Symmetry and statistics

5

Two concepts, of fundamental importance to quantum mechanics, will be discussed in this chapter. The first is that of symmetry. Even though the concept of symmetry is familiar in a wide range of natural sciences, the way symmetry constrains the consequences of quantum mechanics is rather subtle and, at the same time, far-reaching. The second is the symmetry property of the states under the exchange of two identical particles. Identical particles with a half-integer spin (fermions) obey the Fermi–Dirac statistics: the wave functions are totally antisymmetric under the exchange of the particles. Identical particles with an integer spin (bosons) are instead subject to the Bose–Einstein statistics. Their wave functions are totally symmetric.

5.1 Symmetries in Nature

Often the equations of a given physical system can be expressed by using different variables, such as position variables referring to alternative coordinate systems. We talk in general about transformations (e.g. canonical transformations in classical mechanics) of variables in describing the same physics.

A concept closely related is that of symmetry. When a transformation of variables leaves the Hamiltonian formally invariant, when expressed in terms of the new variables[1], we talk about a *symmetry*, or an *invariance* of physical laws. In fact, the equations of motion and the physical laws will look identical in two different descriptions of the same system.

[1] Sometimes not only the form but also the value of the Hamiltonian is left invariant, but here we shall allow for both possibilities.

Symmetries abound in Nature, from atoms and crystals to biological bodies.

A possible consequence of symmetry is the conservation law. Well-known examples from classical mechanics are energy conservation related to the homogeneity of time (the Hamiltonian is invariant under time translation), momentum conservation (if the Hamiltonian is invariant under space translations), and angular momentum conservation (if the space and the potential are isotropic). Electric charge conservation can also be related to the invariance under phase transformations of the wave function of charged particles. In many cases, the conservation law in physics is indeed a consequence of some underlying symmetry.

Symmetries can be classified into two types, discrete and continuous, according to whether the relevant transformations are of discrete or continuous type. There is an approximate left–right symmetry to many biological bodies, including human bodies, which is an example of a discrete symmetry. In elementary particle physics we have an analogous symmetry, parity, which is a good symmetry of strong (nuclear), electromagnetic and gravitational interactions, but is broken by weak interactions[2]. CP, T, and CPT are other important examples of (very good) discrete symmetries of Nature.[3]

[2]In more modern terms, those electroweak interactions associated with the exchange of W and Z bosons violate parity.

[3]C is a "charge conjugation" symmetry, i.e. symmetry under the exchange of particle and anti-particle; T is time reversal. See below.

Symmetries related to continuous set of transformations are known as continuous symmetries. The three-dimensional rotational symmetry group $SO(3)$ (characterized by continuous Euler angles) is an example of a continuous symmetry.

Symmetries may also be divided into two categories: space-time (such as those involving invariance under time or space transformations) and internal symmetries (such as isospin, see below).

A great advance in 20th century theoretical physics was the notion that the requirement of symmetry can be strong enough to determine even the form of the interactions (type of forces). For instance, the form of the derivative[4] interactions of a charged particle with electromagnetic fields is determined by the so-called minimal principle, with the following characteristic way in which the vector and scalar potentials enter the Hamiltonian,

$$H = \frac{(\mathbf{p} - \frac{q}{c}\mathbf{A})^2}{2m} + q\,\phi + \ldots\ .$$

[4]For non-derivative interactions, like $g\mu_B\,\mathbf{s}\cdot\mathbf{B}$ in non-relativistic quantum mechanics, the gauge principle quoted below requires that gauge potentials appear only as electric and magnetic fields, $\mathbf{E}$, $\mathbf{B}$.

As is well known (see Chapter 14), such a form is dictated by the requirement that it should be possible to re-parametrize the electron wave function by an arbitrary phase factor, with time- and space-dependent phase $f(\mathbf{r}, t)$, as

$$\psi(\mathbf{r}, t) \to e^{i\,f(\mathbf{r},t)}\,\psi(\mathbf{r}, t).$$

Even the necessity of the existence of the photon, whose wave function transforms inhomogeneously under gauge transformations, follows from such a requirement. Empirical laws such as the Lorentz force are now understood as a consequence of the minimal principle. This strong form of the symmetry requirement—that the system be invariant under transformations depending on space-time, and that the form of the interactions is uniquely determined by such a requirement—is known as the *gauge principle*.

In the case of electromagnetism, the transformation group is simply the phase transformation—the group $U(1)$—which is commutative (Abelian). C. N. Yang and R. L. Mills [Yang and Mills (1954)] and R. Shaw [Shaw (1954)] extended the gauge principle by constructing a model in which the requirement of local transformation is applied to a set of multi-component wave functions, such as an isospin multiplet. The requirement is now that the theory be invariant under the re-labelling (gauge transformations) of the form

$$\psi(\mathbf{r}, t) \to U(\mathbf{r}, t)\,\psi(\mathbf{r}, t)\,,$$

where $U(\mathbf{r}, t)$ is a matrix representing a group element of $SU(2)$, $SU(3)$, $SO(3)$, etc., depending on the model considered, in general a non-commutative (non-Abelian) group. They are known as Yang–Mills theories today.

It is a truly remarkable fact that the standard model of fundamental interactions—quantum chromodynamics for the strong interactions and the Glashow–Weinberg–Salam model of electroweak interactions—are all theories of this sort (with the $SU(3)$ group in the former and the $SU(2) \times U(1)$ group in the latter). The impressive success of the standard model in describing basically *all* of the known fundamental physical phenomena, with the exclusion of gravitational ones, suggests that a very highly nontrivial conceptual unification underlies the working of Nature ('t Hooft).[5]

[5] To be precise, there is a part of the Glashow–Weinberg–Salam model, related to the so-called Higgs particle, which is not entirely determined by gauge principles. Future experiments, such as the Large Hadron Collider (LHC) experiments which has just started operating at CERN, Geneva, are hoped to give some indications whether the model should be extended and if so in which way.

Finally, a symmetry can be realized in two different ways, either manifest or hidden. The former is the usual way a symmetry is realized in Nature, yielding energy degeneracy among the states belonging to a multiplet of states, transformed among each other by the particular symmetry operation under consideration. However, this is not the only way a symmetry can be realized. It is possible that the physical laws and the Hamiltonian are invariant but the ground state is not.

In the example of the left–right symmetry of the human body, an exact symmetry may be realized in three different ways. Each individual is left–right symmetric, with the heart in the center; or, for each left-hearted person there is another individual with the heart on the right, but otherwise with identical characteristics (a parity partner); or finally, the option that everybody has the heart on the left side, even if all the physical and biological laws are symmetric,[6] i.e., might have allowed for a left-hearted as well as right-hearted people (see Figure 5.1). This last option, which Nature seems to have adopted, is known as "spontaneously broken" symmetry. See Subsection 5.2.1.

[6] Of course, this is a blatant simplification for the sake of discussion. Biological systems are not left–right symmetric at the deeper levels also (e.g. DNA).

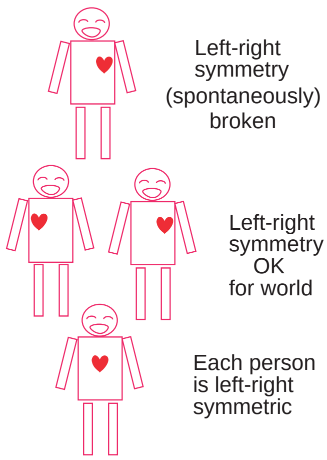

Fig. 5.1 Left–right symmetry might be realized in different ways

A well-known example of spontaneously broken symmetry is the spontaneous magnetization that occurs in certain metals (ferromagnets). Below some critical temperature, all the spins are directed in the same direction, thus "violating" the $SO(3)$ rotational invariance of the Hamiltonian. There are many important applications in solid-state and elementary particle physics of spontaneously broken symmetries.

C. N. Yang, in the concluding talk of the TH 2002 Conference in Paris, characterized the 20th century theoretical physics by three "melodies":[7]

"Symmetry, quantization, and phase factor"

The challenge today is to find out whether we need some new principles or paradigm, in addition to these concepts, to understand Nature at a deeper level, beyond the standard model of fundamental interactions.

