Solid-State Sciences

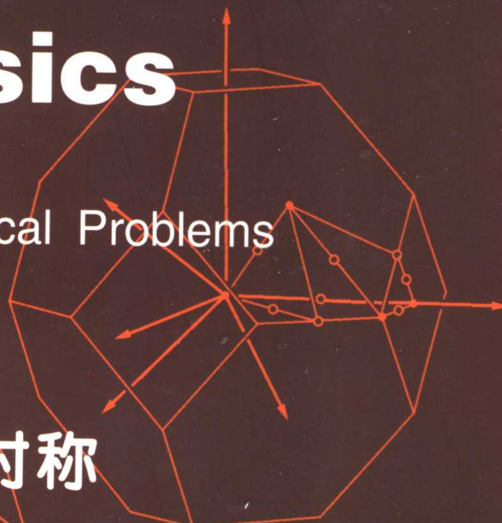
W. Ludwig C. Falter

STUDY EDITION

Symmetries in Physics

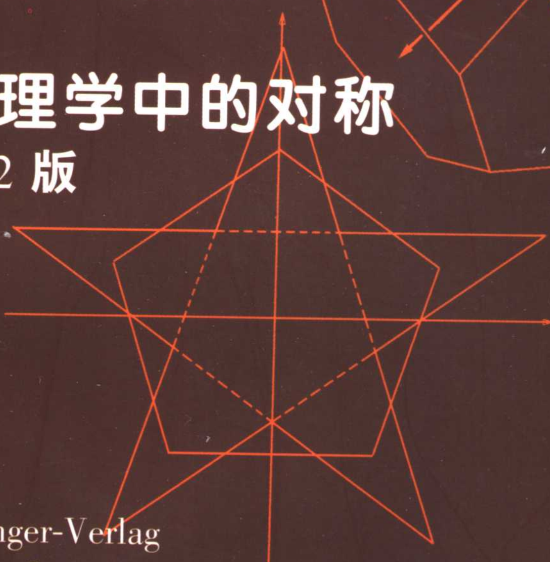
Group Theory Applied to Physical Problems

Second Edition



物理学中的对称

第 2 版



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Group Theory Applied to Physical Problems

Second Extended Edition
With 91 Figures

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Preface

One of the most efficient methods in physics is based on the discussion of the symmetry of a physical system. Group theory and, in particular, representation theory are the mathematical tools for handling the symmetries of such a system. Of course, these fundamental ideas have not changed since the first edition of this book. Only the applications have been extended to new systems and are permanently expanding. Quasicrystals are very new systems in solid-state physics and are discussed in Appendix I. On the other hand, in particle physics, supersymmetry theories have been developed, which combine bosons and fermions. This means that in a study of corresponding models, there is a need for anticommutators (Grassmann algebra) as well as for commutators (Lie algebra). Since these theories are still being developed and since a discussion of the details would go far beyond the scope of this book, we only give some indications in Appendix J.

Other changes are only related to the correction of minor errors or misprints. Often-used symbols and abbreviations are listed in Appendix K.

As already mentioned in the Preface to the First Edition, a short version of the solutions to the exercises may be obtained from the authors.

We thank Prof. Dr. M. Stingl for some advice, Mrs. Schockmann for preparing the manuscript, and especially Dr. H. Lotsch of Springer-Verlag for his good cooperation.

Münster, October 1995 *W. Ludwig · C. Falter*

Preface to the First Edition

The majority of physical systems exhibit symmetries of one kind or another. These symmetries can be used to simplify physical problems (indeed, sometimes a result cannot be achieved in any other way) and also to understand and classify the solutions. The mathematical tools required for this, i.e. group theory, and in particular representation theory, together with their applications to physical problems, were treated by us in a series of seminars and lectures, which now form the basis of this book.

Our main objective is to prepare the necessary mathematical foundations so that they can be used in physics. Most statements are illustrated by examples, which are in many cases simple but occasionally more complicated (especially in connection with space groups). The method of symmetry projections is applied more widely than in most texts of a similar standard, but because this method is a suitable and powerful tool for the systematic reduction of representation spaces to irreducible spaces, and thus for the determination of the eigenstates of the system, it deserves to be better known. This theory finds applications in many areas of physics in which symmetry plays a role. We consider finite, discrete symmetries as well as continuous symmetries and also symmetry breaking, with examples taken from atomic, molecular, solid-state and high-energy physics.

This text is intended mainly for students who have attended basic courses in physics and for researchers working in physics. However, the occurrence of symmetry properties is by no means restricted to physics, so this book should also be useful for people primarily interested in other subjects such as chemistry and physical chemistry. Many problems are included in the text as exercises; a booklet of solutions may be obtained from the authors.

