Chapter 1

Introduction

As far as I can see, all a priori *statements in physics have their origin in symmetry.*
—Hermann Weyl[1]

1.1 Symmetry in Physics

Symmetry is a fundamental human concern, as evidenced by its presence in the artifacts of virtually all cultures. Symmetric objects are aesthetically appealing to the human mind and, in fact, the Greek work *symmetros* was meant originally to convey the notion of "well-proportioned" or "harmonious." This fascination with symmetry first found its rational expression around 400 B.C. in the Platonic solids and continues to this day unabated in many branches of science.

1.1.1 What is a Symmetry?

An object is said to be symmetric, or to have a symmetry, if there is a transformation, such as a rotation or reflection, whereby the object looks the same after the transformation as it did before the transformation. In Fig. 1.3, we show an equilateral triangle, a square, and a circle. The triangle is indistinguishable after rotations of $\frac{1}{3}\pi$ and $\frac{2}{3}\pi$ around its geometric center, or symmetry axis. The square is indistinguishable

[1]In *Symmetry* (Princeton University Press, 1952)

after rotations of $\frac{1}{2}\pi$, π, and $\frac{3}{2}\pi$, and the circle is indistinguishable after *all* rotations around their symmetry axes. These transformations are said to be **symmetry transformations** of the corresponding object, which are said to be **invariant** under such transformations. The more symmetry transformations that an object admits, the more "symmetric" it is said to be. One this basis, the circle is "more symmetric" than the square which, in turn, is more symmetric than the triangle. Another property of the symmetry transformations of the objects in Fig. 1.3 that is central to this course is that those for the triangle and square are *discrete*, i.e., the rotation angles have only discrete values, while those for the circle are *continuous*.

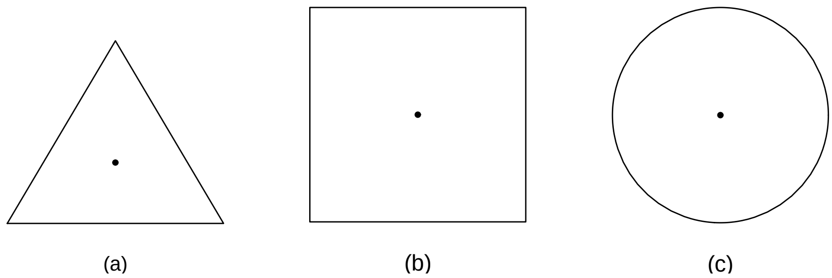

Figure 1.1: An equilateral triangle (a), square (b) and circle (c). These objects are invariant to particular rotations about axes that are perpendicular to their plane and pass through their geometric centers (indicated by dots).

1.1.2 Symmetry in Physical Laws

In the physical sciences, symmetry is of fundamental because there are transformations which leave the laws of physics invariant. Such transformations involve changing the variables within a physical law such that the equations describing the law retain their form when expressed in terms of the new variables. The relationship between symmetry and physical laws began with Newton, whose equations of motion were found to be the same in different frames of reference related by Galilean transformations. Symmetry was also the guiding principle that enabled Lorentz and Poincaré to derive the transformations, now known as Lorentz transformations, which leave Maxwell's equations invariant. The incompatibility between the Lorentz invariance of Maxwell's equations and the Galilean invariance of Newtonian mechanics was, of course, resolved by Einstein's special theory of relativity.

As an example of a symmetry in a physical law, consider the propagation of an impulse at the speed of light c. This is governed by the wave equation, which is obtained from Maxwell's equations:

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\,. \tag{1.1}$$

The Lorentz transformation of space-time coordinates corresponding to a velocity $\boldsymbol{v} = (v, 0, 0)$ is

$$x' = \gamma(x - vt), \quad y' = y, \quad z' = z, \quad t' = \gamma\left(t - \frac{v}{c^2}x\right), \tag{1.2}$$

where $\gamma = (1 - v^2/c^2)^{-1/2}$. When expressed in terms of the transformed coordinates (x', y', z', t'), the wave equation (1.1) is found to retain its form under this transformation:

$$\frac{1}{c^2}\frac{\partial^2 u'}{\partial t'^2} = \frac{\partial^2 u'}{\partial x'^2} + \frac{\partial^2 u'}{\partial y'^2} + \frac{\partial^2 u'}{\partial z'^2}\,. \tag{1.3}$$

This implies that the wave propagates in the same way with the same velocity in two inertial frames that are in uniform motion with respect to one another. The Lorentz transformation is thus a symmetry transformation of the wave equation (1.1) and this equation is said to be **covariant** with respect to these transformations. In general, symmetry transformations of physical laws involve the space-time coordinates, which are sometimes called **geometrical symmetries**, and/or internal coordinates, such as spin, which are called **internal symmetries**.

