2_h, \quad \mathscr{T}, \mathscr{T}_v = v\mathscr{T}, \quad \mathscr{T}_h = h\mathscr{T}, \quad \mathscr{T}_2 = 2_h\mathscr{T}, \tag{137}$$

where v, h are, respectively, reflections in a plane containing the C_∞ axis and in a plane perpendicular to it. (We could have taken, instead of h, the space inversion $i = h2_v$. We follow the tradition of molecular physicists who prefer the notation $C_{\infty h}$ to $C_{\infty i}$.) The corresponding notation for these seven groups with two connected components is

$$C_{\infty v},\ C_{\infty h},\ D_\infty,\ C_\infty \wedge \mathscr{T},\ C_\infty \wedge \mathscr{T}_v,\ C_\infty \wedge \mathscr{T}_h,\ C_\infty \wedge \mathscr{T}_2\ . \tag{138}$$

All other one-dimensional subgroups with four and eight connected components (= 4 or = 8 cosets) are given in Table 9. Remark that Curie (1894) have considered five one-dimensional subgroups $C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}$.

Several groups from the complete list naturally arise as symmetry groups of simple quantum systems.

$C_{\infty v} \wedge \mathscr{T}$ is the symmetry group for the atom in static electric field or for the Rydberg states of heteronuclear diatomic molecule.

$C_{\infty h} \wedge \mathscr{T}_v$ is the symmetry group of an atom in constant magnetic field (Zeeman effect).

$C_\infty \wedge \mathscr{T}_v$ is the maximal common subgroup of $C_{\infty v} \wedge \mathscr{T}$ and $C_{\infty h} \wedge \mathscr{T}_v$. Thus it corresponds to the symmetry of an atom under the simultaneous presence of two parallel magnetic and electric fields.

$D_{\infty h} \wedge \mathscr{T}$ group is the symmetry group for Rydberg states of homonuclear diatomic molecule, or of the quadratic Zeeman effect.

Another interesting quantum example can be given by circularly polarized photon. It is characterized by the group $C_\infty \wedge \mathscr{T}_2$.

Let us now add the physical realization for three-dimensional Lie subgroups of $O(3) \wedge \mathscr{T}$.

Table 9
Description of one-dimensional subgroups of $O(3)\times\mathscr{T}$ with four connected components in terms of continuous and discrete symmetry elements. Sign + means that the corresponding element belongs to the symmetry group

C_∞	C_v	C_h	C_2	$\mathscr{T}$	$\mathscr{T}_v$	$\mathscr{T}_h$	$\mathscr{T}_2$	Group[a]	Perturbations
+	+	+	+					$D_{\infty h}$	Dilation (compression)
+	+			+	+			$C_{\infty v}\wedge\mathscr{T}$	Axis asymmetry
+		+		+		+		$C_{\infty h}\wedge\mathscr{T}$	Double twist
+			+	+			+	$D_\infty\wedge\mathscr{T}$	Uniform twist
+	+					+	+	$C_{\infty v}\wedge\mathscr{T}_h$	Axial current
+		+			+		+	$C_{\infty h}\wedge\mathscr{T}_v$	Angular current
+			+		+	+		$D_\infty\wedge\mathscr{T}_v$	Two opposite angular current
+	+	+	+	+	+	+	+	$D_{\infty h}\wedge\mathscr{T}$	Unperturbed cylinder

[a]Alternative notation for $C_{\infty v}\wedge\mathscr{T}$ is $C_{\infty v}\wedge\mathscr{T}_2$, for $C_{\infty h}\wedge\mathscr{T}_v$ is $C_{\infty h}\wedge\mathscr{T}_2$, for $D_\infty\wedge\mathscr{T}_v$ is $D_\infty\wedge\mathscr{T}_h$, and for $D_{\infty h}\wedge\mathscr{T}$ is $D_{\infty h}\wedge\mathscr{T}_\alpha$ with $\mathscr{T}_\alpha=\mathscr{T}_v,\mathscr{T}_h$, or $\mathscr{T}_2$.

Electric charge has complete $O(3)\wedge\mathscr{T}$ symmetry. In physically reasonable approximation ^{4}He atom in its ground state gives another example of a system with $O(3)\wedge\mathscr{T}$ symmetry.

Spherically symmetric outgoing wave is the system with $O(3)$ symmetry. We can consider space dilation or compression as an example of perturbation breaking the time reversal symmetry. Such a perturbation physically can be realized if an atom is supposed to be in the spherical box with varying radius. ^{4}He atom within the fullerene cage under varying pressure gives approximate physical realization of the effect in the molecular domain.

To realize the $SO(3)\wedge\mathscr{T}$ symmetry group as the symmetry group of a physical system we can take a "relatively" stable particle which is a pseudoscalar. π meson is an example. $\pi^\pm$ can be considered as stable for times much smaller than $\sim 10^{-8}$ s. A macroscopic example of this symmetry group is given by isotropic optically active liquid.

The magnetic monopole gives an example of a system with the invariance symmetry group $SO(3)\wedge\mathscr{T}_s$.

Finally the disintegration of a π meson is the process which is invariant with respect to the $SO(3)$ symmetry group only.

As soon as Curie did not consider explicitly the time reversal he made no difference between static electric field and electric current, for example.

We can propose more formal physical realizations of different one-dimensional subgroups of $O(3)\wedge\mathscr{T}$. Let us consider a homogeneous fixed cylinder as an initial classical object. Its symmetry group is the $D_{\infty h}\wedge\mathscr{T}$ group which is the maximal one-dimensional subgroup of $O(3)\wedge\mathscr{T}$. Further we introduce several elementary excitations (physical perturbations) which correspond to different broken symmetries. In Table 9 we introduce these perturbations, the seven one-dimensional symmetry groups with four connected components are listed in this table. We explain them shortly below.

