Chapter 21
Symmetries and Conservation Laws

It is important and helpful to know all the conserved quantities for a given problem. In quantum mechanics, this means finding all the operators that commute with H. As in classical mechanics, these quantities are closely related to the symmetries of the problem. In the following, this relationship is examined in detail.

Symmetry means simply that there are different 'perspectives' from which a physical system looks the same. In other words, the system is invariant under a certain symmetry operation such as rotation or reflection, and its mathematical description does not change as a result of the transformation.[1] This leads to a remarkable coupling of the geometric and the dynamic properties of a system. In theoretical physics, symmetries are fundamental, because, in a sense, the basic laws of nature result from them, and they are regarded as the most successful principle for the unification of theories.[2]

There are *continuous* and *discrete* symmetries. Continuous symmetry transformations are characterized by a continuous parameter (or possibly several). The following four general continuous symmetries are central in physics[3]:

1. Homogeneity of time or time-translation invariance (the choice of the zero of time (starting time) does not matter).
2. Homogeneity of space or space-translation invariance (the choice of the origin of spacial coordinates (center point) does not matter).

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[1]In general, there are two viewpoints in considering symmetry transformations: the passive viewpoint (the system remains unchanged, but the axes are changed accordingly), and the active viewpoint (the axes remain unchanged, but the system is transformed—which is of course not meant to be a dynamic rotation). Which point of view one prefers is a matter of taste. The best-known example is perhaps the passive and active rotation in two dimensions, which we already mentioned in Chap. 2, Vol. 1.

[2]P.W. Anderson, Nobel Laureate 1972: "It is only a slight exaggeration to say that physics is the study of symmetries."

[3]In special problems, there may of course be additional symmetries (e.g. the Lenz vector in the case of the hydrogen atom).

J. Pade, *Quantum Mechanics for Pedestrians 2*, Undergraduate Lecture Notes in Physics, https://doi.org/10.1007/978-3-030-00467-5_21

3. Isotropy of space or space rotational invariance (the choice of the spatial direction does not matter).
4. Principle of relativity or invariance under specific Galilean transformations[4] (the choice of inertial frame does not matter).

The discrete symmetry transformations are:

1. Invariance under parity inversion, $\mathbf{r} \to -\mathbf{r}$ (the mirror images of all physical processes must be equally possible).
2. Invariance under time reversal $t \to -t$ (physical processes must occur equally both forwards and backwards in time).

One might think that all these symmetries are obvious, but that is not necessarily true. For example, it was previously believed that parity conservation applies to all interactions, but we know now that the weak interaction does not conserve parity (and is also not invariant under time reversal).[5]

Note that all transformations are *Galilean transformations*, i.e. transformations from one non-accelerated reference frame (inertial frame) to another one. Mathematically, the Galilean transformations form a group, the *Galilean group*. The *proper* Galilean group[6] contains the translations in space and time (shifts of the zero points), the rotations about constant angles, and the transformations into a non-rotating reference frame moving uniformly along a straight line with constant velocity v (special Galilean transformations). The full group also includes the reflections (inversions) of space and time.

Continuous symmetries are associated with the existence of conserved quantities, as is summarized in Table 21.1.

This fact is known from classical physics through Noether's theorem, which states that 'To every continuous symmetry of a physical system, there belongs a conserved quantity, and *vice versa*.' In quantum mechanics, also, symmetries lead to conserved quantities[7]—in principle, the situation is the same as in classical mechanics, but it has to be formulated somewhat differently. For if the physics is to remain unchanged by a symmetry operation, then measurable quantities, i.e. eigenvalues and probabilities, must not change. This means that in quantum mechanics, such symmetry transformations are described by *unitary* operators in the Hilbert space (see Chap. 13, Vol. 1).

However, this is not the whole truth, since we must also consider anti-unitary transformations. We have already discussed the reason for this in Chap. 14, Vol. 1:

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[4]Galilean and not Lorentz transformations, because we are considering here nonrelativistic quantum mechanics.

[5]Even Wolfgang Pauli took the validity of the symmetries for granted and consequently declared it as a priori absurd to search for parity-violating processes: "I cannot believe that God is a weak left-hander." He had to revise his views, as is known, after Madame Wu et al., demonstrated parity violation in the beta decay of cobalt-60 atoms in 1956.

[6]Number of parameters: $3 + 1 + 3 + 3 = 10$.

[7]For example, we have seen in an exercise for Chap. 9, Vol. 1 that the angular momentum is conserved in spherically symmetric problems.

Table 21.1 Invariances and conserved quantities

Invariance under	Conserved quantity
Temporal shift	Energy
Spatial shift	Momentum
Spatial rotation	Angular momentum
Change of inertial frame	Velocity of center of mass

All normalized vectors $|\varphi\rangle$ with arbitrary phase are physically equivalent, e.g. the ray $e^{i\alpha}|\varphi\rangle$. Therefore, we cannot require that symmetry transformations be represented by unitary operators only, since this requirement stems from the assumption that the scalar products between states must remain unchanged, i.e. $\langle\varphi' |\psi'\rangle = \langle\varphi |\psi\rangle$. For rays, we need to weaken this assumption to $|\langle\varphi' |\psi'\rangle|^2 = |\langle\varphi |\psi\rangle|^2$. In this situation, a theorem of *Wigner* applies, stating that the last equation can be guaranteed only by *unitary* and *anti-unitary* transformations. With $|\varphi'\rangle = U|\varphi\rangle$, we have for unitary U

$$\langle\varphi' |\psi'\rangle = \langle U\varphi |U\psi\rangle = \langle\varphi |\psi\rangle; \tag{21.1}$$

while for an *anti-unitary* operator U, it holds that

$$\langle\varphi' |\psi'\rangle = \langle U\varphi |U\psi\rangle = \langle\varphi |\psi\rangle^* = \langle\psi |\varphi\rangle. \tag{21.2}$$

We see that an anti-unitary transformation leaves not the scalar products themselves invariant, but, as required, their absolute values.