We are very grateful to Dr. W. Zierau, who gave us much good advice, and to K. Stroetmann, H. Rakel and J. Backhaus for help in preparing the manuscript, the subject index and in proofreading. We are especially indebted to Dr. H. K. V. Lotsch of Springer-Verlag for encouragement and cooperation and to Miss D. Hollis, who improved the style of our sometimes rather "German" English.

Münster, October 1987 *W. Ludwig · C. Falter*

Contents

...διὸ δὴ καὶ χώραν ταῦτα ἄλλα ἄλλην
ἴσχειν, πρὶν καὶ τὸ πᾶν ἐξ αὐτῶν
διακοσμηθὲν γενέσθαι. Καὶ τὸ μὲν δὴ
πρὸ τούτου πάντα ταῦτ'εἶχεν
ἀλόγως καὶ ἀμέτρως....
οὕτω δὴ τότε πεφυκότα ταῦτα πρῶτον
διεσχηματίσατο εἴδεσί τε καὶ ἀριθμοῖς.

Platon, *Timaios*, 53a, b

1. Introduction

Physical systems in general possess symmetry properties. An essential point in the discussion of such systems is to find the relevant symmetries and to classify the properties or the states of the systems with respect to these symmetries. Group theory provides the mathematical tools for the description of symmetries. Within representation theory, methods are developed that allow classification of the physical states of a system with respect to the irreducible representations of the symmetry group.

The symmetries may be of very different natures for different types of objects such as particles (elementary particles, atoms, molecules), many-particle systems (crystals, liquids, fluids), all kinds of fields and macroscopic bodies.

We may distinguish between universal and special symmetries. Examples of *universal symmetries* are the space-time symmetries of systems, that is, the invariance of equations with respect to Poincaré or Lorentz transformations. In many-particle systems, the symmetry with respect to an interchange (permutation) of identical particles is universal. The charge and gauge symmetries of fields also belong to this group of symmetries. In quantum field theory the symmetries may be discrete as well as continuous. Well-known examples of discrete symmetries are the invariances under CPT transformations. The continuous symmetries may be divided into those that do not depend on space-time coordinates (first kind) and those that do (second kind). Invariance of a field theory under gauge transformations of the first kind leads to conservation laws. The number of these laws is equal to the number of parameters involved in the transformation. In the second kind of transformations (local gauge transformations) the parameters depend on the coordinates. Invariance of the theory under such transformations gives rise, in addition to the conservation laws, to interacting fields in the Lagrangian density of the particle fields. Examples are the electromagnetic field, the Yang-Mills fields, and also the gravitational field. Symmetries of this type are also called *dynamical* symmetries. In these cases the interaction is determined by symmetry. On the other hand, the symmetry of an interaction is not always obvious and can only be seen from the phenomena caused by it.

Special symmetries are often of a geometrical nature. Then there are a number of symmetry operations that transform the physical system into itself (spatially). Crystalline symmetries, for example, belong to this category. The number of such operations is finite (or at least enumerable) in general.

The invariance properties of physical systems in space and time, as well as gauge invariances, define the physically conserved quantities, that means observables like momentum, energy, angular momentum, and charges. These quantities then obey conservation laws. This is one of the reasons why symmetry is so important in physics.

In this book, using group theoretical methods we discuss the connection between symmetry and the physical state and show how to simplify a physical problem by using a "given" symmetry. The most important tool in this respect is the representation theory of groups; with its help we can define projectors allowing determination of the symmetry-adapted states. Another essential theorem is that of Wigner and Eckart. It allows statements on matrix elements and transitions, especially in connection with the representation of tensor operators.

In Chaps. 2–10 we consider groups with a countable (discrete, mainly finite) number of elements. This comprises the geometric symmetry groups whose operations leave the distances between two points and the angles between two directions invariant. Apart from this, permutation groups belong to this category, and also further symmetries that sometimes occur in physics.

In the second part (Chaps. 11–14), we discuss continuous symmetry groups and the Lie algebras corresponding to them. Most universal symmetries are included in these groups. Because of the limited size of this book, the essential statements have been explained with the $\mathcal{SU}(n)$ groups, however, a transfer of methods and procedures to other groups in general is possible without difficulty. In the appendix we discuss the Lorentz group, which has infinite-dimensional unitary representations, as an example of a noncompact group.