(i) Homogeneous dilation or compression of the system considered as a time dependent phenomenon. This perturbation breaks the time reversal invariance because time reversal interchanges dilation and compression. The associated symmetry group is $D_{\infty h}$.

(ii) Axis asymmetry can be introduced by a static form of asymmetry (transformation of cylinder into pear-like object) or by a constant electric field parallel to the symmetry axis. The corresponding symmetry group is $C_{\infty v} \wedge \mathscr{T}$.

(iii) Double twist is the static perturbation of the cylinder such that the middle section of the cylinder is twisted in one direction whereas two ends are twisted in the same opposite direction. The corresponding symmetry group is $C_{\infty h} \wedge \mathscr{T}$.

(iv) Uniform twist is just a simple static twist of two opposite ends of the cylinder in opposite directions. The symmetry group is $D_{\infty} \wedge \mathscr{T}$. Much simpler physical realization of the same symmetry group can be reached with a cylinder filled by isotropic optically active liquid.

(v) Axial current can be realized for example as an electric or thermic current along the axis of the cylinder. This perturbation breaks in particular the time reversal invariance. The symmetry group is $C_{\infty v} \wedge \mathscr{T}_h$.

(vi) Angular current can be realized as uniform rotation of the cylinder, or as constant magnetic field parallel to the axis (solenoid magnetic field). The symmetry group is $C_{\infty h} \wedge \mathscr{T}_v$.

(vii) Two opposite angular currents can be constructed with two rotations, two electric circular currents or a magnetic field parallel to the axis and varying linearly (or more generally as an odd function) along the axis and passing through the zero in the equatorial plane of the cylinder. The symmetry group is $D_{\infty} \wedge \mathscr{T}_v$.

There are four plus signs in each column of Table 9. One $+$ stands to unperturbed cylinder and three others correspond to three different four-component groups possessing the same two-component group as a subgroup. Thus each two component symmetry group can be obtained by three different pairs of perturbations taken from Table 9.

Physical interpretation of this construction is as follows. Let us associate with each elementary perturbation the physical situation characterized by the same symmetry. Three different situations are associated with each one component symmetry group. In principle each situation can be considered as a cause or as an effect. The application of Curie principle means that if we apply two (among three possible) situations as a cause, the third could be the effect.

Following realizations can be proposed for illustration.

(a) "Angular current", "axial current", and "uniform twist" have $C_{\infty} \wedge \mathscr{T}_2$ symmetry group as common subgroup. Simultaneous application of "angular current" and "axial current" which we consider as a cause could produce the appearance of a "uniform twist" as an effect. Realization of angular current as a magnetic field and axial current as an electric current enables us to formulate the following physical statement: mechanical twist of a cylinder could be observed if electric current passes along the axis of the cylinder situated along the axis of magnetic field. We can choose two other perturbations as a cause and the third perturbation will be the effect. Two complementary physical statements will be:

(i) Mechanical twist of a cylinder with axial electric current can produce appearance of the axial magnetic field.

(ii) Mechanical twist of an axial magnet can result in the appearance of electric current along the axis of the cylinder.

Naturally each formal perturbation can be realized by different physical situations. For example, instead of electric current and magnetic field we can consider the propagation of a circular polarized light parallel to the cylinder axis.

(b) Another triple of elementary perturbations associated with the symmetry group $C_{\infty h} \wedge \mathscr{T}_h$ are "two opposite angular currents", "axial current", and "double twist". Here and below we give only one (among three possible) choice of cause and effect. Two other effects can be easily deduced.

Simultaneous application of "two opposite angular currents" and axial current gives a system with $C_{\infty h} \wedge \mathscr{T}_h$ symmetry could result in the appearance of a double twist as an effect.

(c) Uniform twist and axis asymmetry together reduce the symmetry to $C_\infty \wedge \mathscr{T}$ and produce the double twist.

(d) Axis asymmetry together with angular current give the symmetry group $C_\infty \wedge \mathscr{T}_v$ and result in appearance of two opposite angular currents.

(e) Axis asymmetry together with axial current give the $C_{\infty v}$ symmetry group which indicates the presence of the dilation.

(f) Double twist plus angular current lead to $C_{\infty h}$ symmetry group and again produce the dilation as an effect.

(g) Uniform twist plus two opposite angular currents yield the D_∞ symmetry group and are accompanied by the dilation as well.

(h) To obtain the C_∞ symmetry group we can apply three elementary excitations, for example, static axis asymmetry, axial current, and angular current.

7.3. Geometrical configurations of N-particle systems. Shape coordinates and their invariant description

To characterize an instantaneous geometrical configuration of the *N-particle* system one should introduce the internal coordinates (shape coordinates in terminology of Littlejohn and Reinsch (1997)) which give the unambiguous description of different geometrical configurations. Naturally, two geometrical configurations of N points in 3-D-space are equivalent if they have the same center of gravity and they can be transformed one into another through orthogonal transformation.

In 3-D-space the $N-1$ Jacobi vectors ($3N-3$ scalar components can be used as variables) are sufficient to characterize the geometrical position of N particle with respect to their center of mass. But at the same time only $3N-6$ variables are algebraically independent as shape coordinates. The problem of the construction of a suitable set of shape coordinates can be reformulated as a description of variables needed to classify the space of orbits of group $SO(3)$ acting on a system of $N-1$ 3-vectors. Each vector belongs to the irreducible representation of $SO(3)$ for $J=1$, where J is the total angular momentum quantum number. In what follows it will be denoted by (1). Thus, we should construct a system of $SO(3)$ invariants for an initial reducible representation $\Gamma = (1) \oplus (1) \oplus \cdots \oplus (1)$. Invariant polynomials forming integrity basis for this initial representation can be used as shape coordinates for the N-body problem.