[7] For the "phase factor", see Chapters 8 and 14.

5.2 Symmetries in quantum mechanics

The presence of a symmetry in a quantum mechanical system is signaled by the existence of a unitary operator U which commutes with the Hamiltonian:

$$[U, H] = 0 \; . \tag{5.1}$$

As a unitary operator satisfies

$$UU^\dagger = U^\dagger U = \mathbf{1}\ ;$$

eqn (5.1) is equivalent to

$$U^\dagger H U = H\ : \tag{5.2}$$

U is a unitary transformation which leaves the Hamiltonian invariant. We have already seen some examples of such operators:

$$U = e^{i\hat{J}\cdot\omega}$$

describes spatial rotations;

$$U = e^{i\hat{p}\cdot r_0/\hbar}$$

represents spatial translations.

Conservation

One of the possible consequences of a symmetry is the conservation of an associated charge. Suppose that the state $|\psi\rangle$ is an eigenstate of a dynamical quantity represented by a Hermitian operator G, such that

$$U \simeq \mathbf{1} - i\epsilon G + \ldots,$$

i.e. G is a generator of U. From eqn (5.1) and eqn (5.2) it follows that

$$[G, H] = 0. \tag{5.3}$$

By assumption

$$G|\psi(0)\rangle = g|\psi(0)\rangle.$$

The state at time $t > 0$ is given by

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle,$$

so that

$$G|\psi(t)\rangle = Ge^{-iHt/\hbar}|\psi(0)\rangle = e^{-iHt/\hbar}G|\psi(0)\rangle = g|\psi(t)\rangle.$$

The system remains an eigenstate of G during the evolution; the charge g is conserved.

Electric charge conservation is similar. The charge operator Q acts on the particle state as follows:

$$Q|e\rangle = -e|e\rangle; \qquad Q|p\rangle = +e|p\rangle;$$
$$Q|n\rangle = 0; \qquad Q|\pi^+\rangle = +e|\pi^+\rangle,$$

etc., where the kets stand for the state of a single electron, a proton, a neutron, and a pion, respectively. Q commutes with the Hamiltonian including all the known forces (the gravitational, electroweak, and strong forces): this fact guarantees that the total electric charge of a system is conserved. In the non-relativistic approximation adopted in most of this book, charge conservation is a consequence of particle number conservation; vice versa, in the relativistic context where particles can be created or annihilated (only the total energy is conserved), electric charge conservation represents a nontrivial selection rules.

In general, conservation means (see Section 2.4.2)

$$0 = i\hbar \frac{dG}{dt} = i\hbar \frac{\partial G}{\partial t} + [G, H] \tag{5.4}$$

For operators which do not depend explicitly on time, this condition reduces to eqn (5.3). The additional term has a simple meaning in terms of symmetry. Let $G(\boldsymbol{\alpha}, t)$ be a generator (or the associated unitary operator) which depends on some parameter and on t. Equation (5.4) is then equivalent to

$$G(\boldsymbol{\alpha}, t) = e^{-iH(t-t_0)/\hbar} G(\boldsymbol{\alpha}, t_0) e^{iH(t-t_0)/\hbar} ,$$

as can be checked by taking the time derivative. The previous equation means

$$G(\boldsymbol{\alpha}, t)\, e^{-iH(t-t_0)/\hbar} = e^{-iH(t-t_0)/\hbar}\, G(\boldsymbol{\alpha}, t_0)\,. \tag{5.5}$$

In words: G is conserved (is a symmetry) *if the transformation of the evolved state is equal to the evolution of the transformed state*, i.e. if the transformation commutes with dynamical evolution. An example will be given below for Galilei boosts.

Degeneracy

Another possible consequence of a symmetry is the degeneracy of energy levels. Consider a stationary state

$$H|\psi_n\rangle = E_n|\psi_n\rangle,$$

and suppose that there exists an operator G which commutes with H. It follows from $[G, H] = 0$ that

$$H\, G\, |\psi_n\rangle = G\, H\, |\psi_n\rangle = E_n\, G|\psi_n\rangle.$$

There are several possibilities. The state $|\psi_n\rangle$ might not be in the domain of the operator G ($G|\psi_n\rangle \notin \mathcal{H}$); G may annihilate $|\psi_n\rangle$, $G|\psi_n\rangle = 0$; or $|\psi_n\rangle$ may happen to be an eigenstate of G:

$$G|\psi_n\rangle = \text{const.}|\psi_n\rangle.$$

In any of these cases no interesting result follows.

If, however, none of the above cases holds (i.e., $G|\psi_n\rangle \in \mathcal{H}$; $G|\psi_n\rangle \neq 0$; $G|\psi_n\rangle \not\propto |\psi_n\rangle$), then it follows that the level n is degenerate: we can find another energy eigenstate, $G\,|\psi_n\rangle$, with the same energy. By acting upon the state $|\psi_n\rangle$ with the operator G repeatedly one expects to find some degenerate set of states. We have already seen several examples of this sort. For instance, if the Hamiltonian commutes with the angular momentum operators L_i, $i = 1, 2, 3$, that is, it is invariant under three-dimensional rotations, an energy level with a given orbital quantum number L is (at least) $2L + 1$ times degenerate. Such a degeneracy can be seen as the result of nontrivial actions of the operators L_x, L_y on an energy (and L_z) eigenstate $|E, \mathbf{L}^2, L_z\rangle$.

5.2.1 The ground state and symmetry

As stated in Section 5.1 the behavior of the ground state under symmetry transformations is of particular importance. In quantum mechanics, with a finite number of degrees of freedom the ground state is *invariant* under symmetry, and unique. Let us discuss this point informally. In the previous paragraph we have shown that if H commutes with a (unitary) operator U and if $|\psi_0\rangle$ is an eigenstate of H, then also $U|\psi_0\rangle$ is an eigenstate with the same energy. If the ground state is unique, it is therefore necessarily invariant. The uniqueness cannot be just a mathematical statement on self-adjoint operators, as the trivial example of a Hamiltonian multiple of the identity clearly has a non-unique ground state. To be a "bona fide" ground state, $|\psi_0\rangle$ must be *stable*, i.e. if we switch a small perturbation λV, the new ground state $|\lambda\rangle$ must satisfy $|\lambda\rangle \to |\psi_0\rangle$ as $\lambda \to 0$. This cannot be true for a ground state belonging to a degenerate subspace. The example of a two-state system

$$H = \begin{pmatrix} E_0 & \lambda V \\ \lambda V & E_0 \end{pmatrix} \tag{5.6}$$

is general enough: we can always think of a perturbation which acts only on the two "degenerate" states $|\pm\rangle$ out of the Hilbert space. In this case the true ground state (even for an infinitesimal non-diagonal element V) $|\lambda\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$ is *not* a small perturbation of a supposed ground state $|+\rangle$ or $|-\rangle$. In any quantum mechanical system with a finite number of degrees of freedom, tunnel effects give rise to non-diagonal elements connecting different ground states.

It is reassuring that a very general theorem states that for "reasonable" Hamiltonians with the usual kinetic terms and two-body interaction potentials, if a ground state exists at all (i.e. if we have a discrete spectrum), then it is unique. This is a generalization of the non-degeneracy theorem of one-dimensional systems. In fact, the theorem proves more: the ground state function can be chosen to be positive everywhere. The interested reader can find a proof in Vol.4 of the book [Reed and Simon (1980b)]. This means that in physically realistic problems the ground state is indeed unique, and then symmetric.

An apparently harmless assumption in eqn (5.6), the existence of a "small" perturbation which can connect different vacuum states, must be reconsidered with more care in the case of systems with *infinite degrees of freedom*. It is precisely here that the situation can change in going from finite to infinite degrees of freedom, such as solids or quantum field theories. In the case of spontaneous magnetization, an infinite energy is required to flip an infinite number of spins, and therefore no non-diagonal elements arise. The system chooses a ground state in which all spins are directed in one direction, at sufficiently low temperatures (where the energetics wins against the entropy effects in the free energy, $E - T\,S$). The rotational symmetry of the Hamiltonian is violated by the ground state.