We note that anti-unitarity is the exception; all transformations considered in the following are unitary, except time reversal, which is anti-unitary.

21.1 Continuous Symmetry Transformations

21.1.1 General: Symmetries and Conservation Laws

Continuous symmetry transformations S are characterized by a continuous parameter α. For $\alpha = 0$, S represents the unit map. The parameter is additive, so that

$$S(\alpha_1 + \alpha_2) = S(\alpha_2)\, S(\alpha_1). \tag{21.3}$$

An example is a rotation about the z axis by the angle α. It is obviously the same if we rotate first by α_1 and then by α_2 or immediately by $\alpha_1 + \alpha_2$.

This symmetry operation is represented in quantum mechanics by a corresponding operator U_S, which acts in the Hilbert space $\mathcal{H}$. We have

$$U_S(\alpha_1 + \alpha_2) = U_S(\alpha_2)\, U_S(\alpha_1), \tag{21.4}$$

where U_S is a *unitary* (i.e. not an anti-unitary) operator. This can be seen because $U_S(\alpha)$ for $\alpha = 0$ is the unit map (which is certainly unitary), from which the transformation for $\alpha \neq 0$ can be continuously deduced.

If (21.4) holds, then *Stone's theorem*[8] applies; it states that a Hermitian operator T_S exists, such that[9]:

$$U_S(\alpha) = e^{-i\alpha T_S}. \tag{21.5}$$

T_S is called the *infinitesimal generator* of the transformation[10] (see the discussion in Chap. 13, Vol. 1 about the propagator). We assume below that U_S and thus also T_S are not time dependent.

What leads to the name 'infinitesimal generator', and what is the relation of symmetry transformations and conservation laws in quantum mechanics? Let us consider the unitary transformation $\left|\psi'\right\rangle = U_S \left|\psi\right\rangle$. For the matrix element $\left\langle\psi\right| H \left|\psi\right\rangle$, it follows that

$$\left\langle\psi\right| H \left|\psi\right\rangle = \left\langle\psi\right| U_S^\dagger U_S H U_S^\dagger U_S \left|\psi\right\rangle = \left\langle\psi'\right| U_S H U_S^\dagger \left|\psi'\right\rangle := \left\langle\psi'\right| H' \left|\psi'\right\rangle. \tag{21.6}$$

Now we require that H be invariant under the symmetry transformation represented by the unitary operator U_S. This means that $H = H' = U_S H U_S^\dagger$. Together with (21.5) and because of $U_S U_S^\dagger = 1$, it follows that

$$U_S H = H U_S \text{ or } [U_S, H] = 0 \text{ or } \left[e^{-i\alpha T_S}, H\right] = 0. \tag{21.7}$$

This equation must be valid for all parameters α, especially for very small or infinitesimal α. In that case, we can expand[11]:

$$e^{-i\alpha T_S} = 1 - i\alpha T_S + O\left(\alpha^2\right). \tag{21.8}$$

This leads directly to

$$[T_S, H] = 0. \tag{21.9}$$

Since we have assumed that T_S is not time dependent, T_S is a constant of the motion, according to Ehrenfest's theorem.

So we have (under the above restrictions and clarifications) the following result: If H is invariant under a continuous symmetry operation that is described in the Hilbert space $\mathcal{H}$ by the unitary operator U_S, then T_S is a conserved quantity, defined

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[8]The full version can be found in Appendix I, Vol. 1.

[9]This relationship is suggested, *inter alia*, by the fact that a function $f(x)$ with the property $f(x + y) = f(x) f(y)$ is given by a (generalized) exponential function a^x.

[10]The sign and any other multiplicative constants cannot be determined at this point ($e^{i\alpha T_S}$, $e^{-i\alpha T_S/\hbar}$, etc.).

[11]Why is one not content with $[U_S, H] = 0$? The answer is because U is unitary, but T is Hermitian and therefore is possibly a measurable variable.

by $U_S = e^{-i\alpha T_S}$. In this way, we have found a direct relationship between symmetries (or geometry) and conserved quantities (or dynamics) in quantum mechanics.

Of course, T_S as a Hermitian operator is a good candidate for a physical observable, and we will indeed discuss below only the latter. For the fundamental transformations mentioned in the introduction, we have:

Time translation (we already know this operator from Chap. 13, Vol. 1)

$$U(t) = e^{-i\frac{tH}{\hbar}}. \tag{21.10}$$

Space translation by a distance $\mathbf{a}$ ($\mathbf{p}$ is the momentum operator):

$$U(\mathbf{a}) = e^{-i\frac{\mathbf{pa}}{\hbar}}. \tag{21.11}$$

Spatial rotation about an axis $\hat{\mathbf{n}}$ by an angle ϑ ($\mathbf{j}$ is the angular-momentum operator):

$$U\left(\hat{\mathbf{n}}, \vartheta\right) = e^{-i\frac{\vartheta\mathbf{j}\cdot\hat{\mathbf{n}}}{\hbar}}. \tag{21.12}$$

Space translation with constant velocity $\mathbf{v}$ (special Galilei transformation or *boost*):

$$U(\mathbf{v}) = e^{-i\frac{\mathbf{v}\cdot\mathbf{G}}{\hbar}} \tag{21.13}$$

with $\mathbf{G} = \mathbf{p}t - m\mathbf{x}$. Due to space and time constraints, the special Galilean transformation is described in detail only in Appendix L, Vol. 2.