Description of the algebra of invariant polynomials for this particular problem was given by Weyl (1939) in terms of generators and relations (syzygies) between them. With increasing N the algebra of invariants becomes very complicated but for low N rather simple and physically clear integrity bases can be proposed.

We list below generating functions for invariants for low N before formulating the general result.

Let us consider the trivial case of one vector ($N = 2$) which corresponds to the (1)-representation of the $SO(3)$ group.

The generating function for invariants has the form

$$g(0 \leftarrow 1) = \frac{1}{1 - t^2} \ . \tag{139}$$

We have one basic invariant which is of the second order $I_1 = x^2$. It can be used to label the orbits. This means that the shape of a two-particle system can be completely characterized by a one polynomial variable, the square of the distance between particles, which is clearly a trivial result.

In the case of a three-particle system we should analyze the system of $SO(3)$ invariants for two vectors (initial representation is $(1)\oplus(1)$). The generating function for invariants has the form

$$g(0 \leftarrow 1\oplus 1) = \frac{1}{(1 - t^2)^3} \ . \tag{140}$$

So to represent invariant functions we have three basic invariants (polynomials of second degree). We can take them (for two vectors $\boldsymbol{x}_1, \boldsymbol{x}_2$) as $I_1 = x_1^2$, $I_2 = x_2^2$, $I_3 = (\boldsymbol{x}_1 \cdot \boldsymbol{x}_2)$. It is clear that $I_1 \geq 0$ and $I_2 \geq 0$, whereas I_3 should satisfy the restriction $I_3^2 \leq I_1 I_2$.

For the four-particle system the generating function for invariants is

$$g(0 \leftarrow 1\oplus 1\oplus 1) = \frac{1 + t^3}{(1 - t^2)^6} \ , \tag{141}$$

which for the first time has a non-trivial numerator. This means that there exist six linearly independent invariants of degree 2 and one auxiliary invariant of degree three. This numerator invariant is algebraically dependent on six basic invariants. Itself, it cannot be represented as a polynomial in basic invariants, but its square can. Natural choice of six basic invariants $\boldsymbol{I} = (I_1, \ldots, I_6)$ (for three vectors, say $\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3$) is

$$\boldsymbol{I} = (y_1^2, y_2^2, y_3^2, (\boldsymbol{y}_1 \cdot \boldsymbol{y}_2), (\boldsymbol{y}_2 \cdot \boldsymbol{y}_3), (\boldsymbol{y}_3 \cdot \boldsymbol{y}_1)) \ . \tag{142}$$

As an auxiliary invariant of the third degree it is natural to take the mixed product $\phi = (\boldsymbol{y}_1 \cdot (\boldsymbol{y}_2 \times \boldsymbol{y}_3))$. It is clear that ϕ^2 is a polynomial in basic invariants. When $\phi \neq 0$ the coordinates $I_1, I_2, I_3, I_4, I_5, I_6$ do not give the unique description of the configuration. The same set $I_1, \ldots, I_6$ describes two different configurations (right and left) which can be distinguished by the sign of the auxiliary invariant ϕ. This means that in the six-dimensional space of basic invariants all internal points of the orbifold have two points as an image in the real configuration space, whereas points on the surface $\phi = 0$ are unique.

For the five-particle system the generating function for invariants starts looking complicated

$$g(0 \leftarrow 1\oplus 1\oplus 1\oplus 1) = \frac{1 + t^2 + 4t^3 + t^4 + t^6}{(1 - t^2)^9} \ . \tag{143}$$

We have for the five-particle system seven non-trivial numerator invariants.

For general N the generating function for invariants can be written in terms of an integral over $SO(3)$ group

$$g_{so(3)}(N;t) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi}\frac{\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\chi}{\det[\boldsymbol{I} - t\boldsymbol{M}(\theta,\phi,\chi)]}\,, \tag{144}$$

where the matrix $\boldsymbol{M}(\theta,\phi,\chi)$ is block diagonal with $N-1$ identical blocks each being the 3×3 Euler rotation matrix $a(\theta,\phi,\chi)$. This integral can be calculated explicitly and the generating function has the following form (Collins and Parsons, 1993)

$$g_{so(3)}(N;t) = \frac{F(t)}{(1-t^2)^{3N-6}} \tag{145}$$

with

$$F(t) = \frac{1}{N-2}\sum_{n=0}^{N-3}\sum_{k=0}^{n}\frac{(n+k)!}{(k!)^2(n-k)!}t^{2k}(1-t)^{2N-6-n-k}(1+t)^{N-3+n-k}\,. \tag{146}$$

7.4. Landau theory of phase transitions

About 60 years ago Landau (1937a, b) has formulated the basic principles of the phenomenological theory of second-order phase transitions which were based on the crucial idea about spontaneous symmetry breaking under phase transition (Landau and Lifshitz, 1958). This approach was generalized later and led to the unified description of completely different physical systems within the unique mathematical formalism.

The essential point of the Landau-type theory is the symmetry breaking occurring under the continuous variation of the physical state of the system. The thermodynamic potential or any other physical quantity which characterizes the phase transition is represented near the transition points as a series expansion in invariant functions for the high-symmetry phase. That is why the mathematical theory of continuous phase transitions is closely related to the description of invariant and covariant polynomials for different chains of groups and that is why the first physical applications of this theory was related with phase transitions in crystal solids. We do not want to enter into this vast field of applications and just restrict ourselves to some basic references which cover this field (Landau and Lifshitz, 1958; Lyubarskii, 1957; Stanley, 1971; Ma, 1976; Izyumov and Syromyatnikov, 1984).

