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CHAPTER I

# Mathematical Preliminaries

The mathematical language of quantum mechanics is introduced in this chapter. It does not contain any physics.

## I.1 The Mathematical Language of Quantum Mechanics

To formulate Newtonian mechanics, the mathematical language of differential and integral calculus was developed. Though one can get some kind of understanding of velocity, acceleration, etc., without differential calculus (in particular for special cases), the real meanings of these physical notions in their full generality become clear only after one is familiar with the idea of the derivative. On the other hand, though, the abstract mathematical definitions of calculus become familiar to us only if we visualize them in terms of their physical realizations. Nowadays, no one would attempt to understand classical mechanics without knowing calculus.

Quantum mechanics, too, has its mathematical language, whose development went parallel to the development of quantum mechanics and whose creation in its full generality was inspired by the needs of quantum physics. This is the language of linear spaces, linear operators, associative algebras, etc., which has meanwhile grown into one of the main branches of mathematics—linear algebra and functional analysis. Although one might obtain some sort of understanding of quantum physics without knowing its mathematical language, the precise and deep meaning of the physical notions in their full generality will not reveal themselves to anyone who does not understand its mathematical language.

A linear space is a set with very little mathematical structure. We will equip it with more structure by defining a scalar product. This notion is again a generalization from the three-dimensional real space $\mathbb{R}^3$.

A linear space is called a *scalar product space* (or *Euclidean space* or *pre-Hilbert space*) if in it a function $(\phi, \psi)$ of the two vectors $\phi, \psi \in \Phi$ is defined which is a complex number and has the following properties

$$(\phi, \phi) \geq 0 \quad \text{and} \quad (\phi, \phi) = 0 \quad \text{iff} \quad \phi = 0. \tag{2.2a}$$

$$(\psi, \phi) = \overline{(\phi, \psi)} \tag{2.2b}$$

(the bar denotes complex conjugate),

$$(\phi, a\psi) = a(\phi, \psi) \tag{2.2c}$$

($a \in \mathbb{C}$, the set of complex numbers),

$$(\phi_1 + \phi_2, \psi) = (\phi_1, \psi) + (\phi_2, \psi). \tag{2.2d}$$

This function is called the *scalar product* of the elements $\phi$ and $\psi$. The usual scalar product in $\mathbb{R}^3$, $(\mathbf{a}, \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}$ clearly fulfills the conditions (2.2a)–(2.2d) with all numbers being real instead of complex.

As in $\mathbb{R}^3$ one calls two vectors $\phi$ and $\psi$ *orthogonal* if

$$(\phi, \psi) = 0. \tag{2.3}$$

With the scalar product defined by (2.2a)–(2.2d) one defines the *norm* $\|\phi\|$ of a vector $\phi$ by

$$\|\phi\| = +\sqrt{(\phi, \phi)}. \tag{2.4}$$

For any vector $\psi$ different from the zero vector one can always define a vector $\hat{\psi} = \psi/\|\psi\|$, which has the property $\|\hat{\psi}\| = 1$ and is called a *normalized* vector.

Sometimes one needs in a linear space a more general notion than the scalar product, the bilinear Hermitian form.

A complex-valued function $h(\phi, \psi)$ of two vector arguments is a *Hermitian form* if it satisfies

$$h(\phi, \psi) = \overline{h(\psi, \phi)}, \tag{2.5b}$$

$$h(\phi, a\psi) = ah(\phi, \psi) \quad (a \in \mathbb{C}), \tag{2.5c}$$

$$h(\phi_1 + \phi_2, \psi) = h(\phi_1, \psi) + h(\phi_2, \psi). \tag{2.5d}$$

If in addition $h$ satisfies

$$h(\phi, \phi) \geq 0 \tag{2.5a}$$

for every vector $\phi$, then $h$ is said to be a *positive Hermitian form*. A positive Hermitian form is called *positive definite* if

$$\text{from} \quad h(\phi, \phi) = 0 \quad \text{follows} \quad \phi = 0 \quad \text{for every vector } \phi. \tag{2.6}$$

Thus a Hermitian form fulfills the conditions (2.2b), (2.2c), and (2.2d), but not the condition (2.2a) for a scalar product. However, a positive definite Hermitian form is, by (2.6), a scalar product.