One can also interpret the facts in such a way that these equations *define* the operators representing the physical quantities of energy, momentum, angular momentum, and position. The denominator $\hbar$ ensures that the exponents are dimensionless. For all these transformations, we have $U(-\xi) = U^\dagger(\xi)$, where ξ is the corresponding set of parameters of the transformation.

21.1.2 Time Translation

The time evolution operator

$$U(t) = e^{-i\frac{tH}{\hbar}}. \tag{21.14}$$

was already derived in Chap. 13, Vol. 1; the precondition was $\frac{\partial H}{\partial t} = 0$. For infinitesimal τ, we have

$$U(\tau) = 1 - i\frac{\tau}{\hbar}H, \tag{21.15}$$

and we can regard H as the infinitesimal generator of a time translation. Since the time in nonrelativistic quantum mechanics is not a measurable variable like the position, there is no commutator as in (21.9); instead, we have simply the result that $\frac{\partial H}{\partial t} = 0$ implies the conservation of energy.

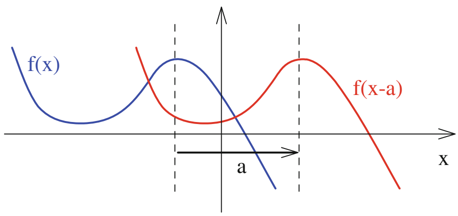

Fig. 21.1 Shift of the function $f(x)$ by a

21.1.3 Spatial Translation

21.1.3.1 Translation and Conservation of Momentum

By means of a particularly simple example, we first want to illustrate once more how a transformation leads to a unitary operator. We start from an (infinitely often differentiable) function $f(x)$. If we shift this function to the right by a, we obtain the new function $f_a(x)$; see Fig. 21.1. This active transformation, which corresponds to a shift of the coordinate system by $-a$, gives the new position $x \to x_a = x + a$. Because of $f_a(x_a) = f(x)$, it follows that $f_a(x) = f(x-a)$. At the position $x - a$, we have the Taylor expansion

$$f(x-a) = \sum_n (-1)^n \frac{a^n}{n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x). \tag{21.16}$$

With the position representation of the momentum operator,

$$p = \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x}, \tag{21.17}$$

it follows that

$$f(x-a) = \sum_n \frac{a^n}{n!} \left(-\frac{ip}{\hbar}\right)^n f(x) = e^{-i\frac{pa}{\hbar}} f(x). \tag{21.18}$$

Thus we have found (for the one-dimensional case) the unitary operator that describes the space translation. It holds that

$$f_a(x) = f(x-a) = e^{-i\frac{pa}{\hbar}} f(x). \tag{21.19}$$

In words: The application of the operator $e^{-i\frac{pa}{\hbar}}$ to a function $f(x)$ shifts it to the right by a. The generalization to the three-dimensional result (21.11) and to the abstract momentum operator is carried out analogously.

The infinitesimal generator of the spatial translation is thus $\mathbf{p}$. From (21.9), we have conservation of momentum if and only if

$$\left[\mathbf{p}, H\right] = 0. \tag{21.20}$$

Correspondingly, if we consider just *one* quantum object, momentum can be conserved only if there is no potential (or more precisely if $\nabla V = 0$).

For N quantum objects, the transformation reads $e^{-i\frac{\mathbf{Pa}}{\hbar}}$, with the total momentum $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$. We consider a closed system, in which all interactions depend only on the mutual distances between the N quantum objects. Hence, the Hamiltonian does not vary due to a spatial shift. According to the above, this means $[\mathbf{P}, H] = 0$, and we see explicitly that the total momentum is conserved, because the Hamiltonian of a closed system is invariant with respect to space translations.

21.1.3.2 Commutation Relation

Using the connection between physical transformations and the associated unitary operators, one can also derive *commutation relations*. We look more closely at the pair position/momentum (one-dimensional). To avoid confusion, we denote the abstract position and momentum operators as X and P, while x and p are eigenvalues. The position operator, for example, fulfills the (idealized) eigenvalue equation $X|x\rangle = x|x\rangle$.

For the derivation of $[X, P] = i\hbar$, we need three elements:

1. We consider a quantum object in the state $|\varphi_0\rangle$, localized around the mean position x_0 with a certain spread Δx. Hence we have

$$\langle\varphi_0| X |\varphi_0\rangle = \langle X\rangle_0 = x_0. \tag{21.21}$$

2. To perform a translation by a, we apply the operator $U(a) = e^{-i\frac{Pa}{\hbar}}$:

$$|\varphi_0\rangle \to |\varphi_a\rangle = U(a)|\varphi_0\rangle = e^{-i\frac{Pa}{\hbar}}|\varphi_0\rangle. \tag{21.22}$$

3. We know that in this translation, the mean position changes according to

$$x_0 \to x_0 + a. \tag{21.23}$$

Thus we obtain for the mean position of the quantum object shifted by a:

$$\langle X\rangle_a = \begin{cases} (21.22)\ \langle\varphi_a| X |\varphi_a\rangle = \langle\varphi_0| U^{-1}(a) XU(a) |\varphi_0\rangle \\ (21.23)\ \ x_0 + a = \langle X\rangle_0 + a = \langle\varphi_0| X + a |\varphi_0\rangle \end{cases} \tag{21.24}$$

Since $|\varphi_0\rangle$ is arbitrary, it follows by comparison that

$$U^{-1}(a) XU(a) = X + a. \tag{21.25}$$

Expanding in powers of a and taking the limit $a \to 0$ (see exercises) leads to the canonical commutation relation for the two *abstract operators* X and P:

$$[X, P] = i\hbar. \tag{21.26}$$

We emphasize that this equation follows *directly* from general principles—without any correspondence principles or similar devices, but only from the three steps (1) to (3), and thus from (21.25) or, in the end, from translational invariance.

