2

Principles of Quantum Mechanics

This introduction describes the mathematical tools used in the formulation of quantum mechanics and the connections between the physical world and mathematical formalism. Such links constitute the fundamental principles of quantum mechanics.[1] They are valid for every specific realization of these principles. Subsequently, their most immediate consequences are presented: the quantum process of measurement and relations of uncertainty. Frequent shortcomings existing in many introductions can thus be avoided.[2]

2.1 Classical Physics

If our vision of a moving object is interrupted by a large billboard, and is resumed after the reappearance of the object, we naturally assume that it has traveled all the way behind the billboard (Fig. 2.1). This is implied in the notion of physical reality, one of the postulates in the famous EPR paradox written by Einstein in collaboration with Boris Podolsky and Nathan Rosen [16]. " If, without in any way disturbing a system, we can predict with certainty the value of a physical quantity, then there is an element of physical reality corresponding to this physical quantity."

[1] Presentations of quantum mechanics resting upon few basic principles start with [15], which remains a cornerstone on the subject.

[2] In many presentations it is assumed that the solution of any wave equation for a free particle is the plane wave $\exp[\mathrm{i}(kx - \omega t)]$. Subsequently, the operators corresponding to the momentum and energy are manipulated in order to obtain an equation yielding the plane wave as solution of differential equations. This procedure is not very satisfactory because: (a) plane waves display some difficulties as wave functions, not being square integrable; (b) quantum mechanics appears to be based on arguments that are only valid within a differential formulation; (c) it leads to the misconception that the position wave function is the only way to describe quantum states.

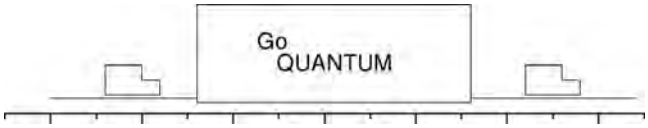

Fig. 2.1. The trajectory of the car behind the billboard as an element of physical reality

This classical framework relies on the acceptance of some preconceptions, most notably the existence of the continuous functions of time called trajectories $\boldsymbol{x}(t)$ [or $\boldsymbol{x}(t)$ and $\boldsymbol{p}(t)$, where $\boldsymbol{p}$ is the momentum of the particle]. The concept of trajectory provides an important link between the physical world and its mathematical description. For instance, it allows us to formulate Newton's second law:

$$\boldsymbol{F}(\boldsymbol{x}) = M\,\frac{\mathrm{d}^2\boldsymbol{x}}{\mathrm{d}t^2}. \tag{2.1}$$

This equation of motion predicts the evolution of the system in a continuous and deterministic way. Since this is a second order equation, the state of a system is determined if the position and velocity of each particle are known at any one time.

Maxwell's theory of electromagnetism is also part of classical physics. It is characterized in terms of fields, which must be specified at every point in space and time. Unlike particles, fields can be made as small as desired. Electromagnetism is also a deterministic theory.

Essential assumptions in classical physics about both particles and fields are:

- The possibility of nondisturbing measurements
- There is no limit to the accuracy of values assigned to physical properties

In fact, there is no distinction between physical properties and the numerical values they assume. Schwinger characterizes classical physics as:

> the idealization of nondisturbing measurements and the corresponding foundations of the mathematical representation, the consequent identification of physical properties with numbers, because nothing stands in the way of the continual assignment of numerical values to these physical properties ([14], p. 11).

Such "obvious" assumptions are no longer valid in quantum mechanics. Therefore, other links have to be created between the physical world and the mathematical formalism.

2.2* Mathematical Framework of Quantum Mechanics

According to classical electromagnetism, an inhomogeneous magnetic field **B** directed along an axis (for instance, the z-axis) should bend the trajectory of particles perpendicular to this axis. The amount of bending of these tiny

magnets will be proportional to the projection μ_z of their magnetic moment $\boldsymbol{\mu}$. Therefore, if the beam is unpolarized (all values $-|\boldsymbol{\mu}| \leq \mu_z \leq |\boldsymbol{\mu}|$ are present), particles are classically expected to impact over a continuous region of a screen. However, it was shown in 1921 by Otto Stern and Walther Gerlach that silver atoms distribute themselves over each of two lines. Since the magnetic moment is proportional to an intrinsic angular momentum called spin ($\boldsymbol{\mu} \propto \mathbf{S}$), it is apparent that only two projections of the spin are allowed by nature [17]. The values of these projections are

$$\pm\frac{1}{2}\,\hbar\,; \qquad \hbar \equiv \frac{h}{2\pi}, \tag{2.2}$$

where h is the Planck constant. It has the dimensions of classical action (energy $\times$ time). (See Table 14.1 and Sect. 5.2.1 for more details.)

Note, however, the fact that a physical quantity may have only two values does not require by itself the abandonment of classical physics. For instance, your PC works upon bits, i.e., classical systems that may be in one of two states.[3] As befits classical systems, their state is not altered upon measurement (thus contributing to the stability of classical computers).

A different description is provided by vectors on a plane. While the sum of the two states of a bit does not make sense, the addition of two vectors on a plane is always another vector. Any vector Ψ may be written as a linear combination (Fig. 2.2a)

$$\Psi = c_x \boldsymbol{\varphi}_x + c_y \boldsymbol{\varphi}_y, \tag{2.3}$$

where c_x, c_y are amplitudes and $\boldsymbol{\varphi}_x$, $\boldsymbol{\varphi}_y$, two perpendicular vectors of module one. This last property is expressed by the relation $\langle \boldsymbol{\varphi}_i \,|\, \boldsymbol{\varphi}_j \rangle = \delta_{ij}$, which is a particular case of the scalar product

$$\langle \Psi \,|\, \Psi' \rangle = c_x^* c_x' + c_y^* c_y'. \tag{2.4}$$

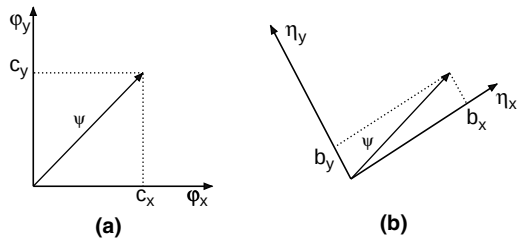

Fig. 2.2. Representation of a vector in two-dimensions. The same vector Ψ can be expressed as the sum of two different systems of basis vectors

[3] Although the bits in your PC function on the basis of quantum processes (for instance, semiconductivity) they are not in themselves quantum systems.

In quantum mechanics we allow complex values of the amplitudes.