Positive Hermitian forms, which are not necessarily scalar products, satisfy the *Cauchy–Schwarz–Bunyakovski inequality*:

$$|h(\phi, \psi)|^2 \leq h(\phi, \phi)h(\psi, \psi). \tag{2.7}$$

If $h$ is positive definite, equality holds iff $\phi = a\psi$ for some $a \in \mathbb{C}$.

A set $M$ in the linear space $\Phi$ is called a *subspace* of $\Phi$ if $M$ is a linear space under the same definitions of the operations of addition and multiplication by a number as given for $\Phi$, i.e., if it follows from $\phi, \psi \in M$ that $a\phi \in M$ and $\phi + \psi \in M$.

An expression of the form $a_1\phi_1 + a_n\phi_n$ is called a *linear combination* of the vectors $\phi_1, \phi_2, \ldots, \phi_n$; the vectors $\phi_1, \phi_2, \ldots, \phi_n$ are said to be *linearly dependent* if there exist numbers $a_1, a_2, \ldots, a_n$, not all zero, for which $a_1\phi_1 + a_2\phi_2 + \cdots + a_n\phi_n = 0$. If the equation $a_1\phi_1 + a_2\phi_2 + \cdots + a_n\phi_n = 0$ holds only for $a_1 = a_2 = \cdots = a_n = 0$, then the vectors $\phi_1, \phi_2, \ldots, \phi_n$ are called *linearly independent*. A space $\Phi$ is said to be *finite-dimensional* and, more precisely, *n-dimensional* if there are $n$ and not more than $n$ linearly independent vectors in $\Phi$. If the number of linearly independent vectors in $\Phi$ is arbitrarily great, then $\Phi$ is said to be *infinite-dimensional*. Every system of $n$ linearly independent vectors in an $n$-dimensional space $\Phi$ is called a *basis* for $\Phi$.

An *isomorphism* between two algebraic structures $\mathscr{A}$ and $\mathscr{B}$ is a one-to-one correspondence between the sets $\mathscr{A}$ and $\mathscr{B}$ (i.e., to every $a \in \mathscr{A}$ there corresponds exactly one $b \in \mathscr{B}$ and vice versa: $a \leftrightarrow b$), which preserves the algebraic operations.

Two linear scalar product spaces $\Phi$ and $\Phi'$ are, thus, isomorphic if from

$$\Phi \ni f \leftrightarrow f' \in \Phi', \qquad \Phi \ni g \leftrightarrow g' \in \Phi' \tag{2.8}$$

it follows that

$$\alpha f + \beta g \leftrightarrow \alpha f' + \beta g', \quad \alpha, \beta \in \mathbb{C} \tag{2.9}$$

and

$$(f, g)_\Phi = (f', g')_{\Phi'}. \tag{2.10}$$

Scalar product spaces (and in particular Hilbert spaces) for which (2.9) and (2.10) are fulfilled are also called isometric. It often happens that two scalar product spaces are isomorphic as linear spaces, i.e., are in a one-to-one correspondence which fulfills (2.9), but are not isomorphic as scalar product spaces, i.e., the correspondence does not fulfill (2.10).

## I.3 Linear Operators

Vectors in $\mathbb{R}^3$ can be transformed into each other. One example is the rotation $R$ of a vector $\mathbf{a}$ into a vector $R\mathbf{a} = \mathbf{b}$. In analogy to this one defines transformations or *linear operators* on a linear space $\Phi$. A function $A$, $A: \Phi \to \Phi$, that maps each vector $\phi$ in a linear space $\Phi$ into a vector $\psi \in \Phi$,

$$A\phi = \psi,$$

is called a linear operator if for all $\phi, \psi \in \Phi$ and $a \in \mathbb{C}$ it fulfills the conditions

$$A(\phi + \psi) = A\phi + A\psi, \tag{3.1}$$

$$A(a\phi) = aA\phi. \tag{3.2}$$

It is called *antilinear* if it fulfills instead of (3.2) the relation

$$A(a\phi) = a^* A\phi, \tag{3.3}$$

where $a^*$ is the complex conjugate of $a$.