From (21.25), one can also deduce (see exercises) that for a function of the position operator $f(X)$, it holds that:

$$[P, f(X)] = \frac{\hbar}{i}\frac{\mathrm{d}f(X)}{\mathrm{d}X}, \tag{21.27}$$

not by assuming a priori that $P = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}X}$—this equation follows rather as a *result* of the derivation, which uses only the abstract operators X and P. Analogously, we obtain:

$$[X, f(P)] = i\hbar\frac{\mathrm{d}f(P)}{\mathrm{d}P}. \tag{21.28}$$

Finally, as a concrete representation, we choose the position representation with $X \to x$, $P \to \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}$. It follows that

$$\left[x, \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right] = i\hbar. \tag{21.29}$$

By the way, all representations of the canonical commutation relations, e.g. (21.26) and (21.29), may be transformed into each other by unitary transformations,[12] and are therefore equivalent.

21.1.4 Spatial Rotation

A spatial rotation about an axis $\hat{\mathbf{a}}$ (unit vector) by the angle γ is described by the unitary operator

$$U_{\hat{\mathbf{a}}}(\gamma) = e^{-i\frac{\gamma\mathbf{j}\hat{\mathbf{a}}}{\hbar}}. \tag{21.30}$$

This is quite analogous to translation (and can be formally written with the usual replacements momentum → angular momentum, etc.). A simple explicit example of a constructive derivation is given in the exercises.[13]

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[12] We repeat the remark that a unitary transformation corresponds to a change of basis in $\mathcal{H}$.

[13] Using as example the matrix representation of $e^{-i\frac{\gamma\mathbf{j}\hat{\mathbf{a}}}{\hbar}}$ for orbital angular momentum $\mathbf{l} = 1$; see Appendix X.2, Vol. 2.

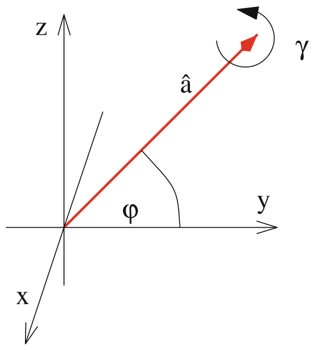

Fig. 21.2 Derivation of the commutation relations for angular momentum

The infinitesimal generator of the spatial rotations is thus the angular momentum (operator) **j**. According to (21.9), conservation of angular momentum is assured if and only if

$$[\mathbf{j}, H] = 0. \tag{21.31}$$

Here, too, we can derive commutation relations directly. We assume that the rotation axis $\hat{\mathbf{a}}$ lies in the $y - z$ plane and makes an angle φ with the y axis; see Fig. 21.2. A rotation about $\hat{\mathbf{a}}$ by the angle γ can then be described as follows:

First we bring the axis of rotation onto the y axis by a rotation through $-\varphi$ around the x axis. Then we rotate the y axis by an angle γ. Finally, we bring the rotation axis back to its old position. In summary, we have for this rotation the two equivalent representations

$$e^{-i\frac{\gamma \mathbf{j}\cdot\hat{\mathbf{a}}}{\hbar}} = e^{-i\frac{\varphi j_x}{\hbar}} e^{-i\frac{\gamma j_y}{\hbar}} e^{i\frac{\varphi j_x}{\hbar}}. \tag{21.32}$$

Again we assume infinitesimal angles φ and γ. As shown below in an exercise, the latter equation leads directly to the commutation relation

$$\left[j_x, j_y\right] = i\hbar j_z. \tag{21.33}$$

The remaining two relations follow by cyclic permutation.

Also of interest are the commutation relations of scalar and vector operators with the angular momentum. A scalar operator S is defined as an operator whose mean value remains invariant under a rotation, while for a vector operator **V**, the mean value must transform as a vector **v** (i.e. like the position vector). As shown in the exercises, a scalar operator S commutes with the angular momentum

$$[\mathbf{j}, S] = 0. \tag{21.34}$$

For a vector operator **V** (such as the position or the momentum), we obtain the commutation relations[14]:

[14] More on vector operators is found in Appendix L, Vol 2.

$$[j_i, V_k] = i\hbar \sum_l \varepsilon_{ikl} V_l. \tag{21.35}$$

Finally, a remark concerning spin 1/2. We have the commutation relations of angular momentum (see Chap. 16)

$$\left[s_i, s_j\right] = i\hbar \sum_k \varepsilon_{ijk} s_k \tag{21.36}$$

or of the Pauli matrices

$$\left[\sigma_i, \sigma_j\right] = 2i \sum_k \varepsilon_{ijk} \sigma_k. \tag{21.37}$$

The unitary rotation transformation may be determined explicitly (see the exercises); the result reads

$$e^{-i\frac{\gamma}{\hbar}\mathbf{s}\cdot\hat{\mathbf{a}}} = e^{-i\frac{\gamma}{2}\sigma\hat{\mathbf{a}}} = \cos\frac{\gamma}{2} - i\sigma\hat{\mathbf{a}}\sin\frac{\gamma}{2}. \tag{21.38}$$

For a rotation by $\gamma = 2\pi$, it follows that

$$e^{-i\pi\sigma\hat{\mathbf{a}}} = -1. \tag{21.39}$$

Hence, a rotation through 2π does not yield the original system; this is obtained only by a rotation through 4π. One might think that this is another oddity of quantum mechanics, but that is not true. Indeed, it is the case also for certain objects in our visual space, such as a Möbius strip. An ant which is running along a Möbius strip has to cover an angle of 4π to arrive back at its starting point; see Fig. (21.3). The real identity rotation for an object in relation to its environment is obviously not the rotation through 2π, but rather through 4π; this situation is not peculiar to quantum mechanics.