1.1.3 Noether's Theorem

Identifying appropriate symmetry transformations is one of the central themes of modern physics since their mathematical expression affects the structure and predictions of physical theories. Work by both mathematicians and physicists, culminating with Emmy Noether, led to the demonstration that there was a deep relationship between symmetry and conservation laws. This is now known as Noether's Theorem:

Noether's Theorem. The covariance of the equations of motion with respect to a continuous transformation with n parameters implies the existence of n quantities, or constants of motion, i.e., **conservation laws.**

In classical mechanics, the conservation of linear momentum results from the translational covariance of Newton's equations of motion, i.e., covariance with respect to transformations of the form $\boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{a}$, for any vector $\boldsymbol{a}$. The conservation of angular momentum similarly results from rotational covariance, i.e., covariance with respect rotations in space: $\boldsymbol{r}' = R\boldsymbol{r}$, where R is a 3×3 rotation matrix. Finally, the conservation of energy results from the covariance of Newton's equations to translations in time, i.e., transformations of the form $t' = t + \tau$.

1.1.4 Symmetry and Quantum Mechanics

The advent of quantum mechanics and later quantum field theory fostered entirely new avenues for investigating the consequences of symmetry. London and Weyl introduced a type of transformation known as a gauge transformation into quantum theory, with total electric charge as the conserved quantity. In the early 1960s, Gell–Mann and Ne'eman proposed the unitary symmetry SU(3) for the strong interactions. This led to the proposal by Gell–Mann and Zweig of a new, deeper, level of quanta, "quarks," to account for this symmetry. Heisenberg, Goldstone and Nambu suggested that the ground state (i.e., the vacuum) of relativistic quantum field theory may not have the full global symmetry of the Hamiltonian, and that massless excitations (Goldstone bosons) accompany this "spontaneous symmetry breaking." Higgs and others found that for spontaneously broken gauge symmetries there are no Goldstone bosons, but instead massive vector mesons. This is now known as the Higgs phenomenon and its verification verification has been the subject of extensive experimental effort.

Another aspect of symmetry, also due to the quantum mechanical nature of matter, arises from the arrangement of atoms in molecules and solids. The symmetry of atomic arrangements, whether in a simple diatomic molecule or a complex crystalline material such as a high-temperature superconductor, affects many aspects of their electronic and vibrational properties and especially their response to external thermal, mechanical, and electromagnetic perturbations. The transformation properties of wavefunctions in quantum mechanics are an example of what is known as **Representation Theory**, which was developed by the mathematicians Frobenius and Schur near the turn of the 20th century. This inspired a huge effort by physicists and chemists to determine the physical consequences of the symmetries of wavefunctions which continues to this day. Notable examples include Bloch's work on wavefunctions in periodic potentials, which forms the basis of the quantum theory of solids, Pauling's work on the chemical interpretation orbital symmetries, and Woodward and Hoffman's work on how the conservation of orbital symmetry determines the course of chemical reactions. Recent scientific advances that highlight the prominent role that symmetry maintains in condensed-matter physics is the discovery of quasicrystals, which have rotational symmetries (e.g., fivefold, as shown in Fig. 1.2) which are incompatible with the translational symmetry of ordinary crystals and are thus sometimes called aperiodic, and the C_{60} form of carbon, known as "Buckminsterfullerene," or "Buckyballs", a name derived from its resemblance to structures (geodesic domes) proposed by R. Buckminster Fuller as an alternative to conventional architecture.

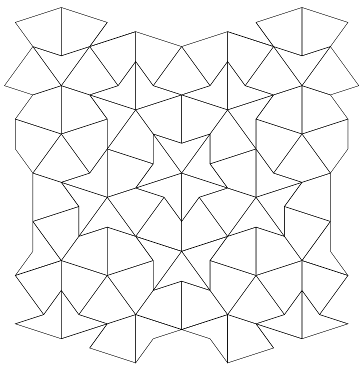

Figure 1.2: A section of a Penrose tile, which has a fivefold rotational symmetry, but no translational symmetry. This two-dimensional structure shares a number of features with quasicrystals.