Appendix A. Group theory: glossary

We give in this appendix some group-theoretical definitions which can be found in various textbooks at different level of abstraction. As group theory for physicists books we recommend Wigner (1959), Weyl (1931), Lyubarskii (1957), and Hamermesh (1964), for more mathematical aspects Hall (1959), Lang (1965), Serre (1977), and Brown (1982).

Group

A group G is a set with a composition law: $\diamond \in M(G\times G, G)$, which is associative:

$$\forall g,h,k\in G,\quad (g\diamond h)\diamond k = g\diamond(h\diamond k)\,, \tag{A.1}$$

which has a neutral element e:

$$\forall g \in G, \quad e \diamond g = g = g \diamond e \tag{A.2}$$

and every element has an inverse one:

$$\forall g \in G, \exists g', \quad g' \diamond g = e = g \diamond g' \ . \tag{A.3}$$

Remark that the neutral element is unique.

There are two usual notations for the group law and the neutral element:

$+, \mathbf{0}$. Examples: the additive group of integers $\mathbb{Z}$, of real or complex numbers, $\mathbb{R}$ or $\mathbb{C}$, the additive group M_{mn} of $m \times n$ matrices with real (respectively, complex) elements. This notation is generally restricted to *Abelian groups*, i.e. the groups with a commutative law: $a + b = b + a$. The inverse element of a is denoted by $-a$ and is called the opposite.

$\times$, ($\mathbf{1}$ or $\boldsymbol{I}$). Examples: the multiplicative groups $\mathbb{R}^\times$,$\mathbb{C}^\times$; the n-dimensional linear groups $GL(n,R)$, $GL(n,C)$, i.e. the multiplicative groups of $n \times n$ matrices on $\mathbb{R}$ or $\mathbb{C}$ with non-vanishing determinant.[25] The inverse element of g is denoted by g^{-1}. Often we will omit the sign $\times$.

In all examples we have just given, the groups have an infinite number of elements. An example of a *finite group* is $\mathscr{S}_n$ the group of permutations of n objects. We shall denote by $|G|$ the number of elements of G.

Subgroup

When a subset $H \subset G$ of elements of G form a group (with the *composition law of G restricted to H*), we say that H is a subgroup of G and we shall denote it by $H \leq G$ (this is not a general convention) or by $H < G$ when we want to emphasize that H is a strict G-subgroup, i.e. H is subgroup of G and $H \neq G$. Note that $A \leq B$, $B \leq G \Rightarrow A \leq G$.

Examples:[26] The subset $U(n)$ of matrices of $GL(n,C)$ which satisfy $m^* = m^{-1}$ is a subgroup of $GL(n,C)$; it is called the n-dimensional unitary group. In particular $U(1) < \mathbb{C}^\times$. Note also that $GL(n,R) < GL(n,C)$.

Since the determinant of the product of two matrices is the product of their determinants, in a group of matrices the matrices of determinant one form the "unimodular subgroup".

Another general example of a subgroup is the one generated by one element. Let $g \in G$ and consider its successive powers: $g, g^2, g^3, \ldots$; The *order of g* is the smallest integer such that $g^n = I$. If no such n exists, we say that g is of infinite order. When g is of finite order n the subgroup generated by g is formed of the distinct powers of g; it is called a cyclic group of order n and it is usually denoted[27] by Z_n. For example $e^{2\pi i/n} \in \mathbb{C}^\times$ generates the cyclic group

$$Z_n = \{e^{2\pi i k/n}, 0 \leq k \leq n-1\} < U(1) < \mathbb{C}^\times \ . \tag{A.4}$$

Remark that the intersection of subgroups of G is a G-subgroup. Generally, the union of subgroups is not a subgroup.

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[25] For $n = 1$, $\mathbb{R}^\times = GL(1,R)$, $\mathbb{C}^\times = GL(1,C)$.

[26] We denote by $m^\top$ the transpose of the matrix m, i.e. $(m^\top)_{ij} = m_{ji}$ and by m^* the Hermitean conjugate of m, i.e. $(m^*)_{ij} = \bar{m}_{ji}$, the complex conjugate of m_{ji}.

[27] We shall sometimes use the notation C_n, but Z_n is very traditional; it comes from the German "Zyklisch". Similarly $\mathscr{S}_n$ is traditional and comes from "substitution".

Lattice

The set of subgroups of a group is an example of a *lattice*. A lattice is a partially ordered set such that for any two given elements, x, y, there exists a unique minimal element among all elements z such that $z > x$ and $z > y$, and similarly for any two given elements, x, y, there exists a unique maximal element among all elements z' such that $z' < x$ and $z' < y$. In particular, a lattice has unique minimal and maximal elements. G is the maximal element of the lattice of its subgroups, the trivial subgroup $\{1\}$ is the minimal one.

Cosets

Let $H < G$. The relation among the elements of G:$x \in yH$ is an equivalence relation; it is reflexive: $x \in xH$, symmetric: $x \in yH \Leftrightarrow y \in xH$, transitive: $x \in yH$, $y \in zH \Rightarrow x \in zH$. The equivalence classes are called *cosets*. We denote by G:H the quotient set, i.e. the set of cosets.