Another crucial property of the vector space is that the same vector Ψ may be expressed as a combination of other sets of perpendicular vectors $\boldsymbol{\eta}_x$, $\boldsymbol{\eta}_y$ along rotated axis (Fig. 2.2b)

$$\Psi = b_x \boldsymbol{\eta}_x + b_y \boldsymbol{\eta}_y. \tag{2.5}$$

This two-dimensional space may be easily generalized to spaces with any number of dimensions, called Hilbert spaces. Here we outline some properties that are specially relevant from the point of view of quantum mechanics. This overview is expanded in Sect. 2.7*:

- Any vector Ψ may be expressed as a linear combination of orthonormal basis states $\boldsymbol{\varphi}_i$ [as in (2.3)]

$$\Psi = \textstyle\sum_i c_i \boldsymbol{\varphi}_i \; ; \qquad c_i = \langle \boldsymbol{\varphi}_i | \Psi \rangle \equiv \langle i | \Psi \rangle, \tag{2.6}$$

$$\langle \boldsymbol{\varphi}_i \,|\, \boldsymbol{\varphi}_j \rangle = \delta_{ij}. \tag{2.7}$$

- Linear operators $\hat{Q}$ act on vectors belonging to a Hilbert space, transforming one vector into another

$$\Phi = \hat{Q}\, \Psi. \tag{2.8}$$

  These operators obey a noncommutative algebra, as shown in Sect. 2.7* for the case of rotations in three-dimensions. We define the commutation operation through the symbol

$$[\hat{Q}, \hat{R}] \equiv \hat{Q}\, \hat{R} \, - \, \hat{R}\, \hat{Q}, \tag{2.9}$$

  where the order of application of the operators is from right to left [$\hat{Q}\hat{R}\,\Psi = \hat{Q}\,(\hat{R}\Psi)$].
- If the vector $\hat{Q}\,\boldsymbol{\varphi}_i$ is proportional to $\boldsymbol{\varphi}_i$, then $\boldsymbol{\varphi}_i$ is said to be an eigenvector of the operator $\hat{Q}$. The constant of proportionality q_i is called the eigenvalue

$$\hat{Q}\, \boldsymbol{\varphi}_i = q_i\, \boldsymbol{\varphi}_i. \tag{2.10}$$

- The scalar product between a vector $\Phi_a = \hat{Q}\, \Psi_a$ and another vector Ψ_b is called the matrix element of the operator $\hat{Q}$ between the vectors Ψ_a and Ψ_b, and it is symbolically represented as[4]

$$\langle \Psi_b | Q | \Psi_a \rangle \equiv \langle b | Q | a \rangle \equiv \langle \Psi_b \,|\, \Phi_a \rangle. \tag{2.11}$$

  The matrix elements of the unit operator are the scalar products $\langle \Psi_a \,|\, \Psi_b \rangle \equiv \langle a \,|\, b \rangle = \langle \Psi_b \,|\, \Psi_a \rangle^*$. The norm $\langle \Psi \,|\, \Psi \rangle^{1/2}$ is a real, positive number.

[4] Dirac called the symbols $\langle a|$ and $|a\rangle$ the bra and ket, respectively [15].

- The Hermitian conjugate $\hat{Q}^+$ of an operator $\hat{Q}$ is defined through the relation
$$\langle b|Q^+|a\rangle = \langle a|Q|b\rangle^*. \tag{2.12}$$
The operator is said to be Hermitian if
$$\hat{Q}^+ = \hat{Q}. \tag{2.13}$$
The eigenvalues q_i of a Hermitian operator are real numbers and the corresponding eigenvectors φ_i constitute a basis set of orthogonal vectors.
- The matrix $\mathcal{U}$ with matrix elements $\mathcal{U}_{ab}$ is said to be unitary if the matrix elements of its inverse are given by
$$\left(\mathcal{U}^{-1}\right)_{ab} \equiv \mathcal{U}^*_{ba}. \tag{2.14}$$
Unitary transformations preserve the norm of the vectors and relate two sets of basis states (see Fig. 2.2)
$$\eta_a = \sum_i \mathcal{U}_{ai}\,\varphi_i \tag{2.15}$$

These abstract mathematical tools (vectors, Hermitian operators and unitary transformations) may be represented through concrete, well-known mathematical objects, such as column vectors and matrices (Chap. 3), or by means of functions of the coordinate and differential operators (Chap. 4).

2.3 Basic Principles of Quantum Mechanics

In this section we present the quantum mechanical relation between the physical world and the mathematical tools that have been outlined in Sect. 2.2*. This relation requires the representation of states, observables, measurements, correlations between particles and dynamical evolution. It is formulated through the quantum principles:

Principle 1. *The state of the system is completely described by a vector* Ψ *– the state vector or state function – belonging to a Hilbert space.*

The state vector Ψ constitutes an unprecedented way of describing physical systems. It is an abstract entity that carries information about the results of possible measurements. It replaces the classical concepts of position and momentum.

The fact that the sum of two-state vectors is another state vector belonging to the same Hilbert space, i.e., describing another state of the system, is usually called the superposition principle. The sum $c_a\Psi_a + c_b\Psi_b$ must not be interpreted in the sense that we have a conglomerate of systems in which some of them are in the state Ψ_a and some in the state Ψ_b, but rather, that the system is simultaneously in both component states. This statement is also valid when the system is reduced to a single particle.

This superposition is fundamentally different from any property of classical particles, which are never found as a linear combination of states associated with different trajectories: a tossed coin may fall as head or tails, but not as a superposition of both.

By establishing that the state vector completely describes the state of the system, Principle 1 assumes that there is no way of obtaining information about the system, unless this information is already present in the state vector. However, for a given problem, one may be interested only in some of the degrees of freedom of the system (e.g., magnetic moment, linear momentum, angular momentum, etc.), not in the complete state vector.

The state vector may be multiplied by an arbitrary complex constant and still represent the same physical state. However, we require that the state vector is normalized, i.e., that its norm has the value 1. Even if we enforce this requirement, an arbitrary overall phase is left, which has no physical significance. This is not the case for the relative phase of the terms in the sum $c_a\Psi_a + c_b\Psi_b$, which encodes important physical information.

The relation between the physical world and states Ψ is more subtle than the classical relation with position and momenta $\boldsymbol{x}, \boldsymbol{p}$. It relies on the following two principles.

Principle 2. *To every physical quantity there corresponds a single linear operator. In particular, the operators $\hat{x}$ and $\hat{p}$, corresponding to the coordinate and momentum of a particle, satisfy the commutation relation*[5]

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar. \tag{2.16}$$

The commutator is defined in (2.9) and the constant $\hbar$ has been already used in (2.2). Its value (Table 14.1) provides an estimate of the domain in which quantum mechanics becomes relevant. Classical physics should be applicable to systems in which the action is much larger than $\hbar$.

This is also fundamentally different from classical physics, for which physical properties are identified with numbers (Sect. 2.1).

Since any classical physical quantity may be expressed as a function of coordinate and momentum $Q = Q(x, p)$, the replacement $x \to \hat{x}$ and $p \to \hat{p}$ in the classical expression $Q(x, p)$ yields the operator $\hat{Q} = Q(\hat{x}, \hat{p})$. Thus, a one-to-one correspondence between operators $\hat{Q}$ and physical quantities or observables Q is established. However, there are also purely quantum operators, such as the spin operators, that cannot be obtained through such substitution.

The operator corresponding to the classical Hamilton function $H(p, x)$ is called the Hamiltonian. For a conservative system,

$$\hat{H} = \frac{1}{2M}\hat{p}^2 + V(\hat{x}), \tag{2.17}$$

where M is the mass of the particle and V the potential.

[5] This commutation relation has been derived from relativistic invariance [18], using the fact that spatial translations [generated by $\hat{p}$, see (4.9)] do not commute with Lorentz transformations even in the limit $c \to \infty$. See also (12.5).

Principle 3. *The eigenvalues q_i of an operator $\hat{Q}$ constitute the possible results of measurements of the physical quantity Q. The probability*[6] *of obtaining the eigenvalue q_i is the modulus squared $|c_i|^2$ of the amplitude of the eigenvector φ_i, if the state vector $\Psi = \sum_i c_i \varphi_i$ is expanded in terms of eigenstates of the operator $\hat{Q}$.*

Since the results of measurements are real numbers, the operators representing observables are restricted to be Hermitian (2.13). In particular, the possible values of the energy E_i are obtained by solving the eigenvalue equation

$$\hat{H}\varphi_i = E_i \varphi_i. \tag{2.18}$$

The above three principles are sufficient for the treatment of static situations involving a single particle. A number of simple, typical, well-known problems of a particle moving in one-dimensional space are discussed in Chaps. 3 and 4. The extension to three-dimensional space is made in Chaps. 5 and 6.