As an application of the $\mathcal{SU}(n)$ groups we consider some aspects of modern gauge theories. Whereas previously one used to start with phenomenological equations, to investigate the interactions and then found the symmetries of the system, we will follow the recent development where one starts with a possible symmetry group for the gauge transformations and the gauge invariance then determines the form of the field equations and the interactions. Thus, in the development of physics it was of no special importance that the system "charged particle–electromagnetic field" is gauge invariant (under an Abelian gauge transformation). But having realized this fact, one can look to see what other gauge-invariant theories are possible if the conserved quantities ("charges") have been previously specified. This leads to new, non-Abelian gauge groups and new interacting fields that couple to the "charges" of the particles. The procedure therefore is the following. One has to look for the "charges" as the conserved quantities, from these one can derive the corresponding gauge invariance of the first kind.

The corresponding gauge invariance then specifies field Lagrangians and interacting fields. The principles of these theories are discussed with some examples in Chap. 14, without claiming to be complete.

For an understanding of the theory of continuous groups, especially Chaps. 12 and 13, the results of Sect. 5.5 are necessary. However, this comparatively difficult section is dispensable for many problems in connection with point and space groups; for these the considerations in Sect. 6.1 are sufficient.

To keep the size manageable we had to restrict ourselves in other respects. Mathematical proofs are given explicitly only as far as they are necessary for an immediate understanding. In many cases they are "simple" enough to be done in the form of an exercise. Thus the reader is strongly advised to solve the exercises; sometimes they are indeed necessary for a handling of the mathematics. In our opinion it was essential to develop the mathematical theory in such a way as to allow direct application to physical problems. Thus statements and theorems are always illustrated with definite examples; then the methods can be immediately transferred to other problems.

One main aim is to show that group theory makes it possible to treat problems from all parts of physics (and molecular chemistry), from classical mechanics to quantum field theory, due to the symmetry inherent in physical systems. Indeed, for many physical theories developed during recent decades, group theory is the central key. In order to demonstrate this we have chosen examples from solid-state as well as molecular physics, including electronic as well as vibrational spectra, and also examples from atomic, nuclear and elementary particle physics. The physical background and the basic relations of the different topics are assumed to be known.

In the applications we often have to use the irreducible representations of the group elements. It was not possible here to give all the irreducible representations of space groups explicitly. For this we have to refer to the existing books of tables, but at the same time we have to state that many things have been tabulated only incompletely. Then the reader has to calculate the irreducible representations, the reduction coefficients, the Clebsch-Gordan coefficients, etc., by himself. The methods are given.

The notation has been standardized in many respects. Where this is the case, we have adapted the generally accepted notation. But there are some fields (e.g. space groups) where several different notations are used. In such cases we had to choose. But the correspondence between different notations can always be established by comparing the definitions. The tables in the Appendix (especially in Appendix A) always allow a comparison.

2. Elements of the Theory of Finite Groups

Most groups which are essential in solid-state physics are finite groups, or at least can be looked upon as being finite; this is the case for the translation group of lattices. Therefore we first have to explain the concepts of the abstract theory of finite groups. This is done in this first section, where we give the basic notations and their relations. All this is illustrated by a simple example.

2.1 Symmetry and Group Concepts: A Basic Example

As an introductory example, we consider an equilateral triangle to which we additionally assign a set of points 1 to 6 (Fig. 2.1). The basic concepts will be illustrated by means of this example, which represents the symmetry of an NH_3 molecule.

The triangle and the set of points are transformed into themselves if the system is rotated about the centre of the triangle by multiples of the angle $2\pi/3$. The axis of rotation, perpendicular to the plane of the triangle, is called a threefold axis, since after three rotations (always through the basic angle $2\pi/3$) the initial situation is restored. These symmetry operations about a threefold axis are denoted by c_3, c_3^2, $c_3^3 = e, \ldots$, where the *rotation* has always to be taken counterclockwise (*positive sense*) and e is the *identity operation* (unit operation), which does not move the triangle. Apart from these rotations, there are reflections σ_v, σ_v', σ_v'' transforming the triangle into itself. These mirror planes contain the threefold axis. We can illustrate the operations best with the mappings produced by them.