In systems with infinite degrees of freedom, a symmetry can thus be realized in two ways: either having a symmetric, unique ground state—in this case, all the excited states will be in various degenerate multiplets, and symmetry is realized in the standard, "manifest" way—or by a ground state which is not symmetric. In the latter case one talks about "spontaneously broken symmetry", even though symmetry is not really broken. In particular, if this second option is realized in a system with a *continuous symmetry*, the system necessarily develops some excitations of zero energy (Nambu–Goldstone excitations).[8]

[8] This is known as the Nambu–Goldstone theorem. See [Nambu (1960), Nambu and Jona-Lasinio (1961), Goldstone, Salam and Weinberg (1962), Strocchi (1985)]. There are many systems in Nature in which a symmetry is realized in the Nambu–Goldstone mode. One of the most remarkable examples in elementary particle physics is the light π mesons, which are best understood as approximate Nambu-Golstone particles, associated with a "hidden" $SU(2)$ symmetry.

5.2.2 Parity ($\mathcal{P}$)

Parity is one of the approximate symmetries of Nature. It is a discrete symmetry, under the spatial reflection

$$\mathbf{r} \to -\mathbf{r}\,.$$

The wave function undergoes a transformation

$$\mathcal{P}\psi(\mathbf{r}) = \psi(-\mathbf{r})$$

while the operators transform as

$$\mathcal{P}\,O(\mathbf{r},\mathbf{p})\,\mathcal{P}^{-1} = O(-\mathbf{r},-\mathbf{p}).$$

If the Hamiltonian is invariant under parity,

$$\mathcal{P}H\mathcal{P}^{-1} = H,$$

or $\mathcal{P}H = H\mathcal{P}$, then parity is conserved. $\mathcal{P}$ is a symmetry operator. As $\mathcal{P}$ commutes with H, the stationary states *can* be chosen to be eigenstates of $\mathcal{P}$ also. The eigenvalues of the latter are limited to be ± 1, as obviously

$$\mathcal{P}^2 = \mathbf{1}\,.$$

The stationary states are then classified into parity-even states

$$\mathcal{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}) = +\psi(\mathbf{r})$$

and -odd states

$$\mathcal{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}) = -\psi(\mathbf{r}).$$

Parity is a good quantum number when the potential is spherically symmetric, $V(\mathbf{r}) = V(r)$. In such a case the angular momentum is also conserved and a state with definite angular momentum will have a definite parity. For instance, in the simple one-particle system (or two-particle system reduced to a one-particle problem for the relative motions), the wave function $R(r)Y_{\ell,m}(\theta,\phi)$ is even or odd according to

$$\mathcal{P} = (-)^{\ell}. \tag{5.7}$$

Such a relation, however, should not obscure the fact that these two symmetries (invariance under three-dimensional rotations and space reflections) are in principle independent concepts. For instance a reflection-invariant potential

$$V(-\mathbf{r}) = V(\mathbf{r}),$$

(such as $V(x^2+2y^2+7z^2)$) is not necessarily spherically symmetric. Vice versa, there are interactions which are invariant under space rotations but not under parity, such as

$$V = g\,\mathbf{r}\cdot\mathbf{s},$$

where $\mathbf{s}$ is the spin operator. Within the context of elementary particle physics, the so-called weak interactions are known to violate parity.

Another example which shows that the relation between parity and angular momentum conservation is not always as simple as eqn (5.7) is a system of more than one particle, which do not interact but are all moving under a common, spherically symmetric potential. (In a very crude approximation an atomic system looks like this.)

The wave function is a product of the wave function of the individual particles, each with a definite angular momentum ℓ_i. The total angular momentum L could take one of the possible values appearing in the decomposition

$$\ell_1 \otimes \ell_2 \otimes \ell_3 \cdots = \ell_1 + \ell_2 + \ldots \ell_N \oplus \ell_1 + \ell_2 + \ldots \ell_N - 1 \oplus \ldots,$$

while parity is simply

$$\mathcal{P} = \prod (-)^{\ell_i}.$$

There is no simple relation between L and $\mathcal{P}$.

Intrinsic parity

An important empirical fact is that each elementary particle carries a definite, intrinsic parity, besides the parity due to the orbital motion. It is a little analogous to the spin of each particle, which is unrelated to its orbital motion. Some of the known elementary particles carry the intrinsic parity

$$\mathcal{P}|\pi\rangle = -|\pi\rangle; \quad \mathcal{P}|K\rangle = -|K\rangle; \quad \mathcal{P}|p\rangle = +|p\rangle;$$

$$\mathcal{P}|n\rangle = +|n\rangle; \quad \mathcal{P}|\bar{p}\rangle = -|\bar{p}\rangle;$$

etc. If a given interaction respects parity, the total parity (the product of the parity of the orbital wave functions and of the intrinsic parities of all particles involved) is conserved in any process.

The spin operator transforms under parity as follows

$$\mathcal{P}\,\mathbf{s}\,\mathcal{P}^{-1} = \mathbf{s},$$

i.e., as an orbital angular momentum. The ordinary momentum operator $\mathbf{p}$ transforms like the position operator:

$$\mathcal{P}\,\mathbf{p}\,\mathcal{P}^{-1} = -\mathbf{p}.$$

In general, the operators can be classified according to their behavior under parity. The momentum, position, vector potential, etc. are *vectors*; the angular momentum operators (including spin operators) are *axial vectors*. Scalar quantities (invariant under rotations) which change sign under parity are known as *pseudo-scalars*, to be compared to ordinary scalars, which are invariant under parity.

Parity, in spite of its natural definition, is not an exact symmetry of Nature: it is only an approximate symmetry. As already anticipated above, weak interactions (in more modern terminology, the exchange of W or Z bosons) violate parity. This is a good reminder of the fact that symmetry is, in general, a property of a given type of interaction (force) rather than being some absolute principle. To the best of our knowledge today, the electromagnetic, strong, and gravitational interactions respect parity.

The explicit form of the parity operator $\mathcal{P}$

It could be of some interest to construct the parity operator in an explicit form, in terms of the operators q and p. Let us first consider a one-dimensional system. For *any* such system, consider the operator

$$A = \frac{p^2}{2} + \frac{q^2}{2} - \frac{\hbar}{2}\,.$$

It is, apart from an additive constant, just the Hamiltonian of a harmonic oscillator with $m = \omega = 1$. By using the known solution of the Heisenberg equation for such an oscillator, see eqns (7.60) and (7.61), we know that after half the period of the evolution q and p change sign:

$$e^{i\frac{1}{\hbar}A\pi}\,p\,e^{-i\frac{1}{\hbar}A\pi} = -p\,, \quad e^{i\frac{1}{\hbar}A\pi}\,q\,e^{-i\frac{1}{\hbar}A\pi} = -q\,. \tag{5.8}$$

But actually the derivation of eqn (5.8) depends *only* on the canonical commutators between q and p, and hence holds in any system. The parity operator is thus given, *in any system*, by

$$\boxed{\mathcal{P} = \exp\left(\frac{i}{\hbar}A\pi\right) = \exp\left[\frac{i}{\hbar}\left(\frac{p^2}{2} + \frac{q^2}{2} - \frac{\hbar}{2}\right)\pi\right]\,.} \tag{5.9}$$

This result might be puzzling at first sight: how can one see that operator (5.9) commutes with a Hamiltonian which is even under parity? Also, what is special about the frequency $\omega = 1$ or $m = 1$?

To clarify these points, first observe that the operator A is certainly self-adjoint and admits a complete basis of orthonormal eigenvectors: the standard eigenstates of a harmonic oscillator. On these states $\mathcal{P}$ acts as follows

$$\mathcal{P}|n\rangle = e^{in\pi}|n\rangle = (-1)^n|n\rangle\,,$$

so $\mathcal{P}$ *is* in fact the parity operator. As any state of any system can be expanded in terms of $\{|n\rangle\}$,

$$\Psi(x,t) = \sum_n c_n(t)\varphi_n(x)\,, \qquad \varphi_n(x) \equiv \langle x|n\rangle\,, \tag{5.10}$$

it follows that $\mathcal{P}$ always acts as the parity operator.