The operations of addition of two operators $A + B$, multiplication of an operator by a complex number $aA$, and multiplication of two operators $AB$, are defined in the following way:

$$(A + B)\phi = A\phi + B\phi, \quad (aA)\phi = a(A\phi), \quad (AB)\phi = A(B\phi), \tag{3.4}$$

for all $\phi \in \Phi$. It is easily verified that $A + B$, $aA$ and $AB$ are linear operators if $A$ and $B$ are linear operators.

Of special interest are the zero operator, denoted 0, and the unit operator or identity operator, denoted $I$, which are defined by

$$0\psi = 0, \quad I\psi = \psi \tag{3.5}$$

for every $\psi \in \Phi$. Note that 0 on the left is the zero operator, while 0 on the right is the zero vector of (2.1c).

For every linear operator $A$ defined on *all* of $\Phi$, one can define an operator $A^\dagger$ by $(A^\dagger\phi, \psi) = (\phi, A\psi)$ for every $\phi, \psi \in \Phi$. The operator $A^\dagger$ is called the *adjoint operator* of $A$. An operator for which $A^\dagger = A$ is called *self-adjoint* or Hermitian.[1]

The definition of linear operators was inspired by the properties of transformations on the three-dimensional space. Linear operators on a linear space $\Phi$ may represent such transformations on the physical three-dimensional space, but they can also have other physical interpretations. In particular, in quantum physics they represent physical observables.

An important notion is the notion of eigenvalue and eigenvector. A symmetric tensor $\mathbb{I}$ in three dimensions can be diagonalized by transforming to its principal axis:

$$\mathbb{I} \cdot \mathbf{a} = \mathrm{I}_{(a)}\mathbf{a}, \tag{3.6a}$$

where $\mathrm{I}_{(a)}$ is the eigenvalue and $\mathbf{a}$ the corresponding eigenvector. Similarly one defines eigenvalues and eigenvectors in a linear space $\Phi$. A nonzero vector $\psi \in \Phi$ is called an eigenvector of the linear operator $A$ if

$$A\psi = \lambda\psi \quad \text{with} \quad \lambda \in \mathbb{C}. \tag{3.6b}$$

$\lambda$ is called the eigenvalue of $A$ corresponding to the eigenvector $\psi$. For a given operator $A$ there may be many (perhaps infinitely many) different

[1] We will usually use the term Hermitian if we do not want to distinguish between the mathematically precisely defined notions *self-adjoint*, *essentially self-adjoint*, and *symmetric*.



eigenvectors with different eigenvalues. There are also linear operators on linear spaces which do not have one single eigenvector in that space.

If $A$ is a Hermitian operator, $A^\dagger = A$, then eigenvectors and eigenvalues have the following properties:

(1) All eigenvalues are real.
(2) If $\phi_1$ and $\phi_2$ are eigenvectors of $A$ with eigenvalues $\lambda_1$ and $\lambda_2$, respectively, and if $\lambda_1 \neq \lambda_2$, then $\phi_1$ and $\phi_2$ are orthogonal to each other, $(\phi_1, \phi_2) = 0$.

The notion of eigenvalue is important in quantum physics: As mentioned above, the operators represent the observables of a physical system. The eigenvalues then represent the numbers which are obtained in a measurement of one of these observables.

An operator $B$ is called the inverse of an operator $A$ if

$$BA = AB = I. \tag{3.7a}$$

It is denoted by

$$B = A^{-1}. \tag{3.7b}$$

A linear operator $U$ is called a unitary operator if

$$U^\dagger U = UU^\dagger = I. \tag{3.8a}$$

Because of (3.7) one defines a unitary operator also by the condition:

$$U^\dagger = U^{-1}. \tag{3.8b}$$

Let $A$ and $B$ be two operators. $A$ and $B$ are said to *commute* if

$$[A, B] \equiv AB - BA = 0. \tag{3.9}$$

$[A, B]$ is called the *commutator* of $A$ and $B$.