Two more principles, concerning many particle systems and the time-evolution of states, are presented in Chaps. 7 and 9, respectively.

2.3.1 Some Comments on the Basic Principles

As in the case of classical mechanics, quantum mechanics may be applied to very different systems, from single-particle to many-body systems to fields. Thus quantum mechanics constitutes a framework in which to develop physical theories, rather than a physical theory by itself.

In the present text we adopt the interpretation that the vector state represents our knowledge about reality, rather than reality itself. This knowledge includes the formulation of the possible tests (measurements) to which the system can be submitted and the probabilities of their outcomes.[7]

We have postulated the existence of new links between the physical world and mathematics: physical quantities are related to (noncommuting) operators; state vectors are constructed through operations with these mathematical entities; the feedback to the physical world is made by predicting as possible results of measurements the eigenvalues of the corresponding operators and the probabilities of obtaining them. This two-way relation between physical world and formalism is not an easy relation. Following David Mermin [19]:

> The most difficult part of learning quantum mechanics is to get a good feeling for how the abstract formalism can be applied to actual phenomena in the laboratory. Such applications almost invariably involve formulating oversimplified abstract models of the real phenomena, to

[6] Notions of probability theory are given in Sect. 2.8*.

[7] Therefore, we have accepted the reduction interpretation of the measurement process. Historically, this was the path followed by most physicists. However, we present one more discussion of the measurement problem in Chap. 12.

> which the quantum formalism can effectively be applied. The best physicists have an extraordinary intuition for what features of the actual phenomena are essential and must be represented in the abstract model, and what features are inessential and can be ignored.

It is almost as useful to state what the principles do not mean, as to say what they do mean. In the following we quote some common misconceptions regarding quantum states [20].

- "The state vector is similar to other fields used in the description of the physical world." It is fundamentally different from the electric or magnetic fields in electromagnetic waves, which carry momentum, energy, etc., and in which any externally caused change propagates at a finite, medium-dependent speed.
- "Energy eigenstates are the only allowed ones." This misconception probably arises from the generalized emphasis on the solution of the eigenvalue equation (2.18) and from its similarity to the correct statement: "Energy eigenvalues are the only allowed energies."
- "A state vector describes an ensemble of classical systems." In the standard Copenhagen interpretation, the state vector describes a single system. In none of the acceptable statistical interpretations is the ensemble classical.
- "A state vector describes a single system averaged over some amount of time." The state vector describes a single system at a single instant.

2.4 Measurement Process

In this section we specify some basic concepts involved in the process of measurement.[8]

2.4.1 The Concept of Measurement

Two or more systems are in interaction if the presence of one leads to changes in the other, and vice versa. Different initial conditions generally lead to different changes, although this may not always be the case.

A measurement is a process in which a system is put in interaction with a piece of apparatus. The apparatus determines the physical quantity or observable to be measured (length, weight, etc.).

There are two important steps in a measurement. The first is the preparation of the system to be measured, i.e., the determination of the initial state. Bohr's definition of the word "phenomenon" refers to "an observation obtained under specified circumstances, including an account of the whole experimental arrangement" [22], p. 64. This should be contrasted with the EPR definition of physical reality (Sect. 2.1).

[8] See also [21], specially Sects. 1.2, 2.1, and 3.6.

The second important step, also crucial in the case of quantum systems, is a (macroscopic) change in the apparatus that should be perceptible by a cognitive system. In many cases this change is produced by a detector at one end of the apparatus. The magnitude of the physical quantity has a value if the change can be represented in numerical form.

2.4.2 Quantum Measurements

The most fundamental difference between a classical and a quantum system is that the latter cannot be measured without being irrevocably altered, no matter how refined the measuring instruments are.[9] This is a consequence of the principles presented in Sect. 2.3.

Assume that a measurement of the physical quantity Q, performed on a system in the state Ψ expanded as in (2.6), yields the result q_j. If the same measurement could be repeated immediately afterwards, the same value q_j should be obtained with certainty. Thus, the measurement has changed the previous value of the coefficients $c_i \rightarrow \delta_{ij}$. In other words, as a result of the measurement, the system jumps to an eigenstate of the physical quantity that is being measured (the reduction of the state vector) (Fig. 2.3). The only exceptions occur when the initial state is already represented by one of the eigenvectors.

Given an initial state vector Ψ, we do not know in general to which eigenstate the system will jump. Only the probabilities, represented by $|c_i|^2$, are

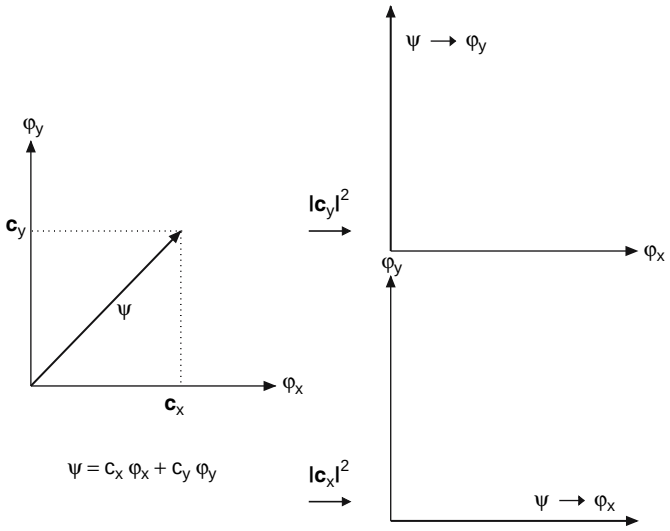

Fig. 2.3. The reduction of the state vector as a result of a measurement

[9] Although classical systems may also be disturbed by measurements, there is always the assumption that the disturbance can be made as small as required, or that it may be predicted by a calculation.

determined. This identification of the probabilities is consistent with the following facts:

- Their value is always positive
- Their sum is 1 (if the state Ψ is normalized)
- The orthogonality requirement (2.7) ensures that the probability of obtaining any eigenvalue $q_j \neq q_i$ vanishes if the initial state of the system is the eigenstate φ_i (see Table 2.1).

The fact that, given a state vector Ψ, we can only predict the probability $|c_i|^2$ of obtaining eigenvalues q_i constitutes an indeterminacy inherent in quantum mechanics. Our knowledge about the system cannot be improved, for instance, through a second measurement, since the state Ψ has been transformed into φ_i.

According to the interpretation adopted in Sect. 2.3.1, it is our knowledge of the system that jumps when we perform a measurement, rather than the physics of the system.

If in the expansion (2.6) there is a subset of basis states φ_k with the same eigenvalue $q_k = q$, the probability of obtaining this eigenvalue is $\sum_k |c_k|^2$. The system is projected after the measurement into the (normalized) state

$$\Psi' = \frac{1}{\sqrt{\sum_k |c_k|^2}} \sum_k c_k \varphi_k. \tag{2.19}$$

The concept of probability implies that we must consider a large number of measurements performed on identical systems, all of them prepared in the same initial state Ψ.

The diagonal matrix element[10] is given by the sum of the eigenvalues weighted by the probability of obtaining them:

$$\langle \Psi | Q | \Psi \rangle = \sum_i q_i |c_i|^2. \tag{2.20}$$

It is also called the expectation value or mean value of the operator $\hat{Q}$. The mean value does not need to be the result q_i of any single measurement, but it is the average value of all the results obtained through the measurement of identical systems.