Invariant subgroup

We could have pointed out that we were using left cosets; similarly we can introduce right cosets Hx. In general $xH \neq Hx$. When left and right cosets are identical, H is called an *invariant subgroup*.[28] We will also write this property $H \lhd G$:

$$H \lhd G \overset{\text{def}}{=} H \leq G, \quad \forall g \in G,\ gH = Hg\ . \tag{A.5}$$

Evidently, *every subgroup of an Abelian group is invariant.*

Every non-trivial group has two invariant subgroups: $\{1\}$ and G itself. The set of invariant G-subgroups forms a lattice (sublattice of the subgroup lattice). Beware that $K \lhd H$, $H \lhd G$ does not imply $K \lhd G$.

Quotient group

When $K \lhd G \Leftrightarrow$ there is a natural group structure on G:K; indeed $gK \diamond hK = (gK)(hK) = gKhK = (gh)K$. We call this group the *quotient group*[29] of G by K and we denote it by G/K. Since the determinant of a matrix is invariant by conjugacy by an invertible matrix, the unimodular subgroups are invariant. The corresponding quotient groups are

$$GL(n, C)/SL(n, C) = \mathbb{C}^{\times}, \quad GL(n, R)/SL(n, R) = \mathbb{R}^{\times}\ ,$$

$$U(n)/SU(n) = U(1), \quad O(n)/SO(n) = Z_2\ .$$

Remark that an index 2 subgroup is always an invariant subgroup.

Conjugacy classes

Two elements $x, y \in G$ are conjugate if there exists a $g \in G$ such that $y = gxg^{-1}$. Conjugacy is an equivalence relation among the elements of a group. A group is therefore a disjoint union of its conjugacy classes. Remark that gh is conjugate to hg. The elements of a conjugacy class have the same order.

[28] An often used synonym is *normal subgroup*.

[29] Sometimes this is called the "factor" group; this is illogical, and even confusing: generally the quotient group cannot be identified with a G-subgroup.

Center

An element which commutes with every element of a group G forms a conjugacy class by itself (this is always the case of the identity); these elements form a subgroup called the *center* of G and often denoted by $C(G)$. The center is an invariant[30] subgroup of G. If the group A is Abelian: $C(A) = A$. Examples:

$$C(GL(n,C)) = \mathbb{C}^{\times} I, \quad C(GL(n,R)) = \mathbb{R}^{\times} I,$$

$$C(U(n)) = U(1)I, \quad C(O(n)) = Z_2 I.$$

The matrices of these centers are multiples of the identity matrix I.

Conjugated subgroups

Two G-subgroups H, H' are said to be *conjugate* if there exists $g \in G$ such that $H' = gHg^{-1}$. This is an equivalence relation among subgroups of a group. We denote by $[H]_G$ the conjugacy class of H. When a subgroup is alone in its conjugacy class, this is an invariant subgroup. We have seen that the subgroups of a group form a lattice. Beware that this is not true for the set of subgroup conjugacy classes.

Centralizer

The *centralizer* of $X \subset G$ is the set of elements of G which commute with **every** element of X; this set is a G-subgroup, we denote it by $C_G(X)$; e.g. the center of G: $C(G) = C_G(G)$.

Normalizer

The *normalizer* of $X \subset G$ is a G-subgroup

$$N_G(X) = \{g \in G, gXg^{-1} = X\} \ . \tag{A.6}$$

Note that $C_G(X) \lhd N_G(X)$.

From the definition of the normalizer, when $H \leq G$, $N_G(H)$ is the largest[31] G-subgroup such that $H \lhd N_G(H)$. For instance: $N_G(H) = G \Leftrightarrow H \lhd G$.

Homomorphism

A group *homomorphism* or, shorter, a *group morphism* between the groups G, H is a map $G \xrightarrow{\rho} H$ compatible with both group laws

$$G \xrightarrow{\rho} H, \quad \rho(xy) = \rho(x)\rho(y), \ \rho(1) = 1 \in H \ . \tag{A.7}$$

This implies

$$\rho(x^{-1}) = \rho(x)^{-1} \ . \tag{A.8}$$

A morphism of a group G into the groups $GL(n,C), GL(n,R), U(n), O(n)$ respectively is called a n-dimensional (complex, real) linear, unitary, orthogonal representation of G.

Kernel and image

The image of the morphism $G \xrightarrow{\rho} H$ is denoted by $\mathrm{Im}\,\rho$. It is a subgroup of H, $\mathrm{Im}\,\rho \leq H$ which includes images of all elements of G.

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[30] It has even a stronger property: it is a characteristic subgroup.

[31] Indeed it is generated by all G-subgroups which contain H as an invariant subgroup.

The kernel $\mathrm{Ker}\,\rho$ of the morphism $G \overset{\rho}{\to} H$ is the set $K \in G$ which is mapped on $1 \in H$. $\mathrm{Ker}\,\rho$ is an invariant subgroup of G. We have the important relation $\mathrm{Im}\,\rho = G/\mathrm{Ker}\,\rho$.

Sequence of homomorphisms

Let us consider the following sequence of homomorphisms of Abelian groups:

$$G_1 \overset{\rho_1}{\to} G_2 \overset{\rho_2}{\to} \cdots G_{n-1} \overset{\rho_{n-1}}{\to} G_n \overset{\rho_n}{\to} G_{n+1} \cdots \ . \tag{A.9}$$

Such a construction, named complex, is quite useful to relate topological and group-theoretical properties. If for all n we have $\mathrm{Im}\,\rho_{n-1} = \mathrm{Ker}\,\rho_n$, the sequence in Eq. (A.9) is an *exact sequence of homomorphisms*.

