Introduction to Louis Michel's lattice geometry through group action

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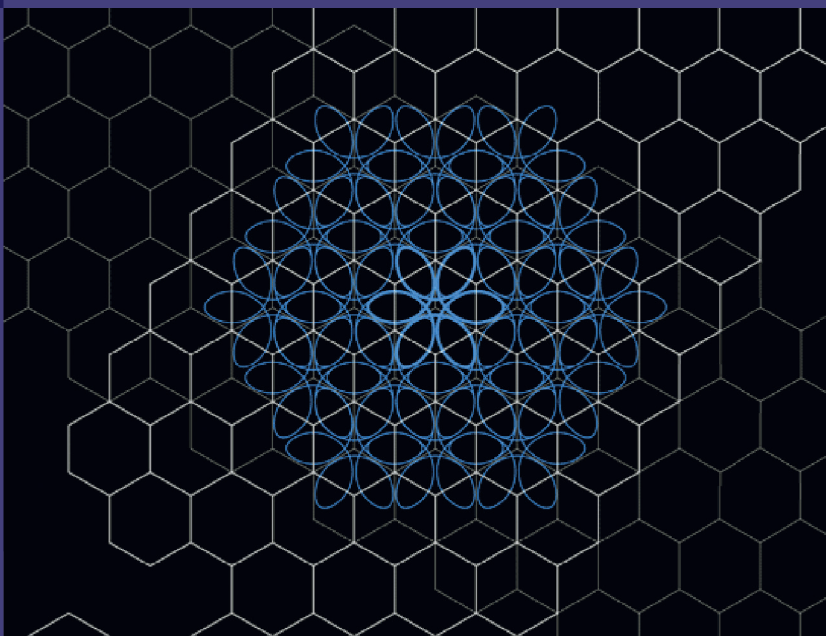

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Preface

This book has a rather long and complicated history. One of the authors, Louis Michel, passed away on the 30 December, 1999. Among a number of works in progress at that time there were a near complete series of big papers on “Symmetry, invariants, topology” published soon after in Physics Reports [75] and a project of a book “Lattice geometry”, started in collaboration with Marjorie Senechal and Peter Engel [53]. The partially completed version of the “Lattice geometry” by Louis Michel, Marjorie Senechal and Peter Engel is available as a IHES preprint version of 2004. In 2011, while starting to work on the preparation of selected works of Louis Michel [19] it became clear that scientific ideas of Louis Michel developed over the last thirty years and related to group action applications in different physical problems are not really accessible to the young generation of scientists in spite of the fact that they are published in specialized reviews. It seems that the comment made by Louis Michel in his 1980’s talk [70] remains valid till now:

“Fifty years ago were published the fundamental books of Weyl and of Wigner on application of group theory to quantum mechanics; since, some knowledge of the theory of linear group representations has become necessary to nearly all physicists. However the most basic concepts concerning group actions are not introduced in these famous books and, in general, in the physics literature.”

After rather long discussions and trials to revise initial “Lattice geometry” text which require serious modifications to be kept at the current level of the scientific achievements, it turns out that probably the most wise solution is to restrict it to the basic ideas of Louis Michel’s approach concentrated on the use of group actions. The present text is based essentially on the preliminary version of the “Lattice geometry” manuscript [53] and on relevant publications by Louis Michel [71, 76, 72, 73, 74], especially on reviews published in Physics Reports [75], but the accent is made on the detailed presentation of the two- and three-dimensional cases, whereas the generalization to arbitrary dimension is only outlined.

Chapter 1

Introduction

This chapter describes the outline of the book and explains the interrelations between different chapters and appendices.

The specificity of this book is an intensive use of group action ideas and terminology when discussing physical and mathematical models of lattices. Another important aspect is the discussion and comparison of various approaches to the characterization of lattices. Along with symmetry and topology ideas, the combinatorial description based on Voronoï and Delone cells is discussed along with classical characterization of lattices via quadratic forms.

We start by introducing in Chapter 2 the most important notions related to group action: orbit, stabilizer, stratum, orbifold, ... These notions are illustrated on several concrete examples of the group action on groups and on vector spaces. The necessary basic notions of group theory are collected in appendix A which should be considered as a reference guide for basic notions and notation rather than as an exposition of group theory.