The uncertainty or standard deviation ΔQ in a given measurement is defined as the square root of the average of the quadratic deviation:

$$\begin{aligned} \Delta Q &= \langle \Psi | \left(Q - \langle \Psi | Q | \Psi \rangle \right)^2 | \Psi \rangle^{1/2} \\ &= \left(\langle \Psi | Q^2 | \Psi \rangle - \langle \Psi | Q | \Psi \rangle^2 \right)^{1/2}, \end{aligned} \tag{2.21}$$

[10] The matrix element is said to be diagonal if the same vector appears on both sides of the matrix element.

where

$$\langle \Psi | Q^2 | \Psi \rangle = \sum_i q_i^2 |c_i|^2. \tag{2.22}$$

2.5 Some Consequences of the Basic Principles

This section displays some consequences of quantum principles in the form of thought experiments. Alternatively, one may obtain the quantum principles as a generalization of the results of such thought experiments (see [23]).

Let us consider a Hilbert space consisting of only two independent states $\varphi_\pm$. We also assume that these states are eigenstates of an operator $\hat{S}$ corresponding to the eigenvalues ± 1, respectively. Thus the eigenvalue equation $\hat{S}\varphi_\pm = \pm\varphi_\pm$ is satisfied. The scalar products $\langle \varphi_+ \,|\, \varphi_+ \rangle = \langle \varphi_- \,|\, \varphi_- \rangle = 1$ and $\langle \varphi_+ \,|\, \varphi_- \rangle = 0$ are verified. There are many examples of physical observables that may be represented by such operator. For instance, the z-component of the spin[11] is frequently used in this book (Sects. 2.2*, 3.1.3, 5.2, 9.2, etc.).

We start by constructing a filter, i.e., an apparatus such that the exiting particles are in a definite eigenstate. In the first part of the apparatus, a beam of particles is split into the two separate $\varphi_\pm$ beams, as in the experiment of Stern and Gerlach (Sect. 5.2.1). In the second part, each beam is pushed toward the original direction. Each separate beam may be masked off at the half-way point. Such an apparatus is sketched in Fig. 2.4a, with the φ_- beam masked off. It will be called a φ-filter. It is enclosed within a box drawn with continuous lines.

Any experiment requires first the preparation of the system in some definite initial state (Sect. 2.4.1). Particles leave the oven in unknown linear combinations Ψ of $\varphi_\pm$ states

$$\Psi = \langle \varphi_+ \,|\, \Psi \rangle \varphi_+ + \langle \varphi_- \,|\, \Psi \rangle \varphi_-. \tag{2.23}$$

They are collimated and move along the y-axis. In the following cases, we prepare the particles in the filtered state φ_+, by preventing particles in the state φ_- from leaving the first filter (Fig. 2.4b).

In the last stage of the experimental setup we insert another filter as part of the detector, in order to measure the degree of filtration. The detector includes also a photographic plate which records the arriving particles and is observed by an experimentalist (Fig. 2.4c).

In the first experiment, we place the detector immediately after the first filter (Fig. 2.4d). If the φ_- channel is also blocked in the detector, every particle goes through; if the channel φ_+ is blocked, nothing passes. The amplitudes

[11] Another example is given by the polarization states of the photon (see Sect. 9.5.2†). Most of the two-state experiments are realized by means of such optical devices.

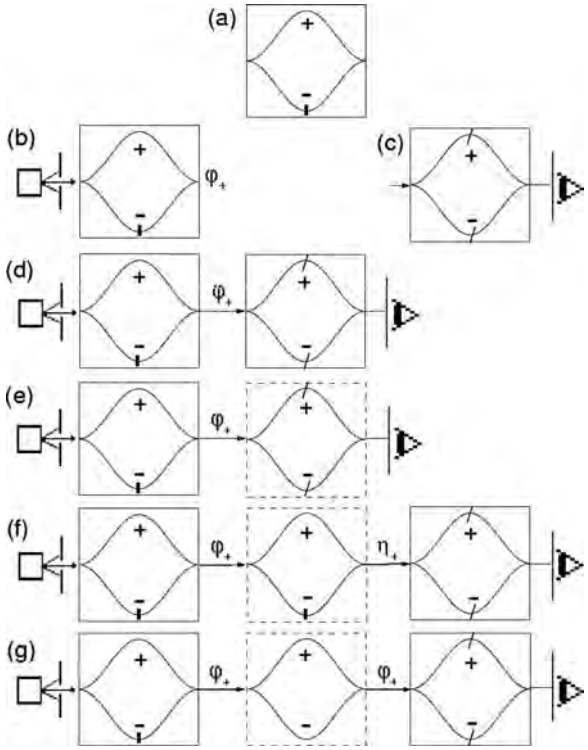

Fig. 2.4. Quantum mechanical thought experiments illustrating the basic principles listed in Sect. 2.3: (**a**) schematic representation of a filter; (**b**) preparation of the state of a particle; (**c**) detector (filter, photoplate, observer); (**d**–**g**) experiments (see text). The vertical bars denote fixed path blocking, while the slanting bars indicate paths that can be either opened or closed. For each experiment we perform a measurement in which the upper channel of the detector is open and the down channel blocked, and another measurement with the opposite features

for these processes are $\langle \varphi_+ \,|\, \varphi_+ \rangle = 1$ and $\langle \varphi_- \,|\, \varphi_+ \rangle = 0$, respectively. The corresponding probabilities, $|\langle \varphi_+ \,|\, \varphi_+ \rangle|^2$ and $|\langle \varphi_- \,|\, \varphi_+ \rangle|^2$, also are 1 and 0.

We now consider another set of basis states $\eta_\pm$, thus satisfying the orthonormality conditions $\langle \eta_+ \,|\, \eta_+ \rangle = \langle \eta_- \,|\, \eta_- \rangle = 1$, $\langle \eta_+ \,|\, \eta_- \rangle = 0$ (Fig. 2.2b). It is easy to verify that an operator $\hat{R}$, satisfying the eigenvalue equation $\hat{R}\,\eta_\pm = \pm\eta_\pm$, does not commute with $\hat{S}$. Let us perform the necessary modifications of the detector filter so that it can block the particles in either of the states $\eta_\pm$. If $\hat{R}$ corresponds the spin component in the x-direction, the required modification of the detector amounts to a rotation of its filter by an angle $\pi/2$ around the y-axis. Dashed boxes represent filters such that particles exit in the $\eta_\pm$ states (η-type filters) (Fig. 2.4e).

A particle exiting the first filter in the state φ_+ reorients itself, by chance, within the second filter. This process is expressed by expanding the states $\varphi_\pm$ in the new basis

$$\varphi_\pm = \langle \eta_+ \,|\, \varphi_\pm \rangle \eta_+ + \langle \eta_- \,|\, \varphi_\pm \rangle \eta_- . \tag{2.24}$$

According to Principle 3, a particle will emerge from the detector filter in the state η_+ with probability $|\langle \eta_+ \,|\, \varphi_+ \rangle|^2$ or in the state η_- with probability $|\langle \eta_- | \varphi_+ \rangle|^2$. If the η_- channel of the second filter is blocked, the particle is either projected into the state η_+ with probability $|\langle \varphi_+ \,|\, \eta_+ \rangle|^2$ or is absorbed with probability $1 - |\langle \varphi_+ \,|\, \eta_+ \rangle|^2 = |\langle \varphi_+ \,|\, \eta_- \rangle|^2$. This result sounds classical: it is the quantum version of the classical Malus law. However, the projection process is probabilistic. Any information about the previous orientation φ_+ is lost.