Examples: If $H \lhd G$ and $G \overset{\rho}{\to} G/H$ we can write

$$1 \to H \overset{i}{\to} G \overset{\rho}{\to} G/H \to 1 \ , \tag{A.10}$$

where $H \overset{i}{\to} G$ is the injection map, i.e. $\forall x \in H$, $i(x) = x \in G$. An exact sequence of this type is named *short exact*. The diagram $1 \to H \overset{i}{\to} G$ means that $\mathrm{Ker}\,i = 1$, i.e. i is injective. $1 \to H$ is the injection of the unit into H. The fact that ρ is surjective is expressed by $G \overset{\rho}{\to} G/H \to 1$. For any homomorphism ρ there is always a short exact sequence

$$1 \to \mathrm{Ker}\,\rho \overset{i}{\to} G \overset{\rho}{\to} \mathrm{Im}\,\rho \to 1 \ . \tag{A.11}$$

Homology groups

Let us now consider a sequence of homomorphisms (A.9) with less restrictive condition on consecutive homomorphisms

$$\mathrm{Im}\,(\rho_{n+1}\rho_n) = 0 \ . \tag{A.12}$$

That is

$$\mathrm{Im}\,\rho_n \subset \mathrm{Ker}\,\rho_{n+1} \ . \tag{A.13}$$

Let $Z_n = \mathrm{Ker}\,\rho_n$ and $B_n = \mathrm{Im}\,\rho_{n-1}$. Elements of G_n are called n-(co)chains, those of Z_n n-(co)cycles, and those of B_n n-(co)boundaries. The groups

$$H_n = Z_n/B_n \ . \tag{A.14}$$

are called the (co)-homology groups of the complex (A.9). We do not discuss here the difference between homology and cohomology, chains and cochains, etc. and just suggest the reader to consult mathematical literature.

If we had $H_n = 0$ for all n, the sequence (A.9) would have been exact. Thus the (co)homology group measures the "lack of exactness" of the sequence.

Euler-Poincaré characteristics

Let $\phi(H_i)$ be rank of the ith homology group. The Euler–Poincaré characteristics of the complex (A.9) is

$$\chi = \sum(-1)^i \phi(H_i) \ . \tag{A.15}$$

Isomorphism

A bijective morphism ρ is called an *isomorphism*. In other words if $\mathrm{Ker}\,\rho = 1_G$, and $\mathrm{Im}\,\rho = H$ than ρ is an isomorphism and $G \sim H$. When we want to classify groups, this will be done up to isomorphism, except if we precise explicitly a more refined classification. Often when we write about "abstract groups" we mean an isomorphism class of groups.[32]

Example. For every prime number p there is (up to isomorphism) only one group of order p: this is Z_p.

Automorphism

An isomorphism from G to G is called an *automorphism* of G. The composition of two automorphisms is an automorphism. Moreover $\forall g \in G$, $I(g) = g$ is the identity automorphism and every automorphism has an inverse; so the automorphisms of G form a group, $\mathrm{Aut}\,G$. The conjugation by a fixed element $g \in G$ induces a G-automorphism: $(gxg^{-1})(gy^{-1}g^{-1}) = g(xy^{-1})g^{-1}$ which is an "inner" automorphism. The set of inner automorphisms forms a subgroup of $\mathrm{Aut}\,G$ that we denote by $\mathrm{In}\,\mathrm{Aut}\,G$. Note that the elements $c \in C(G)$ of the center of G induce the trivial automorphism I_G, so we have the exact sequence:

$$1 \to C(G) \to G \xrightarrow{\theta} \mathrm{In}\,\mathrm{Aut}\,G \to 1\ . \tag{A.16}$$

An automorphism which is not inner, is called outer automorphism. We remark that $\mathrm{In}\,\mathrm{Aut}\,G$ is an invariant subgroup of $\mathrm{Aut}\,G$.

Direct products

Given two groups G_1, G_2, one can form a new group, $G_1 \times G_2$, the direct product of G_1 and G_2: the set of elements of $G_1 \times G_2$ is the product of the set of elements of G_1 and of G_2, i.e. the set of ordered pairs: $\{(g_1, g_2), g_1 \in G_1, g_2 \in G_2\}$, the group law is:

$$(g_1, g_2)(h_1, h_2) = (g_1 h_1, g_2 h_2)\ . \tag{A.17}$$

When $G_1 \neq G_2$, $G_1 \times G_2 \neq G_2 \times G_1$, but they are isomorphic i.e. $G_1 \times G_2 \sim G_2 \times G_1$.

Semi-direct products

Given a morphism $Q \xrightarrow{\theta} K$ one defines the *semi-direct product* as the group whose elements are the pairs (k, q), $k \in K, q \in Q$, and the group law is (using $q \cdot k$ as a short for $(\theta(q))(k)$):

$$(k_1, q_1)(k_2, q_2) = (k_1\, q_1 \cdot k_2, q_1 q_2)\ . \tag{A.18}$$

Here we denote this semi-direct product by $K \rtimes Q$. The semi-direct product of $\mathbb{R}^n$ and $GL(n, R)$ is called the affine group:

$$Aff_n(R) = \mathbb{R}^n \rtimes GL(n, R)\ . \tag{A.19}$$

Similarly we can define the complex affine group: $Aff_n(C) = \mathbb{C}^n \rtimes GL(n, C)$.

[32] In that case we may often use = for isomorphic groups.