e: points and triangle are invariant (do not move)

$$
\begin{aligned}
&c_3: 1 \to 3 \to 5 \to 1 \;; \quad 2 \to 4 \to 6 \to 2 \;; \quad A \to B \to C \to A \;. \\
&c_3^2: 1 \to 5 \to 3 \to 1 \;; \quad 2 \to 6 \to 4 \to 2 \;; \quad A \to C \to B \to A \;. \\
&\sigma_v: 1 \leftrightarrow 2 \;; \quad 3 \leftrightarrow 6 \;: \quad 4 \leftrightarrow 5 \;; \qquad B \leftrightarrow C \;. \\
&\sigma_v': 1 \leftrightarrow 6 \;; \quad 2 \leftrightarrow 5 \;; \quad 3 \leftrightarrow 4 \;; \qquad A \leftrightarrow C \;. \\
&\sigma_v'': 1 \leftrightarrow 4 \;; \quad 2 \leftrightarrow 3 \;; \quad 5 \leftrightarrow 6 \;; \qquad A \leftrightarrow B \;.
\end{aligned}
\tag{2.1.1}
$$

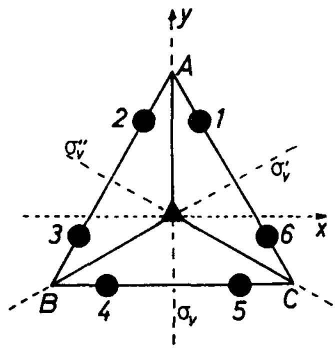

Fig. 2.1. *Arrangement of points, or triangle, having* $\mathscr{C}_{3v}$ *symmetry.* ▲: threefold axis; σ_v, σ_v', σ_v'': mirror planes containing the rotation axis

Table 2.1. The composition (group) table of the symmetry operations of the triangle in Fig. 2.1

a \ b	e	c_3	c_3^2	σ_v	σ_v'	σ_v''
e	e	c_3	c_3^2	σ_v	σ_v'	σ_v''
c_3	c_3	c_3^2	e	σ_v''	σ_v	σ_v'
c_3^2	c_3^2	e	c_3	σ_v'	σ_v''	σ_v
σ_v	σ_v	σ_v'	σ_v''	e	c_3	c_3^2
σ_v'	σ_v'	σ_v''	σ_v	c_3^2	e	c_3
σ_v''	σ_v''	σ_v	σ_v'	c_3	c_3^2	e

With this scheme the effect of successive symmetry operations is also easily depicted; we define the operation in the rightmost position to be performed always *first*, the operation second from the right, second, and so on. The execution of two successive operations is called the *product* (operation), e.g. $\sigma_v c_3$. Generating the corresponding image of $\sigma_v c_3$, we realize that this is identical with that of σ_v', i.e. $\sigma_v c_3 = \sigma_v'$. Accordingly, we find every product of the elements in (2.1.1) to be contained in the set $\{e, c_3, c_3^2, \sigma_v, \sigma_v', \sigma_v''\}$. We further realize that the *products* are *not* always *commutative*; for example, $c_3\sigma_v = \sigma_v''$. For every operation there obviously exists a *reciprocal* or *inverse* operation denoted by c_3^{-1}, σ_v^{-1} and so on. Clearly,

$$e^{-1} = e \ , \qquad c_3^{-1} = c_3^2 \ , \qquad (c_3^2)^{-1} = c_3^{-2} = c_3 \ , \qquad \sigma_v^{-1} = \sigma_v \ , \quad \text{etc.} \tag{2.1.2}$$

The general behavior in constructing products is represented by the so-called *composition (multiplication, group) table* of $(a \cdot b)$ (Table 2.1). We find that in each row and each column of the table every element of the set occurs exactly once. In addition, the inverse elements are readily specified: b and a are inverse to each other if $a \cdot b = e$.

Obviously this example is the geometric realization of a mathematical structure, which is called a group:

Formally, a pair $(\mathcal{G}, \cdot)$ with a set $\mathcal{G}$ of elements and a composition $\cdot$ defines a group if

1) there exists an internal *composition* law $\cdot$ on $\mathcal{G}$;
2) for every pair of elements (a, b) there exists *exactly one element* $c \in \mathcal{G}$ with $c = a \cdot b$;
3) the composition law is *associative*: $(a \cdot b) \cdot c = a \cdot (b \cdot c)$;
4) there exists an *identity (unit) element* with $a \cdot e = a$ for every $a \in \mathcal{G}$;
5) for every element $a \in \mathcal{G}$ there exists an *inverse (reciprocal) element* in $\mathcal{G}$ with $a \cdot a^{-1} = e$. (2.1.3)

