1
Introduction

> When the original German version was first published in 1931, there was a great reluctance among physicists toward accepting group theoretical arguments and the group theoretical point of view. It pleases the author, that this reluctance has virtually vanished in the meantime and that, in fact, the younger generation does not understand the causes and the bases of this reluctance.
>
> *E.P. Wigner (Group Theory, 1959)*

Symmetry is a far-reaching concept present in mathematics, natural sciences and beyond. Throughout the chapter the concept of symmetry and symmetry groups is motivated by specific examples. Starting with symmetries present in nature, architecture, fine arts and music a transition will be made to solid state physics and photonics and the symmetries which are of relevance throughout this book. Finally the square is taken as a first explicit example to explore all transformations leaving this object invariant.

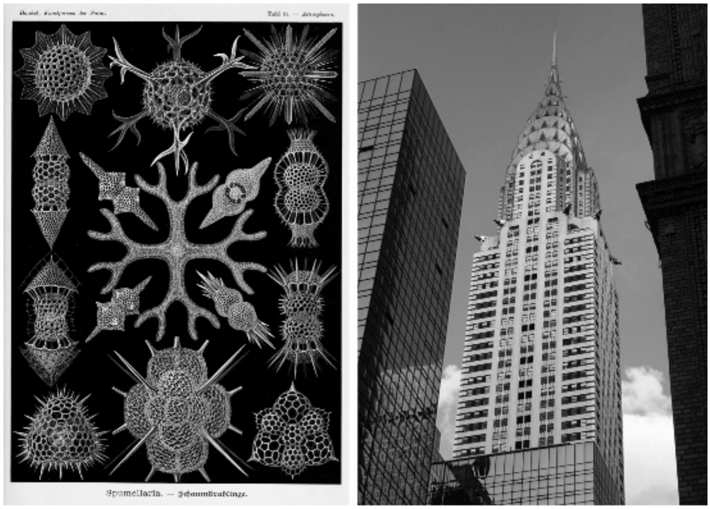
Symmetry and symmetry breaking are important concepts in nature and almost every field of our daily life. In a first and general approach symmetry might be defined as: *Symmetry is present when one cannot determine any change in a system after performing a structural or any other kind of transformation.*

Nature, Architecture, Fine Arts, and Music

One of the most fascinating examples for symmetry in nature is the manifold and beauty of the mineral skeletons of Radiolaria, which are tiny unicellular species. Figure 1.1a shows a table from Haeckel's "Art forms in Nature" [4] presenting a special group of Radiolaria called Spumellaria.

The concept of symmetry can also be found in architecture. Our urban environment is characterized by a mixture of buildings of various centuries. However, every epoch reflects at least some symmetry principles. For example, the Art déco style buildings, like the Chrysler Building in New York City (cf. Figure 1.1b), use symmetry as a design element in a particularly striking manner.

Group Theory in Solid State Physics and Photonics, First Edition. Wolfram Hergert and R. Matthias Geilhufe.



(a) (b)

Figure 1.1 Symmetry in nature and architecture. (a) Table 91 from HAECKEL's 'Art forms in Nature' [4]; (b) Chrysler Building in New York City [5] (© JORGE ROYAN, www.royan.com.ar, CC BY-SA 3.0).

Within the fine arts, the works of M.C. ESCHER (1898–1972) gain their special attraction from an intellectually deliberate confusion of symmetry and symmetry breaking.

In ESCHER's woodcut Snakes [6], a threefold rotational symmetry can be easily detected in the snake pattern. A rotation by 120° transforms the painting into itself. A considerable amount of his work is devoted to mathematical principles and symmetry. The series "Circle Limits" deals with hyperbolic regular tessellations, but they are also interesting from the symmetry point of view. The woodcut, entitled Circle Limit III [6], the most interesting under the four circle limit woodcuts, shows a twofold rotational axis. If the figure is transformed into a black and white version a fourfold rotational axis appears. Obviously, the color leads to a reduction of symmetry [7]. The change of symmetry by inclusion of additional degrees of freedom like color in the present example or the spin, if we consider a quantum mechanical system, leads to the concept of color or SHUBNIKOV groups. A comprehensive overview on symmetry in art and sciences is given by SHUBNIKOV [8]. WEYL [9] and ALTMANN [10] start their discussion of symmetry principles from a similar point of view.