The Euclidean group E_n is the semi-direct product (we write simply Aff_n for $Aff_n(R)$):

$$E_n = \mathbb{R}^n \rtimes O(n) \leq Aff_n \ . \tag{A.20}$$

Group extensions

Given two groups K, Q, a very natural problem is to find all groups E such that $K \lhd E$ and $Q = E/K$. E is called an extension of Q by K. The extension can be represented by a diagram

$$1 \to K \to E \to E/K \to 1 \ , \tag{A.21}$$

which is not an exact sequence. The main problem is to classify different extensions up to equivalence. When E is determined, the action of the group $Q = E/K$ in K is defined. The inner automorphisms of E induce automorphisms of K in a natural way:

$$\forall x \in E, \quad \alpha \in K, \quad \alpha \to x\alpha x^{-1} = f(x)\alpha,$$
$$E \xrightarrow{f} \operatorname{Aut} K.$$

So the problem of finding all group extensions of Q by K can be decomposed in two steps:

(i) Find all homomorphisms g of Q into $\operatorname{Out} K$, they form the set $\operatorname{Hom}(Q, \operatorname{Out} K)$.
(ii) Given Q, K, $g \in \operatorname{Hom}(Q, \operatorname{Out} K)$ find all non-equivalent extensions.

The solution of this mathematical problem is known and given in terms of cohomology groups. The semi-direct product (and it particular case, the direct product) are particular examples of an extensions. But in general case of an extension E of Q by K there is no subgroup of E isomorphic to the quotient Q.

Such an example is given by $SU(2)$ as an extension of $SO(3)$ by Z_2:

$$1 \to Z_2 \to SU(2) \to SO(3) \to 1 \ . \tag{A.22}$$

$SU(2)$ is the group of two-by-two unitary matrices of determinant 1. Its center Z_2 has two elements, the matrices 1 and -1. These matrices are the only square-root of the unit. The three-dimensional rotation group $SO(3)$ is isomorphic to $SU(2)/Z_2$. This group has an infinity of square roots of 1: the rotations by π around arbitrary axis. So $SO(3)$ is not a subgroup of $SU(2)$.

Appendix B. Morse–Bott theory

First of all we extend the concept of non-degeneracy of a function f defined over the manifold M. If N is a connected sub-manifold of M, it will be called a *non-degenerate stationary manifold* for f if and only if at every point of N, $\mathrm{d}f = 0$ and the Hessian is non-degenerate on the normal bundle.

It is natural to extend the notion of the Morse index to non-degenerate stationary manifolds by counting the number of negative eigenvalues of the Hessian on the normal bundle. A function f will be called non-degenerate Morse–Bott-type function if its set $C(f)$ of extrema is a union of non-degenerate stationary manifolds and non-degenerate isolated extrema. These isolated extrema will also be called stationary points of the function, as it is often done in mechanics.

Let now describe shortly what should be done with Morse theory to take into account a priori symmetry of a function f under the action of a (continuous) compact Lie group G on a manifold M. If the action is free (i.e. all stabilizers $G_m = 1$ so there is only one stratum, and all its orbits are principal) the solution is very simple. In this case the orbit space $M|G$ is itself a manifold and we can apply the usual Morse theory to the corresponding function f/G defined over $M|G$. Unfortunately this is not the case for the most part of physically interesting examples.

To extend Morse inequalities to the case of functions possessing a non-degenerate stationary manifold there are two possibilities. There exist more sophisticated Morse inequalities written in terms of usual homology groups for the whole manifold M and for stationary (non-degenerate) sub-manifolds. We have also to consider Poincaré polynomial $P_{C_\alpha}(t)$ for each connected component C_α of the set of stationary points. These last polynomials are needed to write down the polynomial counting stationary points and stationary manifolds of a Morse–Bott function, $\mathscr{M}_f(t)$

$$\mathscr{M}_f(t) = \sum t^{\mu(C_\alpha)} P_{C_\alpha}(t) \,, \tag{B.1}$$

Here $\mu(C_\alpha)$ is the Morse index of the non-degenerate stationary submanifold C_α. If C_α is an isolated stationary point the corresponding Poincaré polynomial reduces to 1. If for example, C_α is a one-dimensional sphere S_1, such a stationary submanifold is counted by a $(1 + t)$ polynomial.

The Morse inequalities now can be formulated in the following statement. All coefficients of the polynomial $Q_f(t)$ defined by Eq. (B.2)

$$\sum t^{\mu(C_\alpha)} P_{C_\alpha}(t) - P_M(t) = (1 + t) Q_f(t) \,, \tag{B.2}$$

are non-negative.

Another way of extending Morse theory to G-invariant functions is based on the possibility to replace everywhere the usual homology by their equivariant analogs. The following theorem is valid.

The equivariant Morse inequalities. For any non-degenerate G invariant f on the compact manifold M, the Morse inequalities hold in the equivariant sense, i.e. Eq. (B.2) can be rewritten as

$$\mathscr{M}_f^G(t) - P_t^G(M) = (1 + t) Q_f^G(t) \tag{B.3}$$

with all coefficients of the polynomial $Q_f^G(t)$ being non-negative. In spite of the fact that this extension seems to be rather simple, the non-triviality lies in the fact that equivariant homology should be calculated. We will not go here into equivariant theory (see Section B.1 for further examples) but just note that naturally the definition of the perfect function may be given in the equivariant sense. Namely, the function is perfect in the equivariant sense if $Q_f^G(t)$ is zero. As it was remarked by Bott (1982), the function may be perfect in the equivariant sense but not in the normal sense. That is why we prefer to use the notion of the simplest Morse–Bott function in the case of continuous symmetry as well and to use the complexity measure by counting the number of connected components of the set of stationary points of the function.

It should be noted that even in the presence of continuous symmetry group the symmetry group action may result in a set of critical orbits which are the isolated points and the simplest Morse–Bott function may possess in such a case only isolated stationary points.