Let us separate all the even and odd eigenstates of A. Any operator in any system has the form of a matrix in such a basis (ee for even–even, etc.),

$$O = \begin{pmatrix} O_{ee} & O_{eo} \\ O_{oe} & O_{oo} \end{pmatrix}\;;$$

in particular, the operator $\mathcal{P}$ itself will have the form

$$\mathcal{P} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\;. \tag{5.11}$$

The point is that this form remains invariant under any unitary transformations (Chapter 7) which leaves the block diagonal form invariant:

$$S = \begin{pmatrix} S_{ee} & 0 \\ 0 & S_{oo} \end{pmatrix} \qquad \Rightarrow \qquad S\,\mathcal{P}\,S^\dagger = \mathcal{P} \tag{5.12}$$

i.e., under transformations under which even and odd states do not get mixed. Now if H is even, clearly the evolution operator is of eqn (5.12) type, and thus commutes with parity.

What if we change the frequency or mass in the definition of the operator A? Namely we now consider the operator

$$\mathcal{P}_\omega = \exp\left[\frac{i}{\hbar}\left(\frac{p^2}{2m} + m\,\omega^2\frac{q^2}{2} - \frac{\hbar\omega}{2}\right)\frac{\pi}{\omega}\right] \equiv \exp\left(\frac{i\pi A_\omega}{\omega\,\hbar}\right)\,.$$

Actually, nothing whatsoever changes. In fact, the eigenstates of the new operator A_ω, $|n_\omega\rangle$, can be obtained by the scale transformation D:

$$D:\,p \to \frac{p}{\sqrt{m\omega}}\,, \qquad D:\,q \to q\sqrt{m\omega}\,; \qquad |n_\omega\rangle = D\,|n\rangle$$

D obviously has the structure of eqn (5.12). It is evident that in the basis $|n_\omega\rangle$ the operator $\mathcal{P}_\omega$ has the form of eqn (5.11), but the point is that it also has the same form in the basis $|n\rangle$; vice versa, the original parity operator $\mathcal{P}$ has the same form in the basis $|n_\omega\rangle$. Indeed, from eqn (5.12) it follows that

$$\langle n_\omega|\mathcal{P}|k_\omega\rangle = \langle n|D^\dagger \mathcal{P} D|k\rangle = \langle n|\mathcal{P}|k\rangle\,.$$

In other words, in spite of appearances, operators $\mathcal{P}_\omega$ and $\mathcal{P}$ are one and the same operator!

The generalization to higher-dimensional systems is straightforward; it suffices to make a product of operators (5.9) for each Cartesian coordinate. Obviously the result of this subsection refers only to "orbital" parity, not to the intrinsic parity carried by elementary particles.

5.2.3 Time reversal

Another important example of a discrete symmetry is time reversal, T. In classical mechanics, Newton's equation for a particle moving under the influence of a conservative force,

$$m\,\ddot{\mathbf{r}} = -\nabla V\,,$$

is invariant under time reversal, $t \to -t$. This means that if a motion from $(\mathbf{r}_1, t_1)$ to $(\mathbf{r}_2, t_2)$ is possible, another motion from $(\mathbf{r}_2, -t_2)$ to $(\mathbf{r}_1, -t_1)$, tracing the same trajectory in the opposite direction, and with $\mathbf{r}(-t) = \mathbf{r}(t)$; $\mathbf{p}(-t) = -\mathbf{p}(t)$, is also a possible solution of the equation of motion. Vice versa, if the force included friction, proportional to velocity, clearly the time-reversed motion would be an impossible motion.

In quantum mechanics, the dynamics is described by the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = H\psi(\mathbf{r}, t). \tag{5.13}$$

For example,

$$H = -\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})$$

for a particle moving in a three-dimensional potential $V(\mathbf{r})$. The transformation $t \to t' = -t$ gives an equation

$$-i\hbar\frac{\partial}{\partial t'}\psi(\mathbf{r}, -t') = H\psi(\mathbf{r}, -t'),$$

in general having a *different* form from the original Schrödinger equation. It might seem to be hardly possible that the quantum mechanical laws be invariant under the time reversal.

Actually there is no reason that the wave function of the time-reversed motion should be given just by $\psi(\mathbf{r}, -t)$. Indeed, upon taking the complex conjugate of the preceding equation, one finds an equation

$$i\hbar\frac{\partial}{\partial t'}\psi^*(\mathbf{r}, -t') = H^*\psi^*(\mathbf{r}, -t'),$$

which more closely resembles the original equation (5.13). The original Schrödinger equation would then be recovered if an (anti-)unitary operator O exists such that

$$O\,H^*\,O^{-1} = H.$$

In such a case, the wave function for the reversed motion can be taken to be

$$\tilde{\psi}(\mathbf{r}, t) = O\psi^*(\mathbf{r}, -t)\,: \tag{5.14}$$

the new wave function $\tilde{\psi}(\mathbf{r}, t)$ satisfies a Schrödinger equation identical to the original one. The time-reversal motion is indeed a possible time evolution in quantum mechanics, in this case.

An operator O such that for any state vectors ψ, ϕ, the relation

$$\langle O\phi|O\psi\rangle = \langle\psi|\phi\rangle$$

holds (see eqn (5.14)) is known as an *anti-unitary* operator. In contrast, for an ordinary unitary operator U the relation

$$\langle U\phi|U\psi\rangle = \langle\phi|\psi\rangle$$

holds for any pair of state vectors. It is evident that under either unitary or anti-unitary transformations, all physical predictions of the theory remain the same. That these are the only possibilities to realize a symmetry in quantum mechanics is known as

Theorem 5.1. (Wigner's theorem) *Every symmetry transformation in quantum mechanics is realized either by a unitary or by an anti-unitary transformation.*

Again, it should be noted that time-reversal symmetry (T) is a property of the particular kind of interaction, rather than being an absolute law of Nature. Although at a macroscopic level it is easy to think of systems which are not conservative, and hence not invariant under T, it is known that at the level of fundamental interactions, T is an extremely good approximate symmetry. As far as we know, gravitational, electromagnetic, and strong interactions respect T, while a small subset of weak interactions due to the exchange of W bosons violate it. (Actually these are more directly connected to the violation of so-called CP symmetry. However, for any theory described by a local Hermitian Hamiltonian the product CPT is a good symmetry—a result known as the CPT theorem. If CPT is an exact symmetry of Nature, then CP violation implies T violation and vice versa.) For a discussion on CP violation in the K^0-$\bar{K}^0$ system, see Supplement Section 22.1.

The great mystery of time-reversal symmetry is that, in spite of the fact that T is almost exactly conserved in fundamental interactions, it is grossly violated in the macroscopic world: it suffices to remember that the second law of thermodynamics—the law of the entropy increase—implies a preferential arrow of time, from the past to the future. It is an extravagant idea to think that the arrow of time is in some way caused by the very tiny amount of T-violating interactions, which are certainly irrelevant to the vast majority of electromagnetic, chemical, and gravitational processes governing the macroscopic world. It is possible that the arrow of time is somehow related to the expansion of the universe. We know that the concept of uniform time evolution itself would have to be modified somehow at the time of the big bang.

5.2.4 The Galilean transformation

Consider two systems of reference, K' and K, moving with respect to each other with a constant relative velocity, $\mathbf{V}$,

$$\mathbf{r} = \mathbf{r}' + \mathbf{V}t \; . \tag{5.15}$$

How is the wave function $\psi'(\mathbf{r}', t)$ in one system related to $\psi(\mathbf{r}, t)$ in the other? To find the transformation law, one may proceed as follows: a plane wave in system K is also seen as a plane wave in system K'. Once we understand how these transform into each other, it must be possible to find out how a generic wave function transforms, as the latter can be composed of plane waves.