Also in music symmetry principles can be found. Tonal and temporal reflections, translations, and rotations play an important role. J.S. BACH's crab canon from *The Musical Offering* (BWV1079) is an example for reflection. The brilliant effects in M. RAVEL's Boléro achieved by a translational invariant theme represent an impressive example as well.

Physics

The conservation laws in classical mechanics are closely related to symmetry. Table 1.1 gives an overview of the interplay between symmetry properties and the resulting conservation laws.

A general formulation of this connection is given by the NOETHER theorem. That symmetry principles are the primary features that constrain dynamical laws was one of the great advances of EINSTEIN in his *annus mirabilis* 1905 [11]. The relevance of symmetry in all fields of theoretical physics can be seen as a major achievement of twentieth century physics.

In parallel to the development of quantum theory, the direct connection between quantum theory and group theory was understood. Especially E. WIGNER revealed the role of symmetry in quantum mechanics and discussed the application of group theory in a series of papers between 1926 and 1928 [11] (see also H. WEYL 1928 [12]). Symmetry accounts for the degeneracy of energy levels of a quantum system. In a central field, for example, an energy level should have a degeneracy of $2l + 1$ (l – angular momentum quantum number) because the angular momentum is conserved due to the rotational symmetry of the potential. However, considering the hydrogen atom a higher 'accidental' symmetry can be found, where levels have a degeneracy of n^2, the square of the principle quantum number. The reason was revealed by PAULI [13, 14] in 1926 using the conservation of the quantum mechanical analogue of the LENZ–RUNGE vector and by FOCK in 1935 by the comparison of the SCHRÖDINGER equation in momentum space with the integral equation of four-dimensional spherical harmonics [15]. FOCK showed that the electron effectively moves in an environment with the symmetry of a hypersphere in four-dimensional space. The symmetry of the hydrogen atom is mediated by transformations of the entire Hamiltonian and not of its parts, the kinetic and the potential energy alone. Such *dynamical symmetries* cannot be found by the analysis of forces and potentials alone. The basic equations of quantum theory and electromagnetism are time dependent, i.e., dynamic equations. Therefore, the symmetry properties of the physical systems as well as the symmetry properties of the fundamental equations have to be taken into account.

Table 1.1 Conservation laws and symmetry in classical mechanics.

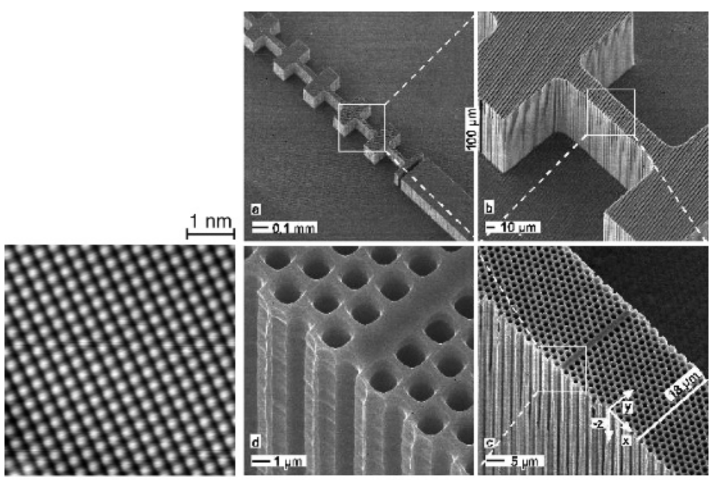
Symmetry property		Conserved quantity
Homogeneity of time (translations in time)	⇒	Energy
Homogeneity of space (translations in space)	⇒	Momentum
Isotropy of space (rotations in space)	⇒	Angular momentum
Invariance under GALILEI transformations	⇒	Center of gravity