Before starting description of lattices, chapter 3 deals with a more general concept, the Delone system of points. Under special conditions Delone sets lead to lattices of translations which are related to the fundamental physical notion of periodic crystals. The study of the Delone set of points is important not only to find necessary and sufficient conditions for the existence of periodic lattices. It allows discussion of a much broader mathematical frame and physical objects like aperiodic crystals, named also as quasicrystals.

Chapter 4 deals with symmetry aspects of periodic lattices. Point symmetry classification and Bravais classes of lattices are introduced using two-dimensional and three-dimensional lattices as examples. Stratification of the ambient space and construction of the orbifolds for the symmetry group action is illustrated again on many examples of two- and three-dimensional lattices. The mathematical concepts necessary for the description of point symmetry of higher dimensional lattices are introduced and the crystallographic restrictions imposed on the possible types of point symmetry groups by periodicity condition are explicitly introduced.

Chapter 5 introduces the combinatorial description of lattices in terms of their Voronoí and Delone cells. The duality aspects between Voronoí and Delone tesselations are discussed. Voronoí cells for two- and three-dimensional lattices are explicitly introduced along with their combinatorial classification as an alternative to the symmetry classification of lattices introduced in the previous chapter. Such notions as corona, facet, and shortest vectors are defined and their utility for description of arbitrary N-dimensional lattices is outlined.

Description of the lattices by using their symmetry or by their Voronoí cells does not depend on the choice of basis used for the concrete realization of the lattice in Euclidean space. At the same time practical calculations with lattices require the use of a specific lattice basis which can be chosen in a very ambiguous way. Chapter 6 discusses a very old subject: the description of lattices in terms of positive quadratic forms. The geometric representation of the cone of positive quadratic forms and choice of the fundamental domain of the cone associated with different lattices is discussed in detail for two-dimensional lattices. The reduction of quadratic forms is viewed through the perspective of the group action associated with lattice basis modification. The correspondence between the combinatorial structure of the Voronoí cell and the position of the point representing lattice on the cone of positive quadratic forms is carefully analyzed. The dimension of the cone of positive quadratic forms increases rapidly with the dimension of lattices. That is why the straightforward geometric visualization becomes difficult for three- and higher dimensional lattices. Nevertheless, for three-dimensional lattices the construction of the model showing the distribution of Bravais lattices and combinatorially different lattices by taking an appropriate section of the cone of positive quadratic forms is possible. This presentation is done on the basis of the very detailed analysis realized by Louis Michel during his lectures given at Smith College, Northampton, USA. Generalizations of the combinatorial description of lattices to arbitrary dimension requires introduction of a number of new concepts, which are shortly outlined in this chapter following mainly the fundamental works by Peter Engel and his collaborators. Symbolic visualization of lattices via graphs is introduced intuitively by examples of 3-, 4-, and partially 5-dimensional lattices without going into details of matroid theory.

Concrete examples of lattices in arbitrary dimensions related to reflection groups are studied in chapter 7. These examples allow us to see important correspondence between different mathematical domains, finite reflection groups, Lie groups and algebra, Dynkin diagrams, ...

Chapter 8 turns to discussion of the comparison between different classifications of lattices introduced in previous chapters and some other more advanced classifications suggested and used for specific physical and mathematical applications in the scientific literature. Among these different classifications we describe the correspondence between geometric and arithmetic classes of lattices and more general crystallographic classes necessary to classify the symmetry of the system of points which are more general than simple regular point lattices. Among the most important for physical applications aspects of lattice symmetry, the notion of enantiomorphism and of time reversal invariance are additionally discussed. The simultaneous use of symmetry and combinatorial classification for three-dimensional lattices is demonstrated by using the Delone approach.

Some physical and mathematical applications of lattices are discussed in chapter 9. These include analysis of sphere packing, covering, and tiling related mainly with specific lattices relevant for each type of problem. More physically related applications are the classification of the regular phases of matter and in particular the description of quasicrystals which are more general than regular crystals. Another generalization of regular lattices includes discussion of lattice defects. Description of different types of lattice defects is important not only from the point of view of classification of defects of periodic crystals. It allows also the study of defects of more formal lattice models, for example defects associated with lattices appearing in integrable dynamical models which are tightly related with singularities of classical dynamical integrable models and with qualitative features of quantum systems associated with lattices of common eigenvalues of several mutually commuting observables.