A set $\mathscr{A}$ is an (*associative*) *algebra with unit element* iff

(a) $\mathscr{A}$ is a linear space.
(b) For every pair $A, B \in \mathscr{A}$, there is defined a product $AB \in \mathscr{A}$ such that

$$(AB)C = A(BC), \tag{3.10a}$$

$$A(B + C) = AB + AC, \tag{3.10b}$$

$$(A + B)C = AC + BC, \tag{3.10c}$$

$$(aA)B = A(aB) = aAB. \tag{3.10d}$$

(c) There exists an element $I \in \mathscr{A}$ such that

$$IA = AI = A \tag{3.11}$$

for all $A \in \mathscr{A}$.

A subset $\mathscr{A}_1$ of an algebra is called a *subalgebra of* $\mathscr{A}$ if $\mathscr{A}_1$ is an algebra with the same definitions of the operations of addition, multiplication by a number, and multiplication as given for $\mathscr{A}$; i.e., if from $A, B \in \mathscr{A}_1$, it follows that $A + B \in \mathscr{A}_1$, $aA \in \mathscr{A}_1$, and $AB \in \mathscr{A}_1$.

An algebra $\mathscr{A}$ is called a **-algebra* if we have on the algebra a **-operation* (involution) $A \mapsto A^\dagger$ that has the following defining properties:

$$\text{(d)}\qquad \begin{aligned}(aA + bB)^\dagger &= \bar{a}A^\dagger + \bar{b}B^\dagger,\\ (AB)^\dagger &= B^\dagger A^\dagger,\\ (A^*)^\dagger &= A,\\ I^\dagger &= I,\end{aligned} \tag{3.12}$$

where $A, B \in \mathscr{A}$ and $a, b \in \mathbb{C}$. From the definitions of the sum and product of operators with a number—given in (3.4)—and from the definition of the formal adjoint operator, one can see that the set of linear operators fulfills all the axioms (a), (b), (c), and (d) of a *-algebra. Thus the set of linear operators in a linear space forms a *-algebra. A *-subalgebra of this algebra is called an *operator *-algebra*. It can be shown that in a certain sense every *-algebra can be realized as an operator *-algebra in a scalar-product space (generalization of the Gelfand–Naimark–Segal reconstruction theorem). In quantum mechanics physical systems are assumed to be described by operator *-algebras.

A set $X_1, X_2, \dots, X_n$ of elements of $\mathscr{A}$ is called a *set of generators*, and $\mathscr{A}$ is said to be *generated* by the $X_i$ ($i = 1, 2, \dots, n$) iff each element of $\mathscr{A}$ can be written

$$A = cI + \sum_{i=1}^{n} c^i X_i + \sum_{i,j}^{n} c^{ij} X_i X_j + \cdots, \tag{3.13}$$

where $c, c^i, c^{ij}, \dots \in \mathbb{C}$.

*Defining algebraic relations* are relations among the generators

$$P(X_i) = 0, \tag{3.14}$$

where $P(X_i)$ is a polynomial with complex coefficients of the $n$ variables $X_i$. An element $B \in \mathscr{A}$,

$$B = bI + \sum b^i X_i + \sum b^{ij} X_i X_j + \cdots, \tag{3.15}$$

where $b, b^i, \dots \in \mathbb{C}$, is *equal* to the element $A$ iff (3.15) can be brought into the same form (3.13) with the same coefficients $c, c^i, c^{ij}, \dots$ by the use of the defining relations (3.14).

## I.4 Basis Systems and Eigenvector Decomposition

As in the three-dimensional space $\mathbb{R}^3$, one can also introduce a system of basis vectors in a general linear space $\Phi$. In $\mathbb{R}^3$ one conveniently chooses a system of three normalized vectors

$$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \qquad \|\mathbf{e}_i\| = 1,$$

which are orthogonal to each other

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, \qquad i, j = 1, 2, 3.$$



Such an *orthonormal basis system* can also always be chosen in a linear scalar product space $\Phi$. We denote these basis vectors in various ways by

$$e_i = |e_i\rangle = |i\rangle, \qquad i = 1, 2, 3, \dots, N. \tag{4.1}$$

Their scalar products are written in one of the following ways:

$$(e_i, e_j) \equiv (e_i|e_j) \equiv \langle i|j\rangle = \delta_{ij}, \qquad i, j = 1, 2, \dots. \tag{4.2}$$

If $\Phi$ is $N$-dimensional then there are $N$ linearly independent vectors in this orthonormal basis system. $N$ can be infinite.