A group is completely defined by its composition table. In our case, composition means the execution of successive operations also denoted as multiplication and written $a \cdot b$ or simply ab. If *all* the multiplications in a group commute, it is an *Abelian group* or *commutative group*. The group table is then symmetric with respect to the principal diagonal. Conditions (2.1.3) require only the existence of a right-identity and right-inverse element. However it follows immediately that these are also left-identity or left-inverse elements as

$$a^{-1} \cdot a = (a^{-1} \cdot a) \cdot (a^{-1} \cdot (a^{-1})^{-1}) = a^{-1} \cdot (a \cdot a^{-1}) \cdot (a^{-1})^{-1}$$
$$= a^{-1} \cdot (a^{-1})^{-1} = e \tag{2.1.4}$$

and

$$e \cdot a = (a \cdot a^{-1}) \cdot a = a \cdot (a^{-1} \cdot a) = a \cdot e = a \ . \tag{2.1.5}$$

Similarly it follows that identity and inverse elements are unique. For, if e and f are both identities, then

$$e = e \cdot f = f$$

because of (2.1.5) and if a^{-1} and $\bar{a}$ are both inverse elements, then

$$\bar{a} = \bar{a} \cdot (a \cdot a^{-1}) = (\bar{a} \cdot a) \cdot a^{-1} = e \cdot a^{-1} = a^{-1} \ .$$

The inverse of a product is given by

$$(a \cdot b)^{-1} \cdot (a \cdot b) = e \rightarrow (a \cdot b)^{-1} \cdot a = b^{-1} \rightarrow (a \cdot b)^{-1} = b^{-1} \cdot a^{-1} \ . \tag{2.1.6}$$

Any nonempty subset of $\mathcal{G}$ satisfying (2.1.3) with the same composition law is called a *subgroup* $\mathcal{U} \subseteq \mathcal{G}$. (2.1.7)

Every group $\mathcal{G}$ possesses $\mathcal{U} = \mathcal{G}$ and $\mathcal{U} = \{e\}$ as trivial subgroups. If more exist, we speak of nontrivial or proper subgroups.

The group described by (2.1.1, 2) and Table 2.1 is denoted by

$$\mathscr{C}_{3v} = \{e, c_3, c_3^2, \sigma_v, \sigma_v', \sigma_v''\} \ . \tag{2.1.8}$$

Subgroups of $\mathscr{C}_{3v}$ are, for example,

$$\mathscr{C}_3 = \{e, c_3, c_3^2\} \qquad \text{and} \qquad \mathscr{C}_s = \{e, \sigma_v\} \ . \tag{2.1.9}$$

The group $\mathscr{C}_{3v}$ is non-Abelian, but $\mathscr{C}_3$ and $\mathscr{C}_s$ are Abelian. The subgroups can be seen directly from the multiplication table; they form a closed set with respect to the composition law.

The triangle, or the set of points, in Fig. 2.1 can also be mapped onto itself by other operations. For example the reflections σ_v can be replaced by twofold rotations c_2, c_2', c_2'', which are rotations by $2\pi/2 = \pi$ about axes lying in the plane of the triangle. The group table does not change formally. Such groups, in which elements and multiplications can be mapped uniquely one to one, i.e. the group table remains unchanged, are called *isomorphic groups*. There are further groups isomorphic ($\cong$) to $\mathscr{C}_{3v}$ which will be described later. Isomorphic groups can express different physical systems (Sect. 3.1). The group containing one threefold main axis and three twofold axes perpendicular to the threefold axis (angle $\pi/3$ between the twofold axes) is called the dihedral group

$$\mathscr{D}_3 = \{e, c_3, c_3^2, c_2, c_2', c_2''\} \ . \tag{2.1.10}$$

It is isomorphic to $\mathscr{C}_{3v}$:

$$\mathscr{D}_3 \cong \mathscr{C}_{3v} \ . \tag{2.1.11a}$$

Starting with an arbitrary given point (e.g. point 1 in Fig. 2.1), we can produce the set of points in Fig. 2.1 by applying special symmetry operations one or more times. In the examples these operations are $p = c_3$ and $q = \sigma_v$ or c_2. Such elements are called *generating elements* or simply *generators of the group*. Elements of a group $\mathscr{G}$ are called generators if any element of $\mathscr{G}$ can be represented by finite products of these generators. The choice of generators is not a unique one. We could also choose alternatively $q = \sigma_v'$ or c_2' or σ_v'' or c_2''. Sometimes it is useful to take more generators than necessary. Any group with a finite number of elements possesses a minimal system of generators, which is called the *basis of the group*. The number of elements in the basis is the rank of *the (finite) group*.

As an example we consider a group defined by two generators p and q with the *generating relations*

$$p^3 = e \ ; \qquad q^2 = e \ ; \qquad (q \cdot p)^2 = e \ . \tag{2.1.12}$$

The group then contains the elements

$$\mathscr{G}_6 = \{e, p, p^2, q, qp, qp^2\} \ . \tag{2.1.13}$$