Appendices can be used as references for basic definitions of group theory (Appendix A), on graphs and partially ordered sets (Appendix B), and for comparison of notations (Appendix C) used by different authors. Also the complete list of orbifolds for 17 two-dimensional crystallographic groups (Appendix D) and for $3D$-irreducible Bravais groups (Appendix E) is given together with short explication of their construction and notation.

The bibliography includes a list of basic books for further reading on relevant subjects and a list of original papers cited in the text, which is obviously very partial and reflects the personal preferences of authors.

Chapter 2

Group action. Basic definitions and examples

This chapter is devoted to the definitions and short explanations of basic notions associated with *group actions*, which play a fundamental role in mathematics and in other fields of science as well. In physics group actions appear naturally in different domains especially when one discusses qualitative features of physical systems and their qualitative modifications.

We also introduce here much of the notation that will be used systematically in this book. Thus this section can be used as a dictionary.

Group action involves two "objects": a group G, and a mathematical structure M on which the group acts. M may be algebraic, geometric, topological, or combinatorial. Aut M, its automorphism group, is the group of one-to-one mappings of M to itself.

Definition: group action. An action of a group G on a mathematical structure M is a group morphism (homomorphism) $G \xrightarrow{\rho}$ Aut M.

The examples we give are designed for the applications we need in this book. Let us start with a very simple mathematical object M, an equilateral triangle in the (two-dimensional) Euclidean plane R^2. The isometries of R^2 that leave this triangle invariant form a group consisting of 6 elements (identity, rotations through $2\pi/3$ and through $4\pi/3$, and reflections across the lines passing through its three vertices and the midpoints of the opposite sides). In the classical notation used by physicists and chemists, this group is denoted D_3. (Alternative notations of groups are discussed in Appendix C).

We can also consider the action of D_3 on other objects, for example on the entire plane (see Figure 2.1). In this case the group morphism $D_3 \xrightarrow{\rho}$ Aut R^2 maps each group element to an automorphism (symmetry transformation) of $M = R^2$. This action is said to be *effective* because each $g \in G$ (other than the identity) effects the displacement of at least one point of the plane.

As another example of the action of D_3, we can take for M a single point, the center of the equilateral triangle. This point is left fixed by every element of D_3; thus this action is not effective.

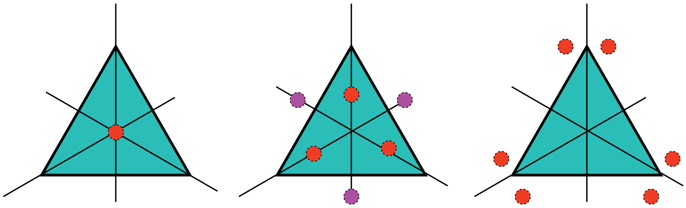


FIG. 2.1 – Orbits of the action of D_3 (the symmetry group of an equilateral triangle) on the 2D-plane. (a) The sole fixed point of the D_3 group action. The stabilizer of this one-point orbit is the whole group D_3. (b) Two examples of orbits consisting of three points. Each point of the orbit has one of the reflection subgroups r_i, $i = 1, 2, 3$, as a stabilizer. The three stabilizers r_i, $i = 1, 2, 3$ form the conjugacy class r of D_3 subgroups. (c) Example of an orbit consisting of six points. The stabilizer of each point of such an orbit and of the orbit itself is a trivial group $C_1 \equiv 1$.

We can also extend the action of D_3 from R^2 to R^3. The rotations through $2\pi/3$ and $4\pi/3$ about the axis passing through the center of the triangle and orthogonal to it generalize the plane rotations in a natural way.

There are two ways to generalize the reflections of D_3 to transformations of 3D-space.

First, we can replace reflection across a line ℓ by reflection in the plane orthogonal to the triangle and intersecting it in ℓ. This gives us a symmetry group whose symbol is C_{3v} (or $3m$ or $*33$). Alternatively, we can replace 2D-reflection across ℓ by rotation in space, through π, around the axis coinciding with that line. This group is denoted D_3 (or 32 [ITC]=[14], or 223 [Conway]=[31]). The groups D_3 and C_{3v} are isomorphic; thus one abstract group has two very different actions on R^3, while their actions on a 2D-dimensional subspace are identical.