An addendum: The question may arise as to why the identity rotation of a photon, which also can assume only two (polarization) states, is not 4π as for the electron with its two (spin) states. The answer is most easily formulated using the *helicity* h, that is the component of the spin of a quantum object in the direction of its momentum, $h = \mathbf{s}\cdot\mathbf{p}/\left|\mathbf{p}\right|$. Relativistic considerations show that for a quantum object with $m_0 \neq 0$ (nonzero rest mass), there are $2s + 1$ different possibilities $(s, s-1, \ldots, -s)$, while

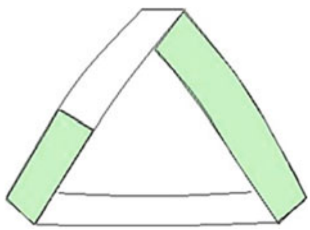

Fig. 21.3 Möbius strip

for $m_0 = 0$ (e.g. a photon), the helicity can assume only the values $h = \pm s$. The spin is responsible for the behavior under a rotation. Since it is $\frac{1}{2}$ for the electron and 1 for the photon, the identity rotation for spin 1 (thus also for a photon with two states) is given by 2π. See also the exercises for Chap. 16.

21.1.5 Special Galilean Transformation

Due to space and time limitations, we consider this case in Appendix L, Vol. 2, and just give the result here. It states that the most general form of a Hamiltonian in three dimensions, compatible with the special Galilean transformation, is given by:

$$H = \frac{1}{2m}\left(\mathbf{p} - \mathbf{f}\left(\mathbf{x}\right)\right)^2 + V\left(\mathbf{x}\right). \tag{21.40}$$

$\mathbf{f}(\mathbf{x})$ can signify e.g. the vector potential $q\mathbf{A}(\mathbf{x})$.

21.2 Discrete Symmetry Transformations

In contrast to the continuous transformations, one cannot deduce the discrete transformations continuously from the unit map. Thus, there are no infinitesimal generators and it is not clear a priori whether the transformations are unitary. The two transformations $\mathcal{T}$ discussed in the following have the property $\mathcal{T}^2 = c$ with $|c| = 1$.[15]

21.2.1 Parity

The parity operator $\mathcal{P}$ reverses the sign of the position, $\mathbf{r} \to -\mathbf{r}$. This process can be represented as a reflection in the plane $z = 0$, followed by a rotation around the z axis by π (for typographic convenience, we use row vectors); see Fig. 21.4:

$$(x, y, z) \underset{\text{reflection}}{\to} (x, y, -z) \underset{\text{rotation by } \pi}{\to} (-x, -y, -z). \tag{21.41}$$

Because rotational invariance is valid in general, one can express parity conservation by the catchy formulation that the *mirror image* of any physical process must be physically possible.

To answer the question of whether the parity operator $\mathcal{P}$ is unitary or anti-unitary, we start with

[15]If $\mathcal{T}^2 = 1$, then the transformation clearly cannot come from a continuous group. For instance, we have for a rotation $(\mathcal{T}_\alpha)^2 = \mathcal{T}_{2\alpha} \neq 1$ for arbitrary angles α.

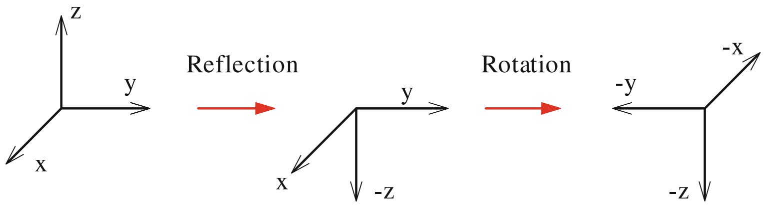

Fig. 21.4 The parity transformation as first a reflection through the $x-y$ plane, followed by a 180° rotation around the z axis

$$\mathcal{P}^2 = 1 \to \mathcal{P} = \mathcal{P}^{-1}. \tag{21.42}$$

We have for a position state $|\mathbf{r}\rangle$:

$$\mathcal{P}\,|\mathbf{r}\rangle = |-\mathbf{r}\rangle \quad \text{or} \quad \langle\mathbf{r}|\,\mathcal{P}^\dagger = \langle-\mathbf{r}|\,, \tag{21.43}$$

and for a general state $|\psi\rangle$:

$$\langle\mathbf{r}|\,\mathcal{P}\,|\psi\rangle = \psi\,(-\mathbf{r}) \quad \text{and} \quad \langle-\mathbf{r}|\,\psi\rangle = \psi\,(-\mathbf{r})\,. \tag{21.44}$$

It follows that

$$\langle-\mathbf{r}| = \langle\mathbf{r}|\,\mathcal{P}. \tag{21.45}$$

The comparison with (21.43) yields finally

$$\langle\mathbf{r}|\,\mathcal{P}^\dagger = \langle\mathbf{r}|\,\mathcal{P} \quad \text{or} \quad \mathcal{P}^\dagger = \mathcal{P} = \mathcal{P}^{-1}. \tag{21.46}$$