In the experiment of Fig. 2.4e, let us replace the detector with the original Stern–Gerlach apparatus sketched in Fig. 5.3. Classical waves may simultaneously increase their intensities at each of the two spots on the screen. However, this would lead to a violation of charge conservation in the case of electrons: quantum mechanics determines probabilities at each spot for just one particle[12]. We are not dealing with classical waves.

We now perform two other experiments which yield results that are spectacularly different from classical expectations. Let us restore the detector filter to the φ-type and introduce a filter of the η-type between the first filter and the detector (Fig. 2.4f). Thus particles prepared in the φ_+ state exit the second filter in the η_+ state. In the spin example, particles leave the first filter with the spin pointing in the direction of the positive z-axis, and the second filter pointing along the positive x-axis. The detector measures the number of particles exiting in one of the $\varphi_\pm$ states (spin pointing up or down in the z-direction). We use now the inverse expansion[13] of (2.24), namely

$$\eta_\pm = \langle \varphi_+ \,|\, \eta_\pm \rangle \varphi_+ + \langle \varphi_- \,|\, \eta_\pm \rangle \varphi_- . \tag{2.25}$$

Thus, the total amplitudes for particles emerging in one of the states $\varphi_\pm$ are[14]

$$\langle \varphi_+ | \eta_+ \rangle \langle \eta_+ | \varphi_+ \rangle \tag{2.26}$$

$$\langle \varphi_- | \eta_+ \rangle \langle \eta_+ | \varphi_+ \rangle . \tag{2.27}$$

[12] An alternative could be that the electron chooses its path just upon entering the second filter. However, this interpretation is inconsistent with the results of experiment 2.4g.

[13] The amplitudes in (2.24) and in (2.25) are related by $\langle \varphi_+ \,|\, \eta_\pm \rangle = \langle \eta_\pm \,|\, \varphi_+ \rangle^*$ and $\langle \varphi_- \,|\, \eta_\pm \rangle = \langle \eta_\pm \,|\, \varphi_- \rangle^*$, according to Table 2.1.

[14] One reads from right to left.

Both components $\varphi_{\pm}$ may emerge from the detector filter, in spite of the fact that the fraction of the beam in the φ_- state was annihilated inside the first filter. There is no way in classical physics to explain the reconstruction of the beam φ_-. This example illustrates the quantum rule concerning the impossibility of determining two observables associated with operators which do not commute: a precise determination of R destroys the previous information concerning S.

The result of this experiment is also consistent with Principle 1 in Sect. 2.3, since the state vector η_+ contains all possible information about the system: its past history is not relevant for what happens to it next. The information is lost in the collision with the blocking mask that has been put inside the second filter.

If we repeat the last experiment, but remove the mask from the second filter (Fig. 2.4g), the total amplitude is given by the sum of the amplitudes associated with the two possible intermediate states

$$\langle\varphi_+|\eta_+\rangle\langle\eta_+|\varphi_+\rangle + \langle\varphi_+|\eta_-\rangle\langle\eta_-|\varphi_+\rangle = \langle\varphi_+\,|\,\varphi_+\rangle = 1 \tag{2.28}$$

$$\langle\varphi_-|\eta_+\rangle\langle\eta_+|\varphi_+\rangle + \langle\varphi_-\,|\,\eta_-\rangle\langle\eta_-|\varphi_+\rangle = \langle\varphi_-\,|\,\varphi_+\rangle = 0, \tag{2.29}$$

where the closure property has been applied [See (2.47)]. All the particles get through in the first case; none in the second case. In going from the amplitude (2.27) to (2.29) we get fewer particles, despite the fact that more channels are opened.

The result of this last experiment is equivalent to an interference pattern. Classically, such patterns are associated with waves. However, unlike the case of waves, particles here are always detected as lumps of the same size on a screen placed in front of the exit side of the detector filter. No fractions of a lump are ever detected, as befits the behavior of indivisible particles. Therefore, these experiments display wave–particle duality[15], which is thus accounted for by Principles 1–3.

The famous question about which of the two intermediate channels the particle went through does not make sense in quantum mechanics, because this path cannot be determined, even in principle. Determination of the path would restore the intensity in both channels of the detector.

It is important that none of the intermediate beams suffers an additional disturbance (for example, the influence of an electric field), which may change the relative phases of the two channels.

Let us again replace the detector in Fig. 2.4f with the original Stern–Gerlach apparatus. Thus we could also obtain information about the order of $\varphi_{\pm}$ states appearing in the detector (provided the counting rate is sufficiently slow). Consistently with Principle 3, this order turns out to be completely

[15] See Sect. 11.1 for a presentation of real two-slit experiments.

random, since relative probabilities $|\langle \varphi_\pm \,|\, \eta_+ \rangle|^2$ are the only information that we can extract from measurements.

2.6 Commutation Relations and the Uncertainty Principle

In this section, it is shown that the commutation relation between two Hermitian operators $\hat{r}, \hat{s}$ determines the precision with which the values of the corresponding physical quantities may be simultaneously determined. Thus Heisenberg uncertainty relations between momenta and coordinates become extended to any pair of observables, and appear as a consequence of their commutation relation.

One assumes two Hermitian operators, $\hat{R}, \hat{S}$, and defines a third (non-Hermitian) operator $\hat{Q}$ such that

$$\hat{Q} \equiv \hat{R} + \mathrm{i}\lambda \hat{S}, \tag{2.30}$$

where λ is a real constant. The minimization with respect to λ of the positively defined norm [see (2.41)]

$$\begin{aligned} 0 \leq \langle \hat{Q}\Psi | \hat{Q}\Psi \rangle &= \langle \Psi | Q^+ Q | \Psi \rangle \\ &= \langle \Psi | R^2 | \Psi \rangle + \mathrm{i}\lambda \langle \Psi | [R, S] | \Psi \rangle + \lambda^2 \langle \Psi | S^2 | \Psi \rangle, \end{aligned} \tag{2.31}$$

yields the value

$$\begin{aligned} \lambda_{\min} &= -\frac{\mathrm{i}}{2} \langle \Psi | [R, S] | \Psi \rangle / \langle \Psi | S^2 | \Psi \rangle \\ &= -\frac{\mathrm{i}}{2} \langle \Psi | [R, S]^+ | \Psi \rangle^* / \langle \Psi | S^2 | \Psi \rangle \\ &= \frac{\mathrm{i}}{2} \langle \Psi | [R, S] | \Psi \rangle^* / \langle \Psi | S^2 | \Psi \rangle. \end{aligned} \tag{2.32}$$

In the second line we have used the definition (2.12) of the Hermitian conjugate. In the last line, the relation $[\hat{R}, \hat{S}]^+ = -[\hat{R}, \hat{S}]$ stems from the Hermitian character of the operators [see (2.40)]. Substituting the value $\lambda_{\min}$ into (2.31) yields

$$0 \leq \langle \Psi | R^2 | \Psi \rangle - \frac{1}{4} \frac{|\langle \Psi | [R, S] | \Psi \rangle|^2}{\langle \Psi | S^2 | \Psi \rangle} \tag{2.33}$$

or

$$\langle \Psi | R^2 | \Psi \rangle \langle \Psi | S^2 | \Psi \rangle \geq \frac{1}{4} |\langle \Psi | [R, S] | \Psi \rangle|^2 . \tag{2.34}$$

The following two operators $\hat{r}, \hat{s}$ have zero expectation value:

$$\hat{r} \equiv \hat{R} - \langle\Psi|R|\Psi\rangle, \qquad \hat{s} \equiv \hat{S} - \langle\Psi|S|\Psi\rangle, \tag{2.35}$$

and the product of their uncertainties is constrained by [see (2.21)]

$$\Delta r \Delta s \geq \frac{1}{2} \left|\langle\Psi|[r,s]|\Psi\rangle\right| . \tag{2.36}$$

Operators corresponding to observables can always be written in the form (2.35). If we prepare a large number of quantum systems in the same state Ψ and then perform some measurements of the observable r in some of the systems, and of s in the others, then the standard deviation Δr of the r-results times the standard deviation Δs of the s-results, should satisfy the inequality (2.36).