We began this discussion with the example of an equilateral triangle in the plane. What is the symmetry group if the triangle is situated in three-dimensional space? Obviously, this group includes the six symmetry transformations forming the two-dimensional group D_3. But now the complete set of transformations leaving the triangle invariant also includes reflection in the plane of the triangle and the composition of this reflection with all the elements of D_3. Thus in R^3 the symmetry group of an equilateral triangle has 12 elements. We denote this larger group by D_{3h}, or $\overline{6}2m$ [ITC], or $*223$ [Conway].

Notice that the action of D_{3h} on the plane of the triangle in R^3 is non-effective, since reflection in that plane leaves all its points fixed. This action, described by the homomorphism $D_{3h} \xrightarrow{\rho} \mathrm{Aut}\ R^2$, has a non-trivial kernel, $\mathrm{Ker}\rho = Z_2$, the group of two elements (the identity and reflection in the plane).

Returning now to the definition of group action, we introduce the following notation. Since the action of a group G on a mathematical structure M is specified by the homomorphism $\rho(g)$ for all $g \in G$, we will write $\rho(g)(m)$ for the transform of any $m \in M$ by $g \in G$, and abbreviate it to $g.m$.[1]

Now we come to a key idea in group action.

Definition: group orbit. The orbit of m (under G) is the set of transforms of m by G; we denote this by $G.m$.

For example (see Figure 2.1), each of the following sets is an orbit of D_3 acting on the two-dimensional plane containing an equilateral triangle:

- three points equally distanced from the center, one on each of the three reflection lines;
- the centroid or, equivalently, the center of mass of the triangle; and
- any set of six distinct points related by the reflections and rotations of the symmetry group D_3.

Figure 2.2 shows orbits of C_{3v}, D_3, and D_{3h} acting on an equilateral triangle in R^3.

Under the action of a finite group, the number of elements in an orbit cannot be larger than the order of the group, and this number always divides the group order. Belonging to an orbit is an equivalence relation on the elements of M and thus M is a disjoint union of its orbits.

For continuous groups an orbit can be a manifold whose dimension cannot exceed the number of continuous parameters of the group. The simplest examples of continuous symmetry groups are the group of rotations of a circle, $SO(2) = C_\infty$, and the circle's complete symmetry group, $O(2) = D_\infty$, which includes reflections. Both C_∞ and D_∞ act effectively on the plane in which the circle lies. In fact their orbits coincide (see Figure 2.3): there is one one-point orbit, the fixed point of the group action, and a continuous family of one-dimensional orbits, each of them a circle.

A second key notion is the stabilizer of an element of M.

Definition: stabilizer. The stabilizer of an element $m \in M$ is the subgroup

$$G_m = \{g \in G,\ g.m = m\}$$

of elements of G which leave m fixed.

If $G_m = G$, then this orbit has a single element and m is said to be a fixed point of M (see Figure 2.1a and Figure 2.3a).

If G is finite, then the number of points in the orbit $G.m$ is $|G|/|G_m|$. Thus if, as in Figure 2.1 b, the stabilizer of a D_3 orbit is a subgroup of order 2, the orbit consists of three points. If $G_m = 1 \equiv e$, the group identity

[1] When G is Abelian and its group law is noted additively, we may use $g + m$ instead of $g.m$ as short for $\rho(g)(m)$, though this use of $+$ is an "abus de langage," since g and m may not be objects of the same type.

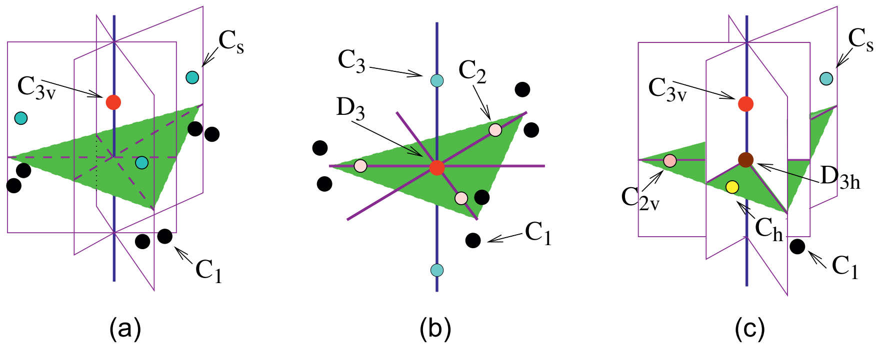


FIG. 2.2 – Generalizing the action of D_3 from R^2 to R^3. (a) Action of the group C_{3v}: three orbits with stabilizers C_{3v} , C_s, and C_1 are shown (s stands for reflection in the indicated plane); (b) Action of the group D_3: four orbits with stabilizers D_3, C_3, C_2, and C_1 are shown. (c) Action of the group D_{3h}: one point from each of six different orbits (D_{3h}, C_{3v}, C_{2v}, C_s, C_h, and C_1) is shown.