1.1 Symmetries in Solid-State Physics and Photonics

In Figure 1.2, two representative examples of solid-state systems are shown. The scanning tunneling microscope (STM) image in Figure 1.2a depicts two monolayers of MgO on a Ag(001) surface in atomic resolution. The quadratic arrangement of protrusions representing one sublattice is clearly revealed. One of the main tasks of solid-state theory is the calculation of the electronic structure of systems starting from the real-space structure.

However, the many-particle Schrödinger equation, containing the coordinates of all nuclei and electrons of a solid cannot be solved directly, neither analytically nor numerically. This problem can be approached by discussing effective one-particle systems, for example, in the framework of density functional theory (cf. [16]). Therefore, it will be sufficient to study Schrödinger-like equations in the following to investigate implications of crystal symmetry.

In the first years of electronic structure theory of solids, principles of group theory were applied to optimize computations of complex systems as much as possible due to the limited computational resources available at that time. Although this aspect becomes less important nowadays, the connection between symmetry in the structure and the electronic properties is one of the main applications of group theory.



(a) (b)

Figure 1.2 Symmetry in solid-state physics and photonics. (a) Atomically resolved STM image of two monolayers of MgO on Ag(001) (from [17], Figure 1) (With permission, Copyright © 2017 American Physical Society.)(b) SEM image of a width-modulated stripe (a) of macroporous silicon on a silicon substrate. The increasing magnification in (b)–(d) reveals a waveguide structure prepared by a missing row of pores. (from [18]). (With permission, Copyright © 1999 Wiley-VCH GmbH.)

Next to the optimization of numerical calculations, group theory can be applied to classify promising systems for further investigations, like in the case of the search for multiferroic materials [19, 20]. In general, four primary ferroic properties are known: ferroelectricity, ferromagnetism, ferrotoroidicity, and ferroelasticity. The magnetoelectric coupling, of special interest in applications, is a secondary ferroic effect. The occurrence of multiple ferroic properties in one phase is connected to specific symmetry conditions a material has to accomplish.

Defects in solids and at solid surfaces play a continuously increasing role in basic research and applications (diluted magnetic semiconductors, p-magnetism in oxides). For example, group theory allows to get useful information in a general and efficient way (cf. [21, 22]) treating defect states in the framework of perturbation theory.

More recently, a close connection between high-energy physics and condensed matter physics has been established, where effective elementary excitations within a crystal behave as particles that were formally described in elementary particle physics. A promising class of materials are Dirac materials like graphene, where the elementary electronic excitations behave as relativistic massless Dirac fermions [23, 24]. Degeneracies and crossings of energy bands within the electronic band structure together with the dispersion relation in the neighborhood of the crossing point are closely related to the crystalline symmetry [25, 26].

In Figure 1.2b, a scanning electron microscope (SEM) image of macroporous silicon is shown. The special etching technique provides a periodically structured dielectric material that is referred to as a photonic crystal. The propagation of electromagnetic waves in such structures can be calculated starting from MAXWELL's equations [27, 28]. The resulting eigenmodes of the electromagnetic field are closely connected to the symmetry of the structured dielectric. Group theory can be applied in various cases within the field of photonics. Subsequently, a few examples are mentioned. The photonic bands of two-dimensional photonic crystals can be classified with respect to the symmetry of the lattice. The symmetry properties of the eigenmodes, found by means of group theory, decide whether this mode can be excited by an external plane wave [29]. Metamaterials are composite materials that have peculiar electromagnetic properties that are different from the properties of their constituents. Group theory can be used for design and optimization of such materials [30]. Group theoretical arguments also help to discuss the dispersion in photonic crystal waveguides in advance. Clearly, this approach represents a more sophisticated strategy in comparison to relying on a trial and error approach [31, 32]. If a magneto-optical material is used for a photonic crystal, time-reversal symmetry is broken due to the intrinsic magnetic field. In this case, the theory of magnetic groups can be used to study the properties of such systems [33].