The plane waves in the two systems are

$$\psi(\mathbf{r}, t) = \exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - Et)\right] \; ; \tag{5.16}$$

$$\psi(\mathbf{r}', t) = \exp\left[\frac{i}{\hbar}(\mathbf{p}'\cdot\mathbf{r}' - E't)\right] \; . \tag{5.17}$$

From classical mechanics we know that the momentum and energy in the two systems are related as follows

$$\mathbf{p} = \mathbf{p}' + m\mathbf{V} \qquad E = E' + \mathbf{V}\cdot\mathbf{p}' + \frac{1}{2}m\mathbf{V}^2 \; . \tag{5.18}$$

By substituting eqns (5.15) and (5.18) into eqn (5.16) one finds that

$$e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r}-Et)} = e^{\frac{i}{\hbar}(\mathbf{p}'\cdot\mathbf{r}'-E't)} e^{\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}'+\frac{1}{2}m\mathbf{V}^2 t)} \; .$$

In the second phase factor on the right-hand side there are no references left to the particular plane wave considered, so the relation should be valid for a generic wave function which can be constructed as a linear combination of the latter:

$$\psi'(\mathbf{r}', t) = e^{-\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}'+\frac{1}{2}m\mathbf{V}^2 t)}\psi(\mathbf{r}, t) \; . \tag{5.19}$$

In eqn (5.19) it is understood that $\mathbf{r}$ is expressed in terms of $\mathbf{r}'$ and t through eqn (5.15).

In the case of a system of many particles, the phase of eqn (5.19) sums up to give

$$m\mathbf{V}\cdot\mathbf{r}' + \frac{1}{2}m\mathbf{V}^2 t \to \sum_i m_i\mathbf{V}\cdot\mathbf{r}_i' + \frac{1}{2}m_i\mathbf{V}^2 t = M_{tot}\mathbf{V}\cdot\mathbf{R}_{CM} + \frac{1}{2}M_{tot}\mathbf{V}^2 t \; .$$

It is thus the center-of-mass coordinate, and the total mass plays the role of the free particle.

Transformation law (5.19) is generally valid, and does not in general imply *invariance* of the dynamical law under Galilean transformations. Of course, we expect that it is the case for the free particles. Let us check that the Schrödinger equation for a free particle indeed remains invariant. The wave function ψ satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2}\psi \; . \tag{5.20}$$

In evaluating the partial derivative of ψ' with respect to time, we must keep in mind that the right-hand side of eqn (5.19) depend on time both explicitly and implicitly through the relation $\mathbf{r} = \mathbf{r}' + \mathbf{V}t$. Thus

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi' &= \left(\frac{1}{2}mV^2\psi + i\hbar\frac{\partial}{\partial t}\psi + i\hbar\mathbf{V}\cdot\frac{\partial}{\partial \mathbf{r}}\psi\right) e^{-\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}' + \frac{1}{2}m\mathbf{V}^2 t)} \\ &= \left(\frac{1}{2}mV^2\psi - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2}\psi + i\hbar\mathbf{V}\cdot\frac{\partial}{\partial \mathbf{r}}\psi\right) e^{-\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}' + \frac{1}{2}m\mathbf{V}^2 t)} \\ &= \left(\frac{1}{2}mV^2\psi - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}'^2}\psi + i\hbar\mathbf{V}\cdot\frac{\partial}{\partial \mathbf{r}'}\psi\right) e^{-\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}' + \frac{1}{2}m\mathbf{V}^2 t)} \ . \end{aligned}$$

In the last step use was made of the fact that $\partial/\partial\mathbf{r} = \partial/\partial\mathbf{r}'$.

On the other hand one can evaluate the kinetic term directly for ψ':

$$\begin{aligned} &-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}'^2}\psi' = \\ &-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial \mathbf{r}'^2}\psi - 2i\frac{1}{\hbar}m\mathbf{V}\cdot\frac{\partial}{\partial \mathbf{r}'}\psi - \frac{m^2}{\hbar^2}\mathbf{V}^2\right] e^{-\frac{i}{\hbar}(m\mathbf{V}\cdot\mathbf{r}' + \frac{1}{2}m\mathbf{V}^2 t)} \ . \end{aligned}$$

Thus one indeed has

$$i\hbar\frac{\partial}{\partial t}\psi' = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}'^2}\psi' \ ;$$

that is, the evolution equation in system K' is identical to that in system K.

The transformation

$$\mathbf{r} \to \mathbf{r} + \mathbf{V}t \ ; \quad \mathbf{p} \to \mathbf{p} + m\mathbf{V}$$

is generated by the unitary operator

$$U = \exp\left[\frac{i}{\hbar}\,\mathbf{V}(\mathbf{p}t - m\mathbf{r})\right] \ .$$

This can be easily checked by considering infinitesimal $\mathbf{V}$. The generator of the transformation is

$$G = \mathbf{p}t - m\mathbf{r}$$

This operator is time dependent. We have, for a Hamiltonian $\mathbf{p}^2/2m$,

$$i\hbar\frac{\partial G}{\partial t} + [G, H] = i\hbar\mathbf{p} + \left[\mathbf{p}t - m\mathbf{r}, \frac{\mathbf{p}^2}{2m}\right] = 0\,,$$

in agreement with eqn (5.4).

We leave it as an exercise to prove the converse: if the system is invariant under Galileo transformation, then the dependence of the center-of-mass coordinates in the Hamiltonian is $\mathbf{P}^2/2M$, where $\mathbf{P}$ is the total momentum and M the total mass.

5.2.5 The Wigner–Eckart theorem

A very powerful theorem that illustrates well the use of the symmetry argument is due to Wigner and Eckart. Consider first a spinless particle, described by a wave function of the form $\psi_0(r)$, a function of the radial coordinate only. Clearly it is invariant under three-dimensional rotations: it represents a state with $\ell = 0$. Now consider instead a state

$$\psi_i(r) = \text{const.}\, \mathbf{r}_i\, \psi_0(r),$$

obtained from the first by applying the position operator. This is a state with $\ell = 1$, being proportional to some combination of $Y_{1,m}(\theta, \phi)$, $m = 1, 0, -1$. The value of the angular momentum ($\ell = 1$) does not depend on the details of the nature of the operator $\mathbf{r}_i$; the same can be said of the state

$$\psi_i^{'}(r) = \text{const.}\, \mathbf{p}_i\, \psi_0(r) \;.$$

Under a three-dimensional rotation a generic operator O transforms as follows:

$$O \to e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, O\, e^{-i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}} \;,$$

while a state transforms like this:

$$|\;\rangle \to e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}|\;\rangle \;.$$

We have already seen that certain states—those with definite angular momentum (J, M)—transform in a simple, universal way (see eqn (4.38)):

$$|J, M\rangle \to \sum_{M'} D^J_{M',M}(\boldsymbol{\omega})\, |J, M'\rangle \;.$$

The rotation matrix for spin J is known once and for all: it depend only on J and does not depend on any other attributes of the particular system considered.

Analogously, certain operators transform in simple manner. Operators such as $\mathbf{r}^2$, $\mathbf{p}^2$, $U(r)$ are all *scalars*: they are invariant under rotations; others, such as $\mathbf{r}$, $\mathbf{p}$, e $\mathbf{J}$, are *vectors*. Quantities transforming as products of vectors are generally known as *tensors*.

To study the properties of transformations of operators under rotations, it is convenient to reorganize the components of tensors so as to make them proportional to the components of some spherical harmonics—they are known as *spherical tensors*—rather than using Cartesian components. For instance, a spherical tensor of rank 1 is equivalent to a vector (A_x, A_y, A_z), but its components are called $T_{1,m}$, $m = 1, 0, -1$, where

$$T_{1,1} = -\frac{A_x + iA_y}{\sqrt{2}}; \quad T_{1,0} = A_z; \quad T_{1,-1} = \frac{A_x - iA_y}{\sqrt{2}} \;. \tag{5.21}$$

In the particular case of the position vector $\mathbf{r}$, the corresponding spherical tensor components are:

$$T_{1,1} = -\frac{x + iy}{\sqrt{2}}; \quad T_{1,0} = z; \quad T_{1,-1} = \frac{x - iy}{\sqrt{2}} \;. \tag{5.22}$$

[9]In the convention used by Landau and Lifshitz eqns (5.21) and (5.22) are multiplied by a factor i.