B.1. Compilation of Bott and Kirwan about the construction of equivariant homology

We follow in this section the equivariant method developed mainly by Bott (1982), Atyah and Bott (1982) and Kirwan (1984, 1988). The starting point for the construction of the equivariant theory is a simple remark that if the group action would be free all problems disappear. Now the idea is to extend the group action to larger space where its action is free and make necessary calculations on this larger space.

First observation. If U is any space on which G acts freely, then the diagonal action of G on $W \times U$ is free. So, to transform our problem into another one with the free group action we should find a space U in which G acts freely and whose homotopy is trivial (i.e. U is contractible).

It is known that such spaces exist, be essentially unique, and play an absolutely essential role in all modern topology. Bott gives examples. For $G = U(1) = S_1$, U is a unit sphere in a complex infinite-dimensional Hilbert space. For $G = U(2)$ the corresponding U space is the space of two-frames in a complex infinite-dimensional Hilbert space.

As soon as U is known for a given G, the homotopy quotient W_G of any action is defined by

$$W_G = (U \times W)/G \,, \tag{B.4}$$

assuming that G acts diagonally on the product.

The construction of W_G enables one to introduce the equivariant version, F^G, of any functor F by imposing

$$F^G(W) = F(W_G) \,. \tag{B.5}$$

This means that the equivariant functor on the initial space W is defined through the ordinary functor on the quotient space W_G.

The space U/G plays the role of the homotopy quotient of the trivial action of G on a point. This space is usually denoted as BG and is referred to as the classifying space of G. It is a topological space which somehow reflects both the algebraic and the topological properties of G.

In the equivariant Morse series a non-degenerate critical point contributes the expression

$$P^G_{\text{point}}(t) = P_{BG}(t) \,. \tag{B.6}$$

Here $P_{BG}(t)$ is the ordinary Poincaré polynomial for BG, the classifying space of G.

If N is a non-degenerate critical manifold consisting of a single orbit $N = G/H$ then this critical submanifold contributes the expression

$$P^G_{G/H}(t) = P_{BH}(t) \,. \tag{B.7}$$

In particular, if the group G acts freely on the critical orbit N, this orbit counts in terms of its index and the ordinary Poincarè polynomial of N/G which in this case is a *point*.

The classifying spaces and their *ordinary homology* play an essential role in the equivariant theory. Concrete example. For $G = U(1)$, the classifying space $U/G = BG$ is a CP_∞ space. Its Poincarè polynomial has the form

$$P_{CP_\infty}(t) = 1 + t^2 + t^4 + t^6 + \cdots = \frac{1}{(1 - t^2)} \,. \tag{B.8}$$

Trivial example. Let us consider the action of the circle S_1 on the two sphere S_2 given by rotation about the z-axis in $\boldsymbol{R}^3$,

$$S_2\colon x^2 + y^2 + z^2 = 1 \ . \tag{B.9}$$

Let us write first Morse counting function and Morse inequalities using ordinary homology for three simple functions z, z^2, $-z^2$.

$$\mathscr{M}_{f=z}(t) = 1 + t^2 \ , \tag{B.10}$$

$$\mathscr{M}_{f=z^2}(t) = (1 + t) + 2t^2 \ , \tag{B.11}$$

$$\mathscr{M}_{f=-z^2}(t) = t(1 + t) + 2 \ , \tag{B.12}$$

As soon as the Poincarè polynomial for the S_2 is $(1 + t^2)$, it is clear that all three functions satisfy Morse inequalities

$$\mathscr{M}_{f=z}(t) - (1 + t^2) = 0 \ , \tag{B.13}$$

$$\mathscr{M}_{f=z^2}(t) - (1 + t^2) = (1 + t)t \ , \tag{B.14}$$

$$\mathscr{M}_{f=-z^2}(t) - (1 + t^2) = (1 + t) \ . \tag{B.15}$$

The function z is perfect in ordinary sense whereas the two others are obviously not perfect.

Equivariant calculations for z and z^2 are given by Bott (1982). The equivariant polynomial for the S_2 is

$$P_t^G(S_2) = \frac{1 + t^2}{1 - t^2}, \quad G = S_1 \ . \tag{B.16}$$

The Morse counting polynomial for the function z

$$\mathscr{M}^G_{f=z}(t) = \frac{1}{1 - t^2} + \frac{t^2}{1 - t^2}, \quad G = S_1 \ , \tag{B.17}$$

includes two contributions from two isolated stationary points. The Morse counting polynomial for the function z^2

$$\mathscr{M}^G_{f=z^2}(t) = 1 + \frac{2t^2}{1 - t^2}, \quad G = S_1 \ , \tag{B.18}$$

includes one contribution from the stationary one-dimensional manifold S_1 corresponding to a circular minimum at $z = 0$ and two contributions from two isolated stationary points which are both maxima. It is easy to see that both functions z, z^2 are perfect in the equivariant sense.

The equivariant Morse counting polynomial for the $(-z^2)$ function includes contributions from two isolated stationary points (two minima) which are

$$\frac{2}{1 - t^2} \, . \tag{B.19}$$

The contribution from the circular maximum at $z = 0$ should be t and

$$\mathscr{M}^G_{f=-z^2}(t) = t + \frac{2}{1 - t^2}, \quad G = S_1 \ , \tag{B.20}$$

but in such a case the difference between the Morse counting equivariant polynomial and the Poincaré equivariant polynomial is

$$\mathscr{M}^{G}_{f=-z^2}(t) - P^{G}(t) = t + \frac{2}{1-t^2} - \frac{1+t^2}{1-t^2} = t + 1\ . \tag{B.21}$$

This result shows that the $(-z^2)$ function satisfies equivariant Morse inequalities, but it is not perfect.

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