1.2 Examples from Quantum Mechanics

1.2.1 One-Dimensional Systems

To appreciate how symmetry enters into the description of quantum mechanical systems, we consider the time-independent Schrödinger equation for the one-dimensional motion of a particle of mass m bound by a potential $V(x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\varphi(x)=E\varphi(x)\,, \tag{1.4}$$

where $\hbar=h/2\pi$, h is Planck's constant, φ is the wavefunction, and E is the energy eigenvalue. By writing this equation as $\mathcal{H}\varphi=E\varphi$, we identify the coordinate representation of the Hamiltonian operator as

$$\mathcal{H}=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\,. \tag{1.5}$$

In the following discussion, we will utilize the fact that the energy eigenvalues of one-dimensional quantum mechanical problems such as that in (1.4) are nondegenerate, i.e., each energy eigenvalue is associated with one and only one eigenfunction.[2]

Suppose that the potential in (1.4) is an even function of x. The mathematical expression of this fact is the invariance of this potential under the inversion transformation $x\to -x$:

$$V(-x)=V(x)\,. \tag{1.6}$$

Examples of such potentials are the symmetric square well and the harmonic oscillator (Fig. 1.3), but the particular form of the potential is unimportant for this discussion. The kinetic energy term in (1.4) is also invariant under the same inversion transformation as the potential, since

$$\frac{\mathrm{d}^2}{\mathrm{d}(-x)^2}=\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{1.7}$$

[2]This follows directly from the fact that this equation, *together with appropriate boundary conditions*, constitute a Sturm–Liouville problem. Other well-known properties of solutions of Schrödinger's equation (real eigenvalues, discrete eigenvalues for bound states, and orthogonality of eigenfunctions) also follow from the Sturm–Liouville theory.

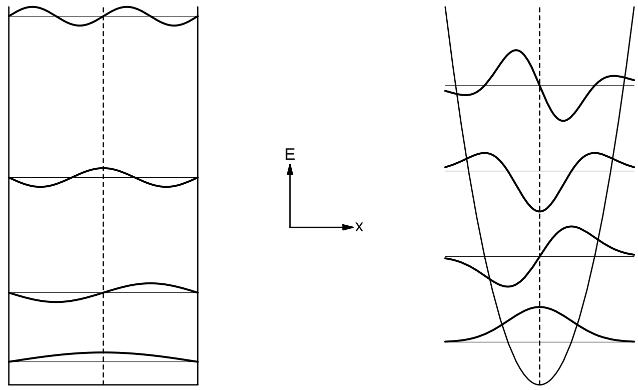

Figure 1.3: The first four eigenfunctions of the Schrödinger equation (1.4) for an infinite square-well potential, $V(x) = 0$ for $|x| \leq L$ and $V(x) \to \infty$ for $|x| > L$ (left), and a harmonic oscillator potential, $V(x) = \frac{1}{2}kx^2$, where k is the spring constant of the oscillator (right). The abscissa is the spatial position x and the ordinate is the energy E, with the vertical displacement of each eigenfunction given by its energy. The origins are indicated by broken lines.

Thus, the Hamiltonian operator in (1.5) is itself invariant under inversion, i.e., inversion is a symmetry transformation of this Hamiltonian. We now use this property of $\mathcal{H}$ to change variables from x to $-x$ in (1.4) and thereby obtain the Schrödinger equation for $\varphi(-x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\varphi(-x) = E\varphi(-x) \tag{1.8}$$

Since E is nondegenerate, there can be only one eigenfunction associated with this eigenvalue, so the $\varphi(-x)$ cannot be linearly independent of $\varphi(x)$. The only possibility is that $\varphi(-x)$ is *proportional* to $\varphi(x)$:

$$\varphi(-x) = A\varphi(x) \tag{1.9}$$

where A is a constant. Changing x to $-x$ in this equation,

$$\varphi(x) = A\varphi(-x) \tag{1.10}$$

and then using (1.9) to replace $\varphi(-x)$, yields

$$\varphi(x) = A^2\varphi(x) \tag{1.11}$$

This requires that $A^2 = 1$, i.e., $A = 1$ or $A = -1$. Combining this result with (1.9) shows that the eigenfunctions φ of (1.4) must be either even

$$\varphi(-x) = \varphi(x) \tag{1.12}$$

or odd

$$\varphi(-x) = -\varphi(x) \tag{1.13}$$

under inversion. As we know from the solutions of Schrödinger's equation for square-well potentials and the harmonic oscillator (Fig. 1.3), both even and odd eigenfunctions are indeed obtained. Thus, not all eigenfunctions have the symmetry of the Hamiltonian, although the ground state usually does.[3] Nevertheless, the symmetry (1.6) does provide a *classification* of the eigenfunctions according to their parity under inversion. This is a completely general result which forms one of the central themes of this course.

1.2.2 Symmetries and Quantum Numbers

The example discussed in the preceding section showed how symmetry enters explicitly into the solution of Schrödinger's equation. In fact, we can build on our discussion in Sec. 1.1.2, and especially Noether's theorem, to establish a general relationship between continuous symmetries and quantum numbers.