In the case of coordinate and momentum operators, the relation (2.16) yields the Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{2.37}$$

We emphasize the fact that this relation stems directly from basic principles and, in particular, from the commutation relation (2.16). It constitutes a limitation upon our knowledge that cannot be overcome, for instance, by any improvement of the experiment.

If the state of the system is an eigenstate of the operator $\hat{r}$, then a measurement of the observable r yields the corresponding eigenvalue. The value of the observable s associated with a noncommuting operator $\hat{s}$ is undetermined. This is the case of a plane wave describing a particle in free space (Sect. 4.3) for which the momentum may be determined with complete precision, while the particle is spread over all space.

Another consequence of the relation (2.36) is that the state vector Ψ may be simultaneously an eigenstate of $\hat{r}$ and $\hat{s}$ only if these two operators commute, since in this case the product of their uncertainties vanishes. Moreover, if the operators commute and the eigenvalues of $\hat{s}$ are all different within a subset of states, then the matrix elements of $\hat{r}$ are also diagonal within the same subset of states (see Sect. 2.7.1*).

Heisenberg conceived the uncertainty relations in order to solve the wave-particle paradox. Pure particle behavior requires localization of the particle, while clear wave behavior appears only when the particle has a definite momentum. Heisenberg's interpretation of this was that each of these extreme classical descriptions is satisfied only when the other is completely untenable. Neither picture is valid for intermediate situations. However, quantum mechanics has to be compatible with the description of the motion of elementary particles (not only with the description of the motion of macroscopic bodies) in terms of trajectories. Heisenberg's answer is that one may construct states Ψ that include a certain amount of localization $\boldsymbol{p}_0(t)$ and $\boldsymbol{x}_0(t)$ in both momentum and coordinate. Thus the motion of a particle has some resemblance to

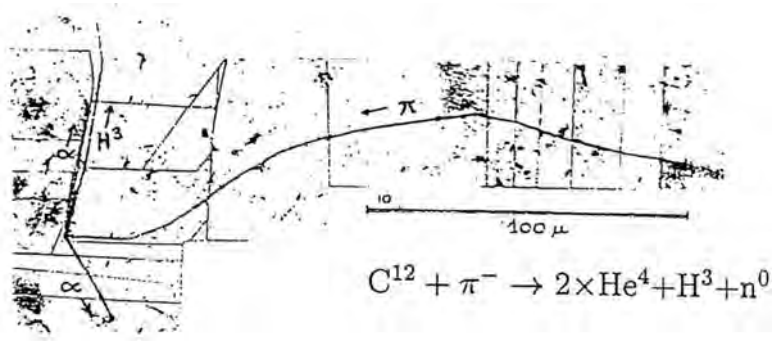

Fig. 2.5. Apparent classical trajectory of a pion (Reproduced with permission from the authors)

classical motion along trajectories. However, there should be a certain spread in the momentum and in the coordinate, such that the amplitudes $\langle \boldsymbol{p}|\Psi\rangle$ and $\langle \boldsymbol{x}|\Psi\rangle$ in momentum eigenstates and position eigenstates allow the uncertainty relations to hold [24].

For an illuminating example, Fig. 2.5 displays the capture of a pion by a carbon nucleus [25]. One can determine the mass, energy and charge of the particles, by measuring the length, the grain density, and the scattering direction of their tracks. Let us assume a pion kinetic energy of 10 MeV. Using the pion mass ($139\,\mathrm{MeV\,c^{-2}}$), one obtains a momentum of $p_\pi = 53\,\mathrm{MeV\,c^{-1}}$. The uncertainty in the direction perpendicular to the track may be estimated from the width of the track $\approx 1\,\mu\mathrm{m}$, which yields $\Delta p_\perp \approx 10^{-7}\,\mathrm{MeV\,c^{-1}}$. The ratio $\Delta p_\perp / p_\pi \approx 10^{-9}$ is too small to produce a visible alteration of the apparent trajectory.

2.7* Hilbert Spaces and Operators

A Hilbert space is a generalization of the Euclidean, three-dimensional space (see Table 2.1). As in ordinary space, the summation $c_a\Psi_a + c_b\Psi_b$ and the scalar product $\langle\Psi_b|\Psi_a\rangle = c_{ab}$ between two vectors are well defined operations.[16] While the constants c_a, c_b, c_{ab} are real numbers in everyday space, it is essential to allow for complex values in quantum mechanics.

Two vectors are orthogonal if their scalar product vanishes. A vector Ψ is linearly independent of a subset of vectors $\Psi_a, \Psi_b, \ldots \Psi_d$ if it cannot be expressed as a linear combination of them[17] ($\Psi \neq c_a\Psi_a + c_b\Psi_b + \cdots + c_d\Psi_d$).

[16] Definitions of these fundamental operations is deferred to each realization of Hilbert spaces [(3.2), (3.4) and (4.1), (4.2)]. In the present chapter we use only the fact that they exist and that $\langle a|b\rangle = \langle b|a\rangle^*$, $\langle a|a\rangle > 0$.

[17] Although the term "linear combination" usually refers only to finite sums, we extend its meaning to include also an infinity of terms.

Table 2.1. Some relevant properties of vectors and operators in Euclidean and Hilbert spaces

	Euclidean space	Hilbert space
vectors	$\boldsymbol{r}$	Ψ
superposition	$\boldsymbol{r} = c_a\boldsymbol{r}_a + c_b\boldsymbol{r}_b$	$\Psi = c_a\Psi_a + c_b\Psi_b$
scalar product	$\langle\boldsymbol{r}_a\|\boldsymbol{r}_b\rangle = \boldsymbol{r}_a{\cdot}\boldsymbol{r}_b = c_{ab}$	$\langle\Psi_a\|\Psi_b\rangle = \langle\Psi_b\|\Psi_a\rangle^* = c_{ab}$
	c_a, c_b, c_{ab} real	c_a, c_b, c_{ab} complex
basis set	$\langle\boldsymbol{v}_i\|\boldsymbol{v}_j\rangle = \delta_{ij}$	$\langle\varphi_i\|\varphi_j\rangle \equiv \langle i\|j\rangle = \delta_{ij}$
dimension ν	3	$2 \le \nu \le \infty$
completeness	$\boldsymbol{r} = \sum_i x_i\boldsymbol{v}_i$	$\Psi = \sum_i c_i\varphi_i$
projection	$x_i = \langle\boldsymbol{v}_i\|\boldsymbol{r}\rangle$	$c_i = \langle\varphi_i\|\Psi\rangle$
scalar product	$\langle\boldsymbol{r}_a\|\boldsymbol{r}_b\rangle = \sum_i x_i^{(a)}x_i^{(b)}$	$\langle\Psi_a\|\Psi_b\rangle = \sum_i (c_i^{(a)})^* c_i^{(b)}$
norm	$\langle\boldsymbol{r}\|\boldsymbol{r}\rangle^{1/2} = \left(\sum_i x_i^2\right)^{1/2}$	$\langle\Psi\|\Psi\rangle^{1/2} = \left(\sum_i \|c_i\|^2\right)^{1/2}$
operators	$\hat{R}_\eta(\theta)\,\boldsymbol{r}_a = \boldsymbol{r}_b$	$\hat{Q}\Psi_a = \Psi_b$
commutators	$\left[\hat{R}_x(\pi/2), \hat{R}_y(\pi/2)\right] \neq 0$	$[\hat{Q}, \hat{R}]$
eigenvalues	$\hat{D}_i\boldsymbol{v}_i = \lambda_i\boldsymbol{v}_i$	$\hat{Q}\varphi_i = q_i\varphi_i$

These last two concepts allow us to define sets of basis vectors φ_i satisfying the requirement of orthonormalization. Moreover, these sets may be complete, in the sense that any vector Ψ may be expressed as a linear combination of them[18] [see (2.6)]. The scalar product $\langle i|\Psi\rangle$ is the projection of Ψ onto φ_i. The scalar product between two vectors Ψ_a, Ψ_b and the square of the norm of the vector Ψ are also given in terms of the amplitudes c_i in Table 2.1.