Hence, $\mathcal{P}$ is unitary. We have[16]:

$$\mathcal{P}\mathbf{r}\mathcal{P} = -\mathbf{r};\, \mathcal{P}\mathbf{p}\mathcal{P} = -\mathbf{p};\, \mathcal{P}^\dagger\mathcal{P} = 1. \tag{21.47}$$

Because of $\mathcal{P}^2 = 1$, $\mathcal{P}$ has the eigenvalues ± 1. If $[H, \mathcal{P}] = 0$, one can always find common eigenfunctions with well-defined parity:

$$H\,|\varphi_\pm\rangle = E_\pm\,|\varphi_\pm\rangle \;\; ; \mathcal{P}\,|\varphi_\pm\rangle = \pm\,|\varphi_\pm\rangle \tag{21.48}$$

i.e. states with even (+) or odd (−) parity. For e.g. the one-dimensional harmonic oscillator, H depends only on x^2 and thus commutes with $\mathcal{P}$. The eigenstates $|n\rangle$ are therefore simultaneously eigenstates of $\mathcal{P}$ and H; $\mathcal{P}\,|n\rangle = (-1)^n\,|n\rangle$. We have seen other examples of eigenfunctions with well-defined parity, e.g. in discussing

[16] Because of e.g. $\mathcal{P}\mathbf{r}f\,(\mathbf{r}) = -\mathbf{r}\mathcal{P}f\,(\mathbf{r})$; from this, it follows that $\mathcal{P}\mathbf{r} = -\mathbf{r}\mathcal{P}$, and thus $\mathcal{P}\mathbf{r}\mathcal{P} = -\mathbf{r}$.

the infinite potential well in Chap. 5, Vol. 1, or in the angular-momentum eigenstates $|l, m\rangle$ (or spherical harmonics) in Chap. 16.[17]

Finally, it remains to ask whether any interaction is parity conserving (i.e. $[H, \mathcal{P}] = 0$). According to current knowledge, this is the case for the strong and electromagnetic interactions, but not for the weak interaction, which occurs e.g. in nuclear beta decay. Essentially, this can be attributed to the fact that there are polar and axial vectors (see Appendix F, Vol. 1), which are affected differently by the parity operator. A *polar vector*, which is transformed like the position vector, is e.g. the momentum:

$$\mathbf{r} \to -\mathbf{r}; \quad \mathbf{p} \to -\mathbf{p}. \tag{21.49}$$

Axial vectors (= *pseudo vectors*) such as the angular momentum vector transform under $\mathbf{r} \to -\mathbf{r}$ in accordance with[18]:

$$\mathbf{l} \to \mathbf{l}. \tag{21.50}$$

Since the angular momentum $\mathbf{l}$ is an axial vector and $\mathbf{l}^2$ is a scalar, both operators commute with $\mathcal{P}$, and we have for the angular momentum eigenstates $\mathcal{P}\,|l, m\rangle = (-1)^l\,|l, m\rangle$ because of $r \to r, \vartheta \to \pi - \vartheta, \varphi \to \varphi + \pi$. Parity violation may occur in a physical process if axial and polar vectors occur simultaneously, for example $\mathbf{p}^2$ and $\mathbf{r} \cdot \mathbf{l}$. The requirement of invariance under parity reversal therefore implies a restriction of which terms may occur in H.

21.2.2 Time Reversal

Time reversal has nothing to do with time travel into the past and the like; a better name would be *reversal of motion*. Invariance under time reversal means the following: Suppose that a system starts in a parameter space at time T at point A and is at point B at time $T + t$. Then invariance under time reversal states that the ‘reverse’ process is possible, namely that a system starts at time $T + t$ at point B and ends up at time $T + 2t$ at point A (for T, one usually chooses $-t$), cf. Fig. 21.5. That this is not self-evident is shown e.g. by the motion of an electron in a homogeneous magnetic field, which is not invariant under time reversal.[19]

[17] Of course, quite generally every state $\psi(\mathbf{r})$ may be divided into an even and an odd part: $\psi(\mathbf{r}) = \psi_+(\mathbf{r}) + \psi_-(\mathbf{r})$, with $\psi_\pm(\mathbf{r}) = \frac{\psi(\mathbf{r}) \pm \psi(-\mathbf{r})}{2}$.

[18] Because of $\mathbf{l} = \mathbf{r} \times \mathbf{p} \to \mathbf{l} = (-\mathbf{r}) \times (-\mathbf{p}) = \mathbf{r} \times \mathbf{p}$. Generally speaking, the product of two polar vectors is a pseudovector.

[19] When forces are conservative, the orbits are time-reversal invariant. Magnetic fields are not conservative.

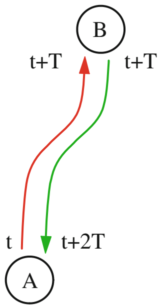

Fig. 21.5 Principle of time reversal. One usually sets $t = -T$

The following plausibility argument suggests that time reversal is an anti-unitary operation[20]: We assume a state with well-defined energy whose time behavior is given by $e^{-i\omega t}$. Under time reversal, this becomes $e^{i\omega t}$, which is obviously equal to the complex conjugate of $e^{-i\omega t}$, $e^{i\omega t} = \left(e^{-i\omega t}\right)^*$. But we know that the complex conjugation is an anti-linear operation, and this should thus also apply to time reversal.

We want to show this fact now in two different ways.