They are proportional to the spherical harmonics[9] $Y_{1,1}, Y_{1,0}$, e $Y_{1,-1}$. (see eqn (4.20).)

The inverse of eqn (5.22) is

$$A_x = -\frac{T_{1.1} - T_{1,-1}}{\sqrt{2}} \; ; \quad A_y = -i\,\frac{T_{1,1} + T_{1,-1}}{\sqrt{2}} \; ; \quad A_z = T_{1,0} \; .$$

The components of a spherical tensor of rank 2 (of "spin 2") are related to those in Cartesian components as follows:

$$\begin{aligned} T_{2,0} &= -\sqrt{\frac{1}{6}}(A_{xx} + A_{yy} - 2A_{zz}) \; ; \\ T_{2,\pm1} &= \mp(A_{xz} \pm iA_{yz}) \; ; \\ T_{2,\pm2} &= \frac{1}{2}(A_{xx} - A_{yy} \pm 2iA_{xy}) \; . \end{aligned}$$

By construction the spherical tensor of "spin" p with $2p+1$ components transform as follows:

$${T_q}^p \Rightarrow e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, {T_q}^p\, e^{-i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}} = \sum_{q'} {D^p}_{q'\,q} T^p_{q'} \; .$$

This means that the action of ${T_q}^p$ on the state $|j, m; n\rangle$ produces a state

$${T_q}^p\, |j, m; n\rangle \; ,$$

which transforms exactly as the direct product of two angular momentum eigenstates

$$|p, q\rangle \otimes |j, m\rangle \; ,$$

i.e.

$$\begin{aligned} {T_q}^p\, |j, m; n\rangle \Rightarrow e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, {T_q}^p\; |j, m; n\rangle &= e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, {T_q}^p\, e^{-i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, e^{i\boldsymbol{\omega}\cdot\hat{\mathbf{J}}}\, |j, m; n\rangle \\ &= \sum_{q',m'} {D^p}_{q'\,q}\, D^j_{m'\,m}\, T^p_{q'}\, |j, m'; n\rangle \; . \end{aligned}$$

As a consequence, one has the following theorem:

Theorem 5.2. (The Wigner–Eckart theorem) *The matrix element*

$$\langle J, M; n'|{T_q}^p|j, m; n\rangle \; ,$$

where n, n' stand for all other quantum numbers (the radial quantum number, type of particle, etc.) are proportional to the Clebsch–Gordan coefficients:

$$\langle J, M; n'|{T_q}^p|j, m; n\rangle = \langle p, j; J, M|p, q, j, m\rangle\langle J, n'\|\mathbf{T}^p\|j, n\rangle \; . \tag{5.23}$$

The proportionality constant, indicated by $\langle J, n'\|\mathbf{T}^p\|j, n\rangle$, called the *reduced matrix element*, depends only on the absolute magnitude of the angular momenta as well as other quantum numbers, but not on the azimuthal quantum numbers. All the dependence on the latter is in the universal Clebsch–Gordan coefficients. Equation (5.23) provides many nontrivial relations among those matrix elements which differ only in the azimuthal quantum numbers M, q, m. In particular, it leads to a set of *selection rules*: the only non-vanishing matrix elements are those with nonzero Clebsch–Gordan coefficients. We talk about *allowed transition*, a terminology borrowed from the analysis of electromagnetic transitions (see Section 9.5).

Let us list some examples, which the reader can verify as an exercise:

1. *Scalar*, $p = 0$. Only the transitions
$$j = J \quad m = M$$
are allowed.
2. *Vector*, $p = 1$. The allowed transitions are
$$|J - j| = \pm 1, 0 \quad ((J = 0) - (j = 0) \text{ forbidden}) \; ; \quad M = m + q \; .$$

5.3 Identical particles: Bose–Einstein and Fermi–Dirac statistics

Closely related to the general concept of symmetry discussed in the preceding section is that of a *symmetry under exchange of identical particles*. Nature abounds with systems made of more than one particle of the same kind; it suffices to think of an atom (with many electrons), a metal (with many atoms of the same species and with many electrons), and in fact, any constituent of the universe.

In quantum mechanics, the wave function of such systems turns out to obey precise properties under the exchange of identical particles: they must be either totally symmetric (for particles with integer spins, known as *bosons*) or totally antisymmetric (for particles with half-integer spins, known as *fermions*). The wave functions are said to obey *Bose–Einstein* (BE) statistics or *Fermi–Dirac* (FD) statistics, respectively.

The restrictions imposed by BE or FD statistics bring about far-reaching and profound consequences in all applications of quantum mechanics, from atoms to macroscopic systems.

Note that by definition two identical particles cannot be distinguished by their intrinsic properties, such as mass, charge, spin. From this point of view, there is no difference between classical and quantum mechanics. What makes particles distinguishable in all cases in classical mechanics is the existence of a definite trajectory (history) for each particle. This allows the particles to be labeled in a convenient way at any reference time, e.g., by the positions they occupy at that precise moment; each particle will maintain its identity during the subsequent time evolution, however complicated it might be.

In quantum mechanics the situation is very different. Owing to the uncertainty relations, there is no precisely defined trajectory for each particle, and the physical state of a system composed, for example, of two identical particles is simply described by a wave function with two sets of arguments,

$$\psi(\xi_1, \xi_2), \qquad \xi \equiv \{\mathbf{r}, \sigma\}, \quad \sigma = s, s-1, \ldots, -s,$$

where σ stands for the third component of the spin. The exchange of the two particles gives rise to the state

$$\psi(\xi_2, \xi_1),$$

which, owing to the identity of the two particles, must represent the same quantum state as $\psi(q_1, q_2)$. According to the principles of quantum mechanics, this implies that

$$\psi(\xi_2, \xi_1) = e^{i\alpha}\, \psi(\xi_1, \xi_2), \tag{5.24}$$

where α is some phase. By repeating the exchange of the two identical particles twice, one must get back to the original wave function, so that

$$e^{2i\alpha} = 1 \ . \tag{5.25}$$

It follows then that

$$e^{i\alpha} = \pm 1, \tag{5.26}$$

in eqn (5.24). This argument can be generalized to a system consisting of N identical particles. The wave function must be either symmetric or antisymmetric under the exchange of any two identical particles.

Which sign should we choose? As already anticipated, in Nature all particles with integer spins (bosons) are described by wave functions which are totally symmetric, while the wave functions of identical particles with half-integer spins (fermions) are totally antisymmetric, i.e., they change sign under the exchange of any pair of particles. We say that bosons obey **Bose–Einstein statistics**, while fermions satisfy **Fermi–Dirac statistics.** Or simply BE or FD statistics, respectively.

For instance, the wave function of two identical spin-$\frac{1}{2}$ fermions (two electrons, two protons, etc.) has the form

$$\Psi = \frac{1}{\sqrt{2}}(\psi(\xi_1, \xi_2) - \psi(\xi_2, \xi_1)) = \frac{1}{\sqrt{2}}(\psi(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) - \psi(\mathbf{r}_2, \sigma_2; \mathbf{r}_1, \sigma_1)), \tag{5.27}$$

where $\sigma_{1,2} = \uparrow, \downarrow$.

In the general case, the identity of the particles is formally expressed by the statement that *every* observable $A(\xi_1, \ldots, \xi_n)$ *is symmetric* under any permutation of the single particle variables. We note that this is a restriction on the number of physically acceptable observables; as an example, for two particles the operator $\mathbf{r}_1$ is not an observable, while $\mathbf{r}_1 + \mathbf{r}_2$ is. Following our discussion in Chapter 2 we see that in this case not every self adjoint operator corresponds to an observable.

Remarks

(i) Within non-relativistic quantum mechanics, the correlation between the spin of the particle and the statistics such a particle obeys (called the spin–statistics relation) is an empirical law. However, it is one of the fundamental results of relativistic quantum mechanics that the spin–statistics correlation follows from the principles of special relativity, of quantum mechanics, and of the positivity of energy. See Section 17.2.3.