The number of states in a basis set is the dimension ν of the associated Hilbert space. It has the value 3 in normal space. In this book, we use Hilbert spaces with dimensions ranging from two to a denumerable infinity.

In ordinary space, vectors are defined by virtue of their transformation properties under rotation operations $\hat{R}_\eta(\theta)$ (η denoting the axis of rotation and θ the angle). These operations are generally noncommutative, as the reader may easily verify by performing two successive rotations of $\theta = \pi/2$, first around the x-axis and then around the y-axis, and subsequently comparing the result with the one obtained by reversing the order of these rotations (Fig. 2.6). Vectors in Hilbert spaces may also be transformed through the action of operators $\hat{Q}$ upon them. The operators $\hat{Q}$ obey a noncommutative algebra. We have defined the commutation operation in (2.9).

In ordinary space, a dilation $\hat{D}$ is an operation yielding the same vector multiplied by a (real) constant. This operation has been generalized in terms

[18] The most familiar case of the expansion of a function in terms of an orthonormal basis set is the Fourier expansion in terms of the exponentials $\exp(\mathrm{i}kx)$, which constitutes the complete set of eigenfunctions corresponding to the free particle case (see Sect. 4.3).

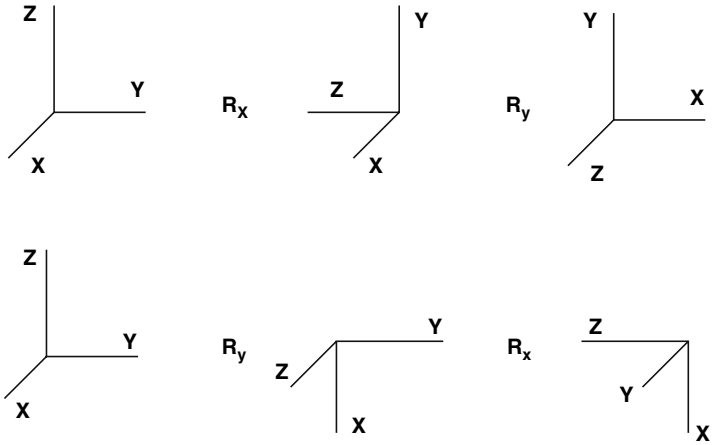

Fig. 2.6. The final orientation of the axes depends on the order of the rotations. R_ν here represents a rotation of $\pi/2$ around the ν-axis

of eigenvectors and eigenvalues in (2.10). In general, linear combinations of eigenvectors do not satisfy the eigenvalue equation.

2.7.1* Some Properties of Hermitian Operators

The Hermitian conjugate operator $\hat{Q}^+$ is defined through (2.12). Similarly, we may write

$$\langle \Psi_b | Q | \Psi_a \rangle = \langle \hat{Q} \Psi_a | \Psi_b \rangle^* = \langle \hat{Q}^+ \Psi_b | \Psi_a \rangle. \tag{2.38}$$

The following properties are easy to demonstrate:

$$\left(\hat{Q} + c\hat{R} \right)^+ = \hat{Q}^+ + c^* \hat{R}^+, \tag{2.39}$$

$$\left(\hat{Q}\hat{R} \right)^+ = \hat{R}^+ \hat{Q}^+. \tag{2.40}$$

According to (2.12), the norm of the state $\hat{Q}\Psi$ is obtained from

$$\langle \hat{Q}\Psi | \hat{Q}\Psi \rangle^{1/2} = \langle \Psi | Q^+ Q | \Psi \rangle^{1/2}. \tag{2.41}$$

Assume now that the state φ_i is an eigenstate of the Hermitian operator $\hat{Q}$ corresponding to the eigenvalue q_i. In this case,

$$\begin{aligned} &\langle i|Q|i\rangle = q_i \langle i \,|\, i \rangle, \qquad \langle i|Q|i\rangle^* = q_i^* \langle i \,|\, i \rangle, \\ &\langle i|Q|i\rangle = \langle i|Q|i\rangle^* \;\rightarrow\; q_i = q_i^*. \end{aligned} \tag{2.42}$$

Therefore, the eigenvalues of Hermitian operators are real numbers.

Consider now the nondiagonal terms

$$\langle j|Q|i\rangle = q_i\langle j\,|\,i\rangle, \qquad \langle i|Q|j\rangle^* = q_j^*\langle i\,|\,j\rangle^* = q_j^*\langle j|i\rangle. \tag{2.43}$$

Then,

$$0 = (q_i - q_j)\langle j\,|\,i\rangle, \tag{2.44}$$

i.e., two eigenstates belonging to different eigenvalues are orthogonal. They may also be orthonormal, upon multiplication by an appropriate normalization constant, which is determined up to a phase.

The eigenvectors of a Hermitian operator constitute a complete set of states for a given system. This means that any state function Ψ, describing any state of the same system, may be expressed as a linear combination of basis states φ_i [see (2.6)].

We define the projection operator (a theoretical filter) $|i\rangle\langle i|$ through the equation

$$|i\rangle\langle i|\varphi_j \equiv \langle i|j\rangle\varphi_i = \delta_{ij}\varphi_i, \tag{2.45}$$

which implies that

$$\sum_i |i\rangle\langle i\,|\,\Psi = \Psi, \tag{2.46}$$

for any Ψ. Thus unity may be expressed as the operator $\sum_i |i\rangle\langle i|$. From this property stems the closure property, according to which the matrix elements of the product of Hermitian operators may be calculated as the sum over all possible intermediate states of products of the matrix elements corresponding to each separate operator:

$$\langle i|QR|j\rangle = \sum_k \langle i|Q|k\rangle\langle k|R|j\rangle. \tag{2.47}$$

2.7.2* Unitary Transformations

The unitary matrix $(\mathcal{U}_{ai}) = (\langle\varphi_i|\eta_a\rangle) = (\langle i|a\rangle)$ in (2.15) transforms the basis set φ_i into the basis set η_a. Such a matrix does not represent a physical observable and it is not therefore required to be Hermitian.