First method: We start from classical mechanics, namely

$$m\frac{\mathrm{d}^2\mathbf{r}(t)}{\mathrm{d}t^2} = \mathbf{F}; \frac{\partial \mathbf{F}}{\partial t} = 0. \tag{21.51}$$

For each solution $\mathbf{r}(t)$, there is a time-reversed solution $\mathbf{r}'(t) = \mathbf{r}(-t)$. We have

$$\mathbf{v}'(t_0) = \left(\frac{\mathrm{d}\mathbf{r}'(t)}{\mathrm{d}t}\right)_{t=t_0} = -\left(\frac{\mathrm{d}\mathbf{r}(-t)}{\mathrm{d}(-t)}\right)_{t=t_0} = -\left(\frac{\mathrm{d}\mathbf{r}(t')}{\mathrm{d}t'}\right)_{t'=-t_0} = -\mathbf{v}(t_0). \tag{21.52}$$

In words: if time is reversed, the position remains the same, but the speed or the momentum changes sign, as is indeed intuitively obvious.

In quantum mechanics, we start from the SEq:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = H(\mathbf{r})\psi(\mathbf{r}, t); \frac{\partial H}{\partial t} = 0; H \in \mathbb{R} \tag{21.53}$$

and obtain (note: H does not depend on t)[21]:

$$i\hbar\frac{\partial\psi(\mathbf{r}, -t)}{\partial(-t)} = H(\mathbf{r})\psi(\mathbf{r}, -t) \rightarrow i\hbar\frac{\partial\psi^*(\mathbf{r}, -t)}{\partial t} = H(\mathbf{r})\psi^*(\mathbf{r}, -t). \tag{21.54}$$

[20]We repeat the remark that an anti-unitary operator B is anti-linear, i.e. $BB^\dagger = B^\dagger B = 1$ and $B\alpha|\varphi\rangle = \alpha^* B|\varphi\rangle$.

[21]The considerations for time-dependent Hamiltonians are more complex and require new concepts (time-ordering operator, etc.); but time reversal is an anti-unitary operator in this case, also.

In other words, with $\psi(\mathbf{r}, t)$, also $\mathcal{T}\psi(\mathbf{r}, t) = \psi'(\mathbf{r}, t) = \psi^*(\mathbf{r}, -t)$ is a solution, where $\mathcal{T}$ is the *time reversal operator*. Since complex conjugation is anti-unitary, this holds also for the the time reversal operator. As in classical mechanics, in quantum mechanics the position remains the same and the momentum changes:

$$\mathbf{r}(t) \to \mathbf{r}(-t)\,;\ \mathbf{p}(t) \to -\mathbf{p}(-t)\,. \tag{21.55}$$

Second method: We write the time evolution of an arbitrary state as $e^{-iHt/\hbar}|\varphi\rangle$ to obtain

$$\mathcal{T}e^{-iHt/\hbar}|\varphi\rangle = e^{iHt/\hbar}\mathcal{T}|\varphi\rangle \to \mathcal{T}e^{-iHt/\hbar}\mathcal{T}^{-1} = e^{iHt/\hbar}. \tag{21.56}$$

For a Hermitian operator B and a unitary or anti-unitary operator U or A, it holds that (see exercises[22]):

$$e^{iUBU^{-1}} = Ue^{iB}U^{-1};\, e^{iABA^{-1}} = Ae^{-iB}A^{-1}. \tag{21.57}$$

If we assume that $\mathcal{T}$ is unitary (i.e. we identify in (21.57) $\mathcal{T} = U$ and $B = -Ht/\hbar$), it follows that

$$\mathcal{T}e^{-iHt/\hbar}\mathcal{T}^{-1} = \begin{cases} e^{iHt/\hbar} \\ e^{-i\mathcal{T}Ht/\hbar\mathcal{T}^{-1}} \end{cases} \text{because of} \begin{matrix} (21.56) \\ (21.57). \end{matrix} \tag{21.58}$$

If we assume, however, that $\mathcal{T}$ is anti-unitary (this means in (21.57) that $\mathcal{T} = A$ and $B = Ht/\hbar$), it follows that

$$\mathcal{T}e^{-iHt/\hbar}\mathcal{T}^{-1} = \begin{cases} e^{iHt/\hbar} \\ e^{i\mathcal{T}Ht/\hbar\mathcal{T}^{-1}} \end{cases} \text{because of} \begin{matrix} (21.56) \\ (21.57). \end{matrix} \tag{21.59}$$

In summary, we obtain

$$\begin{matrix} e^{iHt/\hbar} = e^{-i\mathcal{T}Ht/\hbar\mathcal{T}^{-1}} \\ e^{iHt/\hbar} = e^{i\mathcal{T}Ht/\hbar\mathcal{T}^{-1}} \end{matrix} \ \text{for} \ \begin{matrix} \mathcal{T}\ \text{unitary} \\ \mathcal{T}\ \text{anti-unitary}. \end{matrix} \tag{21.60}$$

For infinitesimal times, we have

$$\begin{matrix} 1 + i\frac{Ht}{\hbar} = 1 - i\mathcal{T}\frac{Ht}{\hbar}\mathcal{T}^{-1} \\ 1 + i\frac{Ht}{\hbar} = 1 + i\mathcal{T}\frac{Ht}{\hbar}\mathcal{T}^{-1} \end{matrix} \to \begin{matrix} H = -\mathcal{T}H\mathcal{T}^{-1} \\ H = \mathcal{T}H\mathcal{T}^{-1} \end{matrix} \ \text{for} \ \begin{matrix} \mathcal{T}\ \text{unitary} \\ \mathcal{T}\ \text{anti-unitary}. \end{matrix} \tag{21.61}$$

Ultimately, from (21.56) and (21.57), it follows that

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[22] In general, every anti-unitary operator A may be represented as the product of a unitary operator U with the operator of complex conjugation K, i.e. $A = UK$. We have $A^{-1} = KU^\dagger$ and $Ki = -iK$.

$$\begin{array}{lcl} \mathcal{T}H + H\mathcal{T} = 0 & \text{for} & \mathcal{T} \text{ unitary} \\ \mathcal{T}H - H\mathcal{T} = 0 & & \mathcal{T} \text{ anti-unitary.} \end{array} \tag{21.62}$$

Now one can argue that the Hamiltonian of a free quantum object contains only $\mathbf{p}^2$, so H must commute with $\mathcal{T}$. Hence, $\mathcal{T}$ is anti-unitary.