The basis system fulfilling (4.2) can be chosen arbitrarily, but it is convenient to choose it such that the particular physical problem under investigation takes its simplest mathematical form. For example, if one describes a rigid body with moment of inertia tensor $\mathbb{I}$ in the usual three-dimensional space, then it is useful to choose the basis system, $\mathbf{e}_i$, $i = 1, 2, 3$ such that

$$\mathbf{e}_i \cdot \mathbb{I} \cdot \mathbf{e}_j = I_{(i)}\delta_{ij},$$

i.e., choose—according to (3.6a)—eigenvectors of the tensor $\mathbb{I}$.

Similarly, it is extremely useful to choose as the basis system for the space of physical states, $\Phi$, eigenvectors of an operator $A$ which represents an important observable of the physical system under investigation (most frequently one chooses for $A$ the energy operator $H$, the position operator $Q$ or the momentum operator $P$). Thus one would want to choose for the basis system a set of vectors $e_i$ which fulfill

$$Ae_i = a_i e_i, \qquad a_i \in \mathbb{C}, \tag{4.3}$$

where the $a_i$ are the eigenvalues. These normalized eigenvectors are often denoted by

$$e_i = |a_i) \quad \text{or} \quad e_i = |a_i\rangle.$$

The symbol $|\ \rangle$ with a letter $\phi$, $a$ or $i$ in it denoting a vector $\phi$, an eigenvalue $a$ or an index $i$ of an eigenvalue is called a *ket*; the symbol $\langle\ |$ with a letter in it is called a *bra*.[2]

In the three-dimensional space $\mathbb{R}^3$ every vector $\mathbf{v}$ can be expanded with respect to a basis system of eigenvectors of any symmetric tensor, i.e.,

$$\mathbf{v} = \sum \mathbf{e}_i v_i, \quad \text{where the} \quad v_i = \mathbf{e}_i \cdot \mathbf{v} \tag{4.4a}$$

are the coordinates or components of the vector $\mathbf{v}$ with respect to the basis of eigenvectors $\{\mathbf{e}_i\}$ of the symmetric tensor $\mathbb{I}$ (3.6a). The same can be proven

[2] P. A. M. Dirac (1958).

for any finite-dimensional linear scalar product space $\Phi$. This means that: For every Hermitian operator $A$ in a finite-dimensional space $\Phi$ there exists a system of eigenvectors

$$Ae_i = a_i e_i, \qquad i = 1, 2, \ldots, N = \text{finite}, \tag{4.3}$$

such that every vector $\phi \in \Phi$ can be written as

$$\phi = \sum_{i=1}^{N} e_i(e_i, \phi) \equiv \sum_{i=1}^{N} e_i(a_i|\phi), \tag{4.4b}$$

where the complex numbers

$$c_i = (e_i, \phi) \equiv (a_i|\phi) \tag{4.5}$$

are the components of the vector $\phi$ with respect to the basis $\{e_i\}$.

The set of $a_i$'s (which are real if $A$ is Hermitian) is called the spectrum of $A$ and the above statement is called the spectral theorem for the operator $A$ in a finite-dimensional space. Equation (4.4b) is called the *spectral decomposition* of the vector $\phi$ or the *eigenvector expansion* of $\phi$.

For infinite-dimensional spaces the above statement is in general not correct. Though there is always a countably infinite set of orthogonal basis vectors, every self-adjoint operator need not have a countably infinite set of eigenvectors which form a basis. Furthermore, quantum physics also requires operators whose set of eigenvalues is a continuous set, or even a union of a discrete set and a continuous set.