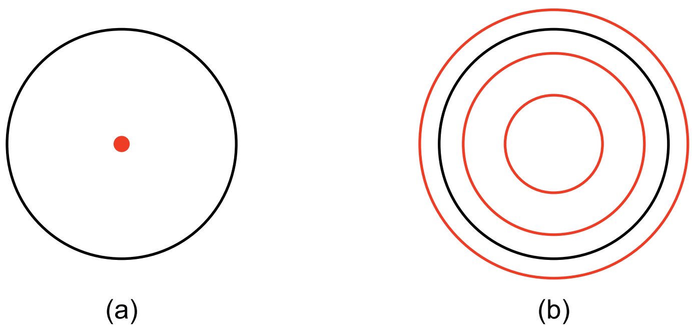
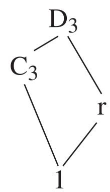


FIG. 2.3 – Orbits of the action of C_∞ and D_∞ on the 2D-plane. (a) The fixed point of these group actions on R^2. (b) Continuous circular orbits.

(Figure 2.1 c), then the size of the orbit is $|G|$ and the orbit is said to be *principal*.[2]

It is easy to prove that $G_{g.m} = gG_mg^{-1}$, from which it follows that the set of stabilizers of the elements of an orbit is a conjugacy class $[H]_G$ of subgroups of G. For example, the stabilizers of the three vertices of an equilateral triangle are the three reflection subgroups, r_i, of D_3, which are conjugate by rotation. This fact allows us to classify (or to label) orbits by their stabilizers, i.e. by the conjugacy classes of subgroups of group G. We recall that the conjugacy

[2] Orbits with trivial stabilizer 1 are always principal but for continuous group actions principal orbits can have nontrivial stabilizers. In that case principal orbits are defined as orbits forming open dense strata, see below.



$\lvert [H]_G \rvert$	$\lvert H \rvert$
1	6
1	3
3	2
1	1

FIG. 2.4 – The lattice of conjugacy classes of subgroups of D_3 group. The table on the right shows, in column 1, the number of elements $|[H]_G|$ in the conjugacy class $[H]_G$ of each type of subgroup. The numbers in the right-hand column are the orders of the subgroup $|H|$.

classes of subgroups of any given group form a partially ordered set: one class is "smaller" than another if it contains a proper subgroup of a group in the other conjugacy class. This partial ordering for D_3 is shown in Figure 2.4.

Orbits with the same conjugacy class of stabilizers are said to be of the same type.

Next, we define the very important notion of stratum.

Definition: stratum. In a group action, a stratum is the union of all points belonging to all orbits of the same type.

By definition, two points belong to the same stratum if, and only if, their stabilizers are conjugate. Consequently we can classify and label the strata of a group action by the conjugacy classes of subgroups of the group.

The three strata of the action of D_3 on R^2 are shown in Figure 2.5. They include the centroid of the triangle (D_3's zero-dimensional stratum), three mirror lines without their intersection point (the one-dimensional stratum), and the complement of these two strata (the two dimensional stratum).

A disc D, minus its center, is one stratum of the action of D_∞ on D; the center is the other.

When they exist, as in the case of the D_3 action on R^2 (Figure 2.1) or the C_∞ action (Figure 2.3) the fixed points form one stratum and the principal orbits form another. Belonging to the same stratum is an equivalence relation for the elements of M or for orbits of a G-action on M. Thus M can be considered as a disjoint union of strata of different dimensions.

We will denote the set of orbits of the action of G on M by $M|G$ and the corresponding set of strata as $M||G$. To belong to the same stratum is an equivalence relation for the elements of M and for elements of the set of orbits, $M|G$. The set of strata $M||G$ is a (rather small in many applications) subset of the set of conjugacy classes of subgroups of G. Thus $M||G$ too has the structure of a partially ordered set $S_i \in M||G$, where by $S_1 < S_2$ we mean that the local symmetry of S_1 is smaller than that of S_2 – i.e. the stabilizers of the points of S_1 are, up to conjugation, subgroups of those of S_2.