The requirement of invariance under time reversal implies a limitation (similar to the case of parity conservation) on which expressions can occur in H. For instance, $\mathbf{p}^2$ and $\mathbf{p}$ or $\mathbf{r} \cdot \mathbf{l}$ cannot occur simultaneously. According to our current knowledge, only the Hamiltonian of the weak interaction is not invariant under time reversal, as indeed it is not invariant under the parity transformation. Another important symmetry is charge conjugation (a better term would be particle-antiparticle exchange). A fundamental theorem of quantum field theory states that any Lorentz-invariant local field theory must be invariant if we simultaneously perform parity inversion, time reversal and charge conjugation (CPT theorem).[23]

Time-reversal invariance leads for certain systems to further-reaching statements. An example is the theorem of Kramers about the degeneracy of eigenstates (Kramers doublets); we sketch it in Appendix M, Vol. 2.

21.3 Exercises

1. Derive the commutation relation (21.26) for position and momentum.
2. Consider the relation between symmetries and conserved quantities by means of the spatial translational invariance of an isolated system of two quantum objects whose interaction depends only on their distance $\mathbf{r}_1 - \mathbf{r}_2$.
3. Let B be a Hermitian operator and U and A a unitary and an anti-unitary operator, resp. Show that:

$$e^{iUBU^{-1}} = Ue^{iB}U^{-1}; e^{iABA^{-1}} = Ae^{-iB}A^{-1}. \tag{21.63}$$

4. Show with the help of the propagator U that eigenvalues of A are conserved, if $[H, A] = 0$.
5. Consider the translation $\mathbf{r}' = \mathbf{r} + \mathbf{a}$ or $T(\mathbf{a})\,\mathbf{r} = \mathbf{r} + \mathbf{a}$. Show that it can be represented by the unitary transformation $U_{T(\mathbf{a})} = \lim_{n\to\infty} \left(1 - \frac{i}{\hbar}\frac{\mathbf{ap}}{n}\right)^n = e^{-\frac{i}{\hbar}\mathbf{ap}}$.

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[23] Only recently, the violation of time-reversal symmetry was detected directly for the first time (CPT invariance, however, remains valid); see J.P. Lee et al., 'Observation of Time-Reversal Violation in the B^0 Meson System', *Phys. Rev. Lett.* 109, 211801 (2012). In this context, entirely new concepts, such as that of the 'time crystal', are emerging; cf. F. Wilczek, 'Quantum Time Crystal', *Phys. Rev. Let.* 109, 160401 (2012). Along with David Gross and David Politzer, Frank Wilczek was awarded the Nobel Prize for Physics in 2004 for the discovery of asymptotic freedom in the theory of strong interactions. See also J. Zhang et al., Observation of a discrete time crystal, *Nature* 543, 217–220 (Mar 2017), and S. Choi et al., Observation of discrete time-crystalline order in a disordered dipolar many-body system, *Nature* 543, 221–225 (Mar 2017).

6. Determine the commutator of P with an arbitrary function of X, without using $P = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}X}$ from the outset (this is to be derived). Use

$$U^{-1}(a)\, X^2 U(a) = U^{-1}(a)\, XU(a)\, U^{-1}(a)\, XU(a) = (X+a)^2\,; \quad (21.64)$$

and analogously

$$U^{-1}(a)\, X^n U(a) = (X+a)^n \quad (21.65)$$

as well as the power-series expansion of the function $f(X) = c_0 + c_1 X + c_2 X^2 + \ldots$.

7. Show that a rotation through the angle φ around the z axis is represented by $e^{-i\alpha l_z}$.

8. Using (21.32),

$$e^{-i\frac{\gamma \mathbf{j}\hat{\mathbf{a}}}{\hbar}} = e^{-i\frac{\varphi j_x}{\hbar}} e^{-i\frac{\gamma j_y}{\hbar}} e^{i\frac{\varphi j_x}{\hbar}}, \quad (21.66)$$

derive the commutation relations for the angular momentum.

9. A scalar operator is defined as an operator whose mean value is invariant under a rotation. Derive the result $[\mathbf{j}, S] = 0$.

10. A vector operator is an operator $\mathbf{V}$ whose mean value transforms like a vector $\mathbf{v}$ under a rotation through an angle γ about an axis $\hat{\mathbf{a}}$, i.e. as

$$\mathbf{v}' = \cos\gamma \cdot \mathbf{v} + \sin\gamma \cdot \left(\hat{\mathbf{a}} \times \mathbf{v}\right) + (1-\cos\gamma)\left(\hat{\mathbf{a}} \times \mathbf{v}\right) \cdot \hat{\mathbf{a}}. \quad (21.67)$$

Derive $[j_i, V_k] = i\hbar \sum_l \varepsilon_{ikl} V_l$.[24]

11. Formulate explicitly the unitary operator $e^{-i\frac{\gamma}{2}\sigma\hat{\mathbf{a}}}$ for spin 1/2; σ is the vector $\sigma = (\sigma_1, \sigma_1, \sigma_1)$ and $\hat{\mathbf{a}}$ a 3-dimensional unit vector.

[24] More on vector operators in Appendix G, Vol. 2.