It could have been that all operators which appear in quantum physics have the property that the set of their eigenvalues is discrete. That would have been the case if the measurement for every observable in quantum physics could only lead to a discrete set of numbers. Then only an infinite-dimensional generalization of (4.3) and (4.4) would be needed. However, there are observables in physics whose measurement can lead to any number out of a continuous set of numbers (e.g., the observables momentum and position can in many cases take any value $x$ with $-\infty < x < +\infty$). Therefore we need not only the infinite-dimensional generalization (which can be obtained in the Hilbert space) but also the continuous, infinite-dimensional generalization of (4.3) and (4.4). There exist in fact spaces $\Phi$—or more precisely, there exist topologies for infinite-dimensional linear spaces—for which the generalization of the finite-dimensional spectral decomposition can be proven for all self-adjoint operators needed in physics.[3] This generalization is the nuclear spectral theorem. As the eigenvector decomposition is so important for physics we will only use spaces for which this theorem is valid.

We cannot present the mathematics here and will explain the discrete and continuous eigenvector decomposition in an infinite-dimensional space in analogy to the finite-dimensional case (4.4b) or (4.4a). We consider the discrete and continuous cases separately; the general case of an arbitrary self-adjoint operator of physics will be a combination of these two cases.

[3] These spaces $\Phi$ and their conjugates $\Phi^\times$ (cf. Section I.7 below) (and the closely related theory of distributions) and the triplet $\Phi \subset \mathscr{H} \subset \Phi^\times$ they form with the Hilbert space $\mathscr{H}$ did in fact not exist when they were needed for quantum mechanics. The creation of these mathematical structures was inspired by the development of quantum theory.



We will call the self-adjoint operator with a discrete set of eigenvalues $H$ and the operator with a continuous set of eigenvalues $Q$. Then the spectral theorem asserts:

There exists a system of eigenvectors $|E_n\rangle$ in the discrete case and $|x\rangle$ in the continuous case;

$$H|E_n\rangle = E_n|E_n\rangle, \qquad E_n = E_0, E_1, E_2, \ldots, \tag{4.3d}$$

$$Q|x\rangle = x|x\rangle; \qquad -\infty \le m \le x \le M \le +\infty, \tag{4.3c}$$

such that *every* $\phi \in \Phi$ can be expanded in terms of these eigenvectors:

$$\phi = \sum_{n=0}^{\infty} |E_n\rangle(E_n|\phi\rangle, \tag{4.4d}$$

$$\phi = \int_m^M dx\,|x\rangle\langle x|\phi\rangle, \tag{4.4c}$$

and $\phi = 0$ if and only if all its components are zero, i.e., $(E_n|\phi\rangle = 0$ for all $E_n$ and $\langle x|\phi\rangle = 0$ for all $x$.[4]

A system of eigenvectors $|E_n\rangle$ or $|x\rangle$ with these properties is called *complete* or a *basis system*. Thus the spectral theorem asserts the existence of a complete system of eigenvectors of a self-adjoint operator. $(E_n|\phi\rangle$ or $\langle x|\phi\rangle$ are called the coordinates or components of $\phi$ with respect to the basis system $\{|E_n\rangle\}$ or $\{|x\rangle\}$, respectively. They are, as in the three-dimensional case, the scalar products of the eigenvectors with $\phi$:

$$\langle x|\phi\rangle = (|x\rangle, \phi), \tag{4.5c}$$

$$(E_n|\phi\rangle = (|E_n\rangle, \phi). \tag{4.5d}$$

Thus $(E_n|\phi\rangle$ is the infinite-dimensional generalization of the $v_i$ in (4.4a), and $\langle x|\phi\rangle$ is the continuous infinite-dimensional generalization of $v_i$.

Whereas the $|E_n\rangle$ are proper eigenvectors, the $|x\rangle$ are called generalized eigenvectors, or, *eigenkets*. Though we can manipulate them as if they were proper eigenvectors, mathematically there is an important difference between the discrete basis vectors $|E_n\rangle$ and the continuous basis vectors $|x\rangle$: the $|E_n\rangle$ are in $\Phi$ while the $|x\rangle$ are in $\Phi^\times$, the space of continuous antilinear functionals over $\Phi$. We shall define and explain these mathematical notions in Section I.7. Here we shall try to convey the meaning of these generalized eigenvectors by analogy to the finite-dimensional case.