Consider the time-dependent Schrödinger equation for a free particle of mass m in one dimension:

$$i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2}\,. \tag{1.14}$$

The solutions to this equation are plane waves:

$$\varphi(x,t) = \mathrm{e}^{i(kx-\omega t)}\,, \tag{1.15}$$

where k and ω are related to the momentum and energy by $p = \hbar k$ and $E = \hbar\omega$. In other words, the quantum numbers k and ω of the

[3] A notable exception to this is the phenomenon of *spontaneous symmetry-breaking* discussed in Sec. 1.1, where the symmetry of the equations of motion and the boundary conditions is not present in the observed solution for the ground state.

solutions to Eq. (1.14) correspond to the momentum and energy which, because of the time- and space-translational covariance of this equation, correspond to conserved quantities. Thus, quantum numbers are associated with the symmetries of the system. Similarly, for systems with rotational symmetry, such the hydrogen atom or, indeed, *any* atom, the appropriate quantum numbers are the energy and the angular momentum, the latter producing two quantum numbers, as required by Noether's theorem, because the transformations have two degrees of freedom.

1.2.3 Matrix Elements and Selection Rules

One of the most important uses of symmetry is to identify the matrix elements of an operator which are required to vanish. Continuing with the example in the preceding section, we consider the matrix elements of an operator $\mathcal{H}'$ whose position representation $\mathcal{H}'(x)$ has a definite parity. The matrix elements of this operator are given by

$$\mathcal{H}'_{ij} = \int \varphi_i(x)\mathcal{H}'(x)\varphi_j(x)\,\mathrm{d}x \tag{1.16}$$

where the range of integration is symmetric about the origin. If $\mathcal{H}'$ has even parity, i.e., if $\mathcal{H}'(-x) = \mathcal{H}'(x)$, as in (1.6), then these matrix elements are nonvanishing only if $\varphi_i(x)$ and $\varphi_j(x)$ are both even or both odd, since only in these cases is the integrand an even function of x. This is called a **selection rule**, since the symmetry of $\mathcal{H}'(x)$ determines, or selects, which matrix elements are nonvanishing.

Suppose now that $\mathcal{H}'(x)$ has odd parity, i.e., $\mathcal{H}'(-x) = -\mathcal{H}'(x)$. The matrix elements in (1.16) now vanishes if $\varphi_i(x)$ and $\varphi_j(x)$ are both even or both odd, since these choices render the integrand an odd function of x. In other words, the selection rule now states that only eigenfunctions of *opposite* parity are coupled by such an operator. Notice, however, that the use of symmetry only identifies which matrix elements *must* vanish; it provides no information about the *magnitude* of the nonvanishing matrix elements.

Suppose that

$$\mathcal{H}'(x) = Ax \tag{1.17}$$

where A is a constant, i.e., $\mathcal{H}'(x)$ is proportional to the coordinate x. Such operators arise in the quantum theory of transitions induced by an electromagnetic field.[4] $\mathcal{H}'(x)$ clearly has odd parity, so the matrix elements (1.16) are nonvanishing only if $\varphi_i(x)$ and $\varphi_j(x)$ have *opposite* parity. But, if

$$\mathcal{H}'(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{1.18}$$

which is the coordinate representation of the kinetic energy operator, then the matrix elements (1.16) are nonvanishing only if $\varphi_i(x)$ and $\varphi_j(x)$ have the *same* parity.

Selection rules are especially useful if there are **broken symmetries**. For example, the Hamiltonian of an atom, which is the sum of the kinetic energies of the electrons and their Coulomb potentials, is invariant under all rotations. But when an atom is placed in an electric or magnetic field, the Hamiltonian acquires an additional term which is *not* invariant under all rotations, since the field now defines a preferred direction. These are the Stark and Zeeman effects, respectively. A similar situation is encountered in quantum field theory when, beginning with a Lagrangian that is invariant under certain symmetry operations, a term is added which does not have this invariance. If the symmetry-breaking terms in these cases are small, then selection rules enter into the perturbative calculation around the solutions of the symmetric theory.

1.3 Summary

The notion of symmetry implicit in all of the examples cited in this chapter is endowed with the algebraic structure of "groups." This is a topic in mathematics that had its beginnings as a formal subject only in the late 19th century. For some time, the only group that was know and whose properties were studied were permutation groups. Cauchy played a major part in developing the theory of permutations, but it was the English mathematician Cayley who first formulated the notion of an abstract group and used this to identify matrices and quaternions

[4] E. Merzbacher, *Quantum Mechanics* 2nd edn. (Wiley, New York, 1970), Ch. 18.

as groups. In a later paper, Cayley showed that every finite group could be represented in terms of permutations, a result that we will prove in this course. The fact that geometric transformations, as discussed in this chapter, and permutations, share the same algebraic structure is part of the richness of the subject and is rooted in its history as an adjunct to the study of algebraic solutions of equations. In the next chapter, we discuss the basic properties of groups that form the basis of this course.