(ii) The rule that *all* particles with half-integer spin (or integer spin) obey Fermi–Dirac (vis à vis Bose–Einstein) statistics, is internally consistent. Consider the nucleon (a collective name for the two constituent particles of atomic nuclei—the proton and neutron) which has spin $\frac{1}{2}$ and is therefore a fermion. Two identical nuclei, composed of n nucleons, would have integer or half-integer spins, according to whether n is even or odd, respectively. But as the exchange of the two identical nuclei is equivalent to the exchange of n pairs of nucleons, it follows that the wave function of the former is either symmetric (n even) or antisymmetric (n odd).

(iii) From a formal point of view, the wave function of N identical particles can be regarded as a representation of the permutation groups of N objects. The (standard) assumption that the wave function for definite positions and for definite spin components is a well-defined complex number, apart from an arbitrary phase, corresponds to the hypothesis that the wave functions form a one-dimensional representation of the permutation group. Under this condition result (5.25), and hence eqn (5.26), follows inevitably.[10]

(iv) The above consideration hinges upon one more aspect of the physical world: the topological structure of the configuration space. In fact, in order to discuss the meaning of the exchange of the two particles clearly, it is necessary to place the two particles at two distinct points. Say one of the particles is at $\{0\}$ and the other particle is at a generic point $\{x\}$. Clearly the repeated exchange of the two particles is equivalent to the particle at $\{x\}$ going around the point $\{0\}$ and coming back to the original point. The three-dimensional space minus a point, $\mathbf{R}^3/\{0\}$, is simply - connected,[11]

$$\pi_1(\mathbf{R}^3/\{0\}) = \mathbb{1}\,.$$

Therefore property (5.25) is necessary for the theory to be consistent: the wave function cannot make a jump as the loop is gradually shrunk to zero.

(v) The above discussion shows, however, that some two-dimensional systems may admit exceptions to the rule. Indeed a two-dimensional space minus a point is topologically equivalent to a circle, S^1, and its fundamental group is $\mathbb{Z}$. In this case a more general statistics is possible. Excitations (called the *anyons*) obeying these more general statistics with a nontrivial phase in eqns (5.25) and (5.26),

[10] By losing this assumtion, it is logically possible to construct a quantum theory with a more general type of statistics (*parastatistics*). However, no physical particles or systems are known which make use of such unusual kinds of statistics.

[11] The symbol $\pi_1(M)$ (the fundamental group of the space M) represents the group of equivalent classes of the map from a circle S^1 to the space M. Any space in which a closed loop can be smoothly shrunk to a point is *simply connected*, with the trivial fundamental group, $\pi_1(M) = \mathbb{1}$; a map from a circle to a circle can be classified by positive or negative winding numbers, so $\pi_1(S^1) = \mathbb{Z}$; a torus has $\pi_1(T^1) = \mathbb{Z} \times \mathbb{Z}$, and so on.

known as *the fractional statistics*, are known to play an important role in the physics of the quantum Hall effect, and, perhaps, in high-T superconductors.

The operation of symmetrization or antisymmetrization of the wave function with respect to the exchanges of identical particles can be realized by

$$\mathcal{S} = \frac{1}{N!}\sum_P P\,; \qquad \mathcal{A} = \frac{1}{N!}\sum_P \epsilon_P\, P\,, \tag{5.28}$$

where P represents all possible permutations of $(12\ldots N)$ particles and $\epsilon_P = \pm 1$ according to the whether P is an even or odd permutation.[12] They act as projection operators,

$$\mathcal{S}^2 = \mathcal{S}; \quad \mathcal{A}^2 = \mathcal{A}; \quad \mathcal{S}\mathcal{A} = 0\ .$$

[12] Any permutation can be constructed as a product of an even or odd number of exchanges of a pair of objects: even though the way a given permutation can be constructed this way is not unique, the parity of each permutation is well defined.

On the other hand, the Hamiltonian of N identical particles is clearly invariant under the exchange of the operators (momenta, position, spin, etc.) referring to these particles. Therefore the operation of symmetrization or antisymmetrization commutes with the evolution operator,

$$e^{-iHt/\hbar}\ :$$

the statistics is consistent with and maintained during the time evolution of the system.

As the symmetric states and antisymmetric states are orthogonal,

$$\langle\psi_S|\psi_A\rangle = \langle\psi_S|\mathcal{S}\mathcal{A}|\psi_A\rangle = 0\,,$$

a given system of N identical particles (with a definite statistics) will never mix with or leak to systems with a "wrong" statistics. This guarantees that all the constructions of quantum mechanics, completeness, unitarity (total probability is equal to unity), etc. remain valid even under the restriction of states with definite statistics.

5.3.1 Identical bosons

Consider now systems of N identical bosons. In the simplest case of two identical particles without spin, interacting with a potential $V(\mathbf{r})$, where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, the wave function can be factorized as

$$\Psi = \Phi(\mathbf{R})\psi(\mathbf{r}), \qquad \mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2},$$

where $\Phi(\mathbf{R})$ describes the center of mass, $\psi(\mathbf{r})$ the relative motion. The condition that Ψ be symmetric under the exchange of the two particles implies that

$$\psi(-\mathbf{r}) = \psi(\mathbf{r}).$$

Thus only those motions with even values of angular momenta $\ell = 0, 2, \ldots$ are allowed.

To discuss the more general case, it is often useful to consider as a basis of the states

$$|p_{i_1}\rangle \otimes |p_{i_2}\rangle \ldots |p_{i_N}\rangle \equiv |p_{i_1}, p_{i_2} \ldots, p_{i_N}\rangle \,, \tag{5.29}$$

with reference to the composite system

$$\boxed{\mathcal{H}^{(N)} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_N \,.} \tag{5.30}$$

Such a description in terms of *single-particle states* $|p_{i_k}\rangle$ $(k = 1, \ldots, N)$ is particularly useful in the case of N particles weakly interacting (so that in the first approximation they can be considered to be non-interacting). Of course, the states (5.29) form a valid basis of the composite system even when the interactions are important.

For general N the state vector has the form

$$|p_{i_1}, \ldots, p_{i_N}\rangle_{\mathcal{S}} = \left(\frac{N_1! N_2! \ldots N_r!}{N!}\right)^{1/2} \sum_{P'} P' \, |p_{i_1}, \ldots, p_{i_N}\rangle, \tag{5.31}$$

$$N_1 + N_2 + \ldots + N_r = N,$$

where N_i stands for the number of particles which "occupy" the single-particle state, p_i, which labels all the quantum numbers, including spin.

For $N = 2$, and in the coordinate representation, the wave function takes the possible form

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} \frac{1}{\sqrt{2}}[\,\psi_{p_1}(\mathbf{r}_1)\psi_{p_2}(\mathbf{r}_2) + \psi_{p_2}(\mathbf{r}_1)\psi_{p_1}(\mathbf{r}_2)\,] \,, & (p_1 \neq p_2), \\ \psi_{p_1}(\mathbf{r}_1)\psi_{p_1}(\mathbf{r}_2) \,, & (p_1 = p_2). \end{cases}$$

Note that the probability that the particles occupy the same position $\mathbf{r}_1 \simeq \mathbf{r}_2$ is *twice* what is expected in classical mechanics. An analogous argument can be made in the momentum representation.

A word of caution is appropriate here. The states (5.31) form a basis in the tensor space (5.30). A generic state is described by a linear combination of such vectors. This means that while it is true that any N-boson wave function satisfies the symmetry property

$$\Phi(\xi_1, \xi_2, \ldots, \xi_N) = \Phi(\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_N}) \,,$$

for every permutation $(1, 2, \ldots, N) \to (i_1, i_2, \ldots, i_N)$, this does not imply that it can be written as a symmetrization of a product of single particle wave functions.[13]

These properties of the wave functions of the identical bosons, whether they are elementary particles, atoms, or molecules, underlie certain extraordinary phenomena. An example is the phenomenon of Bose–Einstein condensation, in which a macroscopic number of, for example, atoms occupy the same quantum states, behaving *as if* described by a single wave function. These states are realized in Nature at very low temperatures, near absolute zero, such as liquid helium (*superfluidity*); more recently, BE condensation of gaseous atoms has been realized [Ketterle (2002)] or more recently, even for various molecules. The phenomenon of superconductivity is also related to this.