The inverse transformation to (3.14) is written as

$$\varphi_i = \sum_a \langle a\,|\,i\rangle\eta_a. \tag{2.48}$$

Therefore, the inverse transformation $\mathcal{U}^{-1}$ is the transposed conjugate:

$$\mathcal{U}^{-1} = (\langle a\,|\,i\rangle) = \mathcal{U}^+, \qquad \mathcal{U}^+\mathcal{U} = \mathcal{U}\mathcal{U}^+ = \mathcal{I}, \tag{2.49}$$

where $\mathcal{I}$ is the unit matrix. A matrix satisfying (2.49) is said to be unitary [see (2.14)]. Equation (2.49) implies that

$$\sum_i \langle a|i\rangle\langle i|b\rangle = \langle a|b\rangle = \delta_{ab},$$
$$\sum_a \langle i|a\rangle\langle a|j\rangle = \langle i|j\rangle = \delta_{ij}. \tag{2.50}$$

If states are transformed according to $\eta = \mathcal{U}\varphi$, then the state $\mathcal{U}\hat{Q}\varphi$ ($\hat{Q}$ = physical operator) may be written as

$$\mathcal{U}\hat{Q}\varphi = \mathcal{U}\hat{Q}\mathcal{U}^+\mathcal{U}\varphi = \hat{R}\eta, \tag{2.51}$$

which yields the rule for the transformation of operators, namely

$$\hat{R} = \mathcal{U}\hat{Q}\mathcal{U}^+. \tag{2.52}$$

In addition to the norm, unitary transformations preserve the value of the determinant and the trace:

$$\det(\langle a|R|b\rangle) = \det(\langle i|Q|j\rangle),$$
$$\text{trace}\,(Q) \equiv \sum_i \langle i|Q|i\rangle = \text{trace}\,(R) \equiv \sum_a \langle a|R|a\rangle. \tag{2.53}$$

2.8* Notions of Probability Theory

Probability theory studies the likelihood P_i that the outcome q_i of an event will take place. Probability may be defined as

$$P_i \equiv \lim_{N\to\infty} \frac{n_i}{N}, \tag{2.54}$$

where n_i is the number of outcomes q_i of a total of $N \equiv \sum_i n_i$ outcomes. Since the limit $N \to \infty$ is never attained, N should in practice be made large enough to ensure that the fluctuations become sufficiently small.

The limits of P_i are

$$0 \le P_i \le 1. \tag{2.55}$$

If $P_i = 0$, the outcome q_i cannot occur; if $P_i = 1$, it will take place with certainty.

If two events (i, j) are statistically independent, the probability that both i and j take place is given by the product

$$P_{(i\,\text{and}\,j)} = P_i P_j. \tag{2.56}$$

If two events are mutually exclusive, the probability that one or the other occur is the sum

$$P_{(i\,\text{or}\,j)} = P_i + P_j. \tag{2.57}$$

The collection of P_is is called the (discrete) probability distribution. The concepts of average $\langle Q\rangle$, root mean square $\langle Q^2\rangle^{1/2}$ and standard deviation ΔQ, applied in Sect. 2.4, are given by

$$\langle Q\rangle = \sum_i q_i\, P_i,$$

$$\langle Q^2\rangle^{1/2} = \left(\sum_i q_i^2 P_i\right)^{1/2}, \tag{2.58}$$

$$\Delta Q = \langle (Q - \langle Q\rangle)^2\rangle^{1/2} = \left(\langle Q^2\rangle - \langle Q\rangle^2\right)^{1/2}.$$

In the case of a continuous distribution, the sums $\sum_i$ are replaced by integrals $\int \mathrm{d}x$. Instead of probabilities P_i, one defines probability densities $\rho(x)$ such that

$$1 = \int_{-\infty}^{\infty} \rho(x)\mathrm{d}x, \qquad \langle Q\rangle = \int_{-\infty}^{\infty} q(x)\rho(x)\mathrm{d}x. \tag{2.59}$$

Problems

Problem 1. Assume that the state Ψ is given by the linear combination $\Psi = c_1\Psi_1 + c_2\Psi_2$, where the amplitudes c_1, c_2 are arbitrary complex numbers, and both states Ψ_1, Ψ_2 are normalized.

1. Normalize the state Ψ, assuming that $\langle 1|2\rangle = 0$.
2. Find the probability of the system being in the state Ψ_1.

Problem 2. Use the same assumptions as in Problem 1, but $\langle 1|2\rangle = c \neq 0$.

1. Find a linear combination $\Psi_3 = \lambda_1\Psi_1 + \lambda_2\Psi_2$ that is orthogonal to Ψ_1 and normalized.
2. Express the vector Ψ as a linear combination of Ψ_1 and Ψ_3.

Problem 3. Prove the equations (2.39) and (2.40). Hint: Apply successively the definition of Hermitian conjugate to the operators $\hat{Q}, \hat{R}$. For instance, start with $\langle \Psi_b|QR|\Psi_a\rangle = \langle \hat{R}\Psi_a|Q^+|\Psi_b\rangle^*$.

Problem 4. Show that

$$[\hat{Q}, \hat{R}] = -[\hat{R}, \hat{Q}], \qquad [\hat{Q}\hat{R}, \hat{S}] = [\hat{Q}, \hat{S}]\hat{R} + \hat{Q}[\hat{R}, \hat{S}]. \tag{2.60}$$

Problem 5. Find the commutation relation between the coordinate operator $\hat{x}$ and the one-particle Hamiltonian (2.17). Discuss the result in terms of the simultaneous determination of energy and position of a particle.

Problem 6. Find the commutation relations

1. $[\hat{p}^n, \hat{x}]$, where n is an integer.
2. $[f(\hat{p}), \hat{x}]$. Hint: Expand $f(\hat{p})$ in power series of $\hat{p}$ and apply 1.

Problem 7. Verify that the commutation relation (2.16) is consistent with the fact that the operators $\hat{x}$ and $\hat{p}$ are Hermitian.

Problem 8. Assume the basis set of states φ_i.

1. Calculate the effect of the operator $\hat{R} \equiv \sum_i |i\rangle\langle i|$ on an arbitrary state Ψ.
2. Repeat for the operator $\hat{R} \equiv \prod_i (\hat{Q} - q_i)$, assuming that the equation $\hat{Q}\varphi_i = q_i\varphi_i$ is satisfied.

Problem 9. Find the relation between the matrix elements of the operators $\hat{p}$ and $\hat{x}$ in the basis of eigenvectors of the Hamiltonian (2.17).

Problem 10. Consider the eigenvalue equations

$$\hat{F}\varphi_1 = f_1\varphi_1 \; ; \quad \hat{F}\varphi_2 = f_2\varphi_2 \; ; \quad \hat{G}\eta_1 = g_1\eta_1 \; ; \quad \hat{G}\eta_2 = g_2\eta_2 \; ,$$

and the relations

$$\varphi_1 = \frac{1}{\sqrt{5}}\,(2\eta_1 + \eta_2) \; ; \qquad \varphi_2 = \frac{1}{\sqrt{5}}\,(\eta_1 - 2\eta_2) \; .$$

1. Is it possible to simultaneously measure the observables F and G?
2. Assume that a measurement of F has yielded the eigenvalue f_1. Subsequently G and F are measured (in this order). Which are the possible results and their probabilities?

Problem 11. Consider eigenstates φ_p of the momentum operator. Assume that the system is prepared in the state

$$\Psi = \frac{1}{\sqrt{6}}(\varphi_{2p} + \varphi_p) + \sqrt{\frac{2}{3}}\varphi_{-p}.$$

1. What are the possible results of a measurement of the kinetic energy K, and what are their respective probabilities?
2. Calculate the expectation value and standard deviation of the kinetic energy.
3. What is the vector state after a measurement of the kinetic energy that has yielded the eigenvalue $k_p = p^2/2M$?

Problem 12. Evaluate in m.k.s. units possible values of the precision to which the velocity and the position of a car should be measured in order to verify the uncertainty relation (2.37).

Problem 13. A 10 MeV proton beam is collimated by means of diaphragms with a 5 mm aperture.

1. Show that the spread in energy ΔE_{H} associated with the uncertainty principle is negligible relative to the total spread $\Delta E \approx 10^{-3}$ MeV.
2. Calculate the distance x that a proton has to travel in order to traverse 5 mm in a perpendicular direction, if the perpendicular momentum is due only to the uncertainty principle.