The goal of this book is to discuss the variety of possible applications of computational group theory as a powerful tool for actual research in photonics and electronic structure theory. Specific examples using the *Mathematica* package GTPack will be provided.

1.2
A Basic Example: Symmetries of a Square

As a first example, the symmetry of a square is discussed (Figure 1.3). The square is located in the xy-plane. In general, the whole xy-plane could be covered completely by squares leading to a periodic arrangement like that of the STM image from the two MgO layers on Ag(001) in Figure 1.2a. Subsequently, operations that leave the square invariant are identified.[1)]

First, *rotations* of $0, \pi/2, \pi,$ and $3\pi/2$ in the mathematical positive direction around the z-axis represent such operations. A rotation by an angle of 0° induces no change at all and is therefore named *identity element E*. Instead of the rotation by $3\pi/2$ a rotation by $-\pi/2$ can be considered. Furthermore, a rotation by an angle of $\varphi + n2\pi,\ n = 1, 2, \ldots$ is equivalent to a rotation by φ and is not considered as a new operation. In total, four inequivalent rotational operations are found.

Next to rotations leaving the square invariant, *reflection lines* can be identified. Performing a reflection, the perpendicular coordinates with respect to the line change their sign. In the present example, the x-axis is such a reflection line and furthermore a symmetry operation. By a reflection along this line, the point 1 becomes 4, 2 becomes 3, and vice versa. If the symmetries are considered in three dimensions, a reflection might be expressed by a rotation with angle π around the normal direction of the reflection line (here it is the y-axis) followed by an *inversion* (the inversion changes the signs of *all* coordinates). A rotation around the y-axis interchanges the points 1 and 2 and 4 and 3 as well. After applying an inversion the points 1 and 3 and 2 and 4 are interchanged. Additionally, the y-axis and the two diagonals of the square are reflection lines.

In total there are eight inequivalent symmetry elements, four rotations and four reflections. Those elements form the *symmetry group* of the square. The combination of two symmetry elements, i.e., the application one after another, leads to another element of the group.

In Figure 1.4, a square is presented with different coloring schemes. It can be verified that the use of color in Figure 1.4b–d reduces the symmetry. The symmetry groups of the colored squares are *subgroups* of the group of the square of

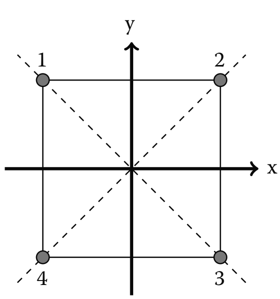


Figure 1.3 Square with coordinate system and reflection lines. The vertices are numbered only to explain the effect of symmetry operations.

1) Symmetry operations are restricted here to the xy-plane, i.e., are orthogonal coordinate transformations in x and y represented by 2×2 matrices.

Figure 1.4 Symmetry of a square: Square colored in different ways.

Figure 1.4a. As an example: In Figure 1.4c the diagonal reflection lines still exist, but but the mirror symmetry along the x- and y-axis is broken. Furthermore, the fourfold rotation axis is reduced to a twofold rotation axis. While the square itself represents a geometrical symmetry, the color scheme might be thought to be connected with a physical property like the spin, in terms of spin-up (black) and spin-down (white).

In the next sections, the basics of group theory are introduced. The symmetry group of the square will be kept as an example. Referring to Figure 1.2b, a hexagonal arrangement of pores can be seen for the photonic crystal. The symmetry group of a hexagon has 12 elements.

Task 1 (Symmetry of the square and the hexagon)**.** The Notebook **GTTask_1.nb** contains a discussion of the symmetry properties of the colored squares of Figure 1.4. Extend the discussion to a regular hexagon and its different colored versions to get familiar with *Mathematica* and GTPack.