[13] For example, $\psi(x_1, x_2) = e^{-(x_1+x_2)^2}$ is symmetric but is not a symmetrization of a product. Of course, ψ can be expanded in series of plane waves $(e^{ik_1x_1}e^{ik_2x_2} + e^{ik_2x_1}e^{ik_1x_2})$ of the form (5.31).

5.3.2 Identical fermions and Pauli's exclusion principle

Again let us start with the simplest case of two identical spin-$\frac{1}{2}$ particles (e.g., two protons), described by a wave function of the same form as eqn (5.27). If the two particles interact through a potential depending on the relative position $\mathbf{r}$ only, the wave function can be factorized as

$$\Psi = \Phi(\mathbf{R})\psi(\mathbf{r}), \qquad \mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2},$$

where $\Phi(\mathbf{R})$ describes the free motion of the center of mass. The relative wave function now depends on the spin states as well. The spin states of of two spin-$\frac{1}{2}$ particles can always be decomposed into states of spin 1 (the spin triplet),

$$|\uparrow\uparrow\rangle, \qquad \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}, \qquad |\downarrow\downarrow\rangle,$$

and a state of spin 0 (the spin singlet),

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} .$$

The triplet states are symmetric under the exchange of two spins, while the singlet state is antisymmetric. It follows that the corresponding orbital wave function must have the opposite parity,

$$\psi_{1\,m}(-\mathbf{r}) = -\psi_{1\,m}(\mathbf{r}), \quad (m = 1, 0, -1), \qquad \psi_{0\,0}(-\mathbf{r}) = \psi_{0\,0}(\mathbf{r}).$$

Thus the angular momenta of the relative motion of two identical spin-$\frac{1}{2}$ particles are restricted to odd (total spin 1) or even (total spin 0) values only.

If the basis of direct-product states (5.29) is used, one has, for $N = 2$, a wave function of the form

$$|p_1, p_2\rangle_{\mathcal{A}} = \frac{1}{\sqrt{2}} \left(|p_1\rangle|p_2\rangle - |p_2\rangle|p_1\rangle\right) . \tag{5.32}$$

More generally, the states of a system composed of N identical fermions can be written as

$$\mathcal{A}\,|p_1\rangle\,|p_2\rangle\,\ldots|p_N\rangle = \frac{1}{N!}\sum_P \epsilon_P\, P\,|p_1\rangle\,|p_2\rangle\,\ldots|p_N\rangle\ ,$$

which in the coordinate representation takes the form of the *Slater determinant*

$$\psi_{\{p_i\}}(\xi_1, \xi_2, \ldots \xi_N) = \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \psi_{p_1}(\xi_1) & \psi_{p_1}(\xi_2) & \ldots & \psi_{p_1}(\xi_N) \\ \psi_{p_2}(\xi_1) & \psi_{p_2}(\xi_2) & \ldots & \psi_{p_2}(\xi_N) \\ \vdots & \ddots & \ddots & \vdots \\ \psi_{p_N}(\xi_1) & \psi_{p_N}(\xi_2) & \ldots & \psi_{p_N}(\xi_N) \end{vmatrix} .$$

The ξs denote both orbital and spin variables.

Thus the wave functions of more than one identical fermion vanish whenever two fermions occupy the same state,

$$\psi_{\{p_i\}}(\xi_1, \xi_2, \dots \xi_N) = 0, \quad \text{if} \quad p_j = p_k, \quad j \neq k \; .$$

The rule that the two identical fermions cannot occupy the same quantum state is known as **Pauli's exclusion principle**. Pauli's exclusion principle is absolutely fundamental in all applications of quantum mechanics to systems involving identical fermions, such as atomic nuclei, atoms, molecules, solids, gases and neutron stars.

The Slater determinants can thus be regarded as the *basis* in the Hilbert space of N fermions. A general wave function is given by a linear combination of Slater determinants. For the application of these constructions to atoms, see Chapter 15.

In a more general case, one has, in the presence of identical fermions,

$$\Psi(\xi_1, \xi_2, \dots, \xi_N) = \epsilon_P \Psi(\xi_{i_1}, \xi_{i_2}, \dots, \xi_{i_N})$$

for each permutation $P : (1, 2, \dots, N) \to (i_1, i_2, \dots, i_N)$. Note that Pauli's principle in the restricted sense stated above refers to those situations in which single-particle quantum numbers give a good description of the system, which is not always the case.

In atoms, the electronic configurations are basically constrained by Pauli's principle becasuse two electrons (in the same spin state) cannot stay in the same atomic orbit. The periodic nature of elements essentially originates from Pauli's principle and the quantization of the atomic orbits. See Chapter 15.

Guide to the Supplements

In Supplement 20.8 we give a brief account of the permutation group $\mathcal{S}_N$ and of the Young tableaux. In Supplement 20.9 a practical problem is solved: how to write the matrix elements of operators between multi-particle states. These formulas will be used in the construction of wave functions for heavy atoms.

Supplements 20.10 and 20.11 are a brief introduction to the Fock representation and to the non-relativistic version of second quantization. These supplements are meant to help in understanding the relation between non-relativistic quantum mechanics and quantum field theory. See Chapter 17 for more about *relativistic* quantum field theories and the theory of elementary particles.

Problems

(5.1) A particle of spin $J = 1$ and unknown parity decays at rest into two identical spin-$\frac{1}{2}$ particles.

(a) Compute the orbital angular momentum of the final particles and the total spin.

(b) Determine the parity of the decaying particle, assuming that in the decay, parity is conserved.

(c) Let us suppose that the initial particle is in the state $|J, J_z\rangle = |1, 0\rangle$. Write explicitly the final state with an unknown radial function, but with explicit use of spherical harmonics and spin states.

Let us now suppose that one measures the spin projections of the final particles with Stern–Gerlach-type apparatus, for two particles emitted in the directions (θ, φ) and

$$(\pi - \theta, \varphi + \pi) \,.$$

(d) For fixed values of (θ, φ), write the normalized spin wave function of the final state.

(e) Compute the probability that a particle is emitted in the direction (θ, φ) with $s_z = \frac{1}{2}$.

(f) Compute the probability that a simultaneous measurement of $(s_y(1), s_y(2))$ gives $(\frac{1}{2}, \frac{1}{2})$.

(5.2) A deuteron d is a nucleus with charge +1, composed of a proton (p) and a neutron (n). The deuteron has spin 1 and parity +. A negative pion π^-, with charge -1 and spin 0, can be bound to the deuteron to form a sort of "deuterium atom". Let us suppose that this system is formed in the lowest Bohr orbit.

(a) Compute the ratio between the Bohr radius of this system and the standard Bohr radius, and compute the binding energy of the system. Some masses needed for the computation are listed below, in MeV/c^2:

$$M_{\pi^-} = 139.6\,; \;\; M_{e^-} = 0.51\,;$$
$$M_d = 1\,875.6\,; \;\; M_p = 938.3\,.$$

(b) The bound system described above decays with the reaction $\pi^- + d \to n + n$. Both angular momentum and parity are conserved in the decay. Discuss if one can determine the intrinsic parity of the π^- from these data.

(c)) Compute the angular distribution of neutrons in the final state, knowing that in the initial state $J_z = 0$.

(d)) Explain why the hydrogen atom does not decay via a somewhat analogous process, $e^- + p \to n + \nu$, where ν is the (electron) neutrino.

(5.3) Write the explicit form of the completeness relation for a system of two free identical particles.

(5.4) Write the Hamiltonian and the Heisenberg equations for a system of particles interacting with a potential $U(\mathbf{x}_1, \mathbf{x}_2)$ in the second quantization formalism.

(5.5) Consider a simplified version of the Young experiment, limiting the dynamics to two single "modes" of the electromagnetic field that describe a photon passing from slit 1 or 2 respectively. Use a Fock formalism to describe the photon's beam, and compute the probability of measuring a photon through slit 1 k times in a single-photon experiment repeated n times. Show that the same probability is obtained by measuring k photons in a single experiment with a beam of n photons. Describe in this model the interference.