The set of eigenvalues $E_n$ in (4.3d) is called the spectrum of the operator $H$. If $H$ has a discrete set of eigenvalues, the spectrum is called discrete. All the corresponding eigenvectors $|E_n\rangle$ enter into the discrete basis vector expansion (4.4d) and there are no further eigenvectors with discrete eigenvalue that enter into the basis vector expansion (4.4d). The set of continuous eigenvalues $x$, whose eigenvectors enter into the generalized eigenvector expansion (4.4c), is called the continuous spectrum of the operator $Q$.

[4] The simple nondegenerate form (4.4d), (4.4c) is valid if the operator $A$ ($H$ or $Q$) is cyclic, i.e., if there exists an $f \in \Phi$ such that $A^n f = f_{(n)}$ generate the entire space $\Phi$, which means that any $\phi \in \Phi$ can be written as $\phi = \sum_n f_{(n)} c_{(n)}$ where $c_{(n)}$ are complex numbers. Degenerate spectra, which occur when more than one quantum number is needed, will be discussed later in the text.

In general—and this depends upon the properties of the space $\Phi$—there are more generalized eigenvectors of $Q$—i.e., kets which fulfill (4.3c) and whose precise definition will be given in Section I.7—than enter in the eigenvector expansion (4.4c). Their generalized eigenvalues we will not include in the definition of the continuous spectrum. Whereas the discrete eigenvalues of a self-adjoint operator are always real, the generalized eigenvalues need not be real; they can be real or complex, and even if they are real they need not necessarily belong to the spectrum, i.e., appear in the integral (4.4c). But for a self-adjoint operator there is always a real subset of the set of generalized eigenvalues whose eigenvectors are complete.

The most general form of the spectral theorem for an operator $A$ representing a physical observable is a combination of (4.4d) and (4.4c):

$$\phi = \sum |a_i\rangle\langle a_i|\phi\rangle + \int da\, |a\rangle\langle a|\phi\rangle, \tag{4.4g}$$

where the sum is over the discrete spectrum and the integral is over the (absolutely) continuous spectrum of $A$. It can happen that some or all values $a_i$ appearing in the sum also appear in the integral. Then they are called discrete eigenvalues in the continuous spectrum. If this happens for $a_k$ then $|a_k\rangle$, is still orthogonal to all $|a\rangle$ including $|a_k\rangle$, i.e.,

$$\langle a_k|\phi^c\rangle = 0 \quad \text{for} \quad \phi^c = \int da\, |a\rangle\langle a|\phi^c\rangle.$$

The spectral theorem (4.4b), (4.4d), (4.4c), and (4.4g)—which we have to accept here without proof[5]—is the central statement, from which the other results of this section follow.

To see that the coordinates $(E_n|\phi)$ are indeed what their notation indicates, namely the scalar product of the vector with the basis vector $|E_n)$, we calculate the scalar product of (4.4d) with the eigenvector $|E_m)$. From (4.4d), it follows that

$$(|E_m), \phi) = \sum_{n=0}^{\infty} (|E_m), |E_n))(E_n|\phi). \tag{4.6d}$$

Since $|E_m)$ and $|E_n)$ are eigenvectors of the same Hermitian operator $H$, if $E_n \neq E_m$ they must be orthogonal to each other,

$$(|E_m), |E_n)) = 0. \tag{4.7'}$$

For $E_n = E_m$ we normalize them:

$$(|E_n), |E_n)) = \| |E_n) \|^2 = 1. \tag{4.7''}$$

[5] The finite-dimensional case (4.4b) is easily reduced to the problem of the number of roots of a polynomial of degree $N$, as shown in Section I.5 below in particular by Equation (5.17). Equations (4.4d) and (4.4c) need much more mathematical preparation, cf. I. M. Gelfand *et al.* (1964), Vol. 4, or K. Maurin (1968).



This we combine and write

$$(|E_m), |E_n)) = (E_m|E_n) = \delta_{E_n E_m} = \delta_{nm}; \qquad n, m = 1, 2, \ldots, \tag{4.7d