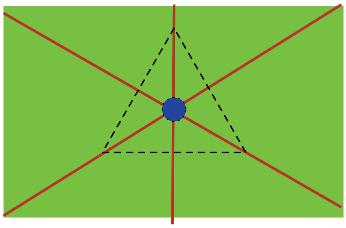


FIG. 2.5 – The strata of D_3 action on R^2. Black point in the center represents the zero-dimensional D_3-stratum. The rays without their common intersection point form the one-dimensional r-stratum. The six two-dimensional regions of the plane form the two-dimensional principal stratum with trivial stabilizer.

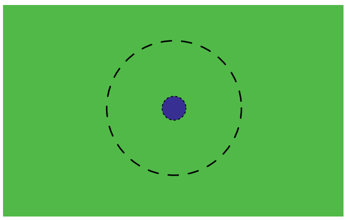


FIG. 2.6 – Strata of the action of C_∞ (or D_∞) on R^2. The black point forms the zero-dimensional stratum. The whole plane without the point is the two-dimensional principal stratum.

Beware: a less symmetric stratum might have a larger dimension than a more symmetric one. The set of strata is partially ordered by local symmetry, not by size.

The example of the action of D_3 on R^2, discussed above, leads to three strata: the zero dimensional stratum D_3, the one-dimensional stratum r, and the two-dimensional principal stratum 1, which is open and dense. Only three conjugacy classes of subgroups of D_3 (see Figure 2.5) appear as local symmetry of strata. The natural partial order between strata is $1 < r < D_3$.

The action of C_∞ (the group of pure rotational symmetries of a circle or of a disk) on R^2 leads to two strata (see Figure 2.6). The zero-dimensional stratum consists of one point, the center. The two-dimensional principal stratum is the whole plane minus that point. Note that the action of D_∞ on R^2 has the same two strata, but their stabilizers now are different.

Finally, we define the notions of orbit space and orbifold.

Definition: orbit space. The set of orbits appearing in an action of G on M is the orbit space $M|G$.

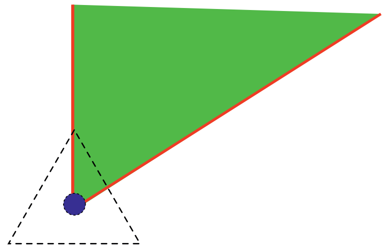


FIG. 2.7 – Orbifold of D_3 action on R^2. The black point represents the D_3-orbit consisting of one point. Two rays form 1D-set of r-orbits consisting each of three points. The shaded region is a two-dimensional set of principal $C_1 \equiv 1$ orbits, consisting each of six points.

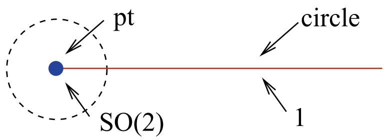


FIG. 2.8 – Orbifold of the action of C_∞ on R^2. Black filled point - the orbit with stabilizer $SO(2)$ consisting of one point. Solid line - the set of 1D-orbits, each orbit being a circle.

If M contains only one orbit, i.e. if any $m \in M$ can be transformed into any other element of M by the group action, the action is said to be *transitive* and M is called a *homogeneous space* (with respect to G and ρ). Examples of homogeneous spaces and their associated groups include

- a circle (not a disk!), $G = D_\infty$;
- R^n, and G the group of translations in R^n.
- a sphere S_n in $(n+1)$-dimensional space and $G = SO(n+1)$.

Definition: orbifold. The orbifold of a group action is a set consisting of one representative point from each of its orbits.

Thus, the space of orbits for the action of D_3 on R^2 can be represented as a sector of the plane (see Figure 2.7). The space of orbits for the action of C_∞ on R^2 can be represented as a one-dimensional ray with a special point at the origin (see Figure 2.8).

Let us consider the space of orbits of a (three-dimensional) D_3 action on a two-dimensional sphere surrounding an equilateral triangle (see Figure 2.9). Assume that its action on R^2 (see Figure 2.2 b) coincides with the action of the 2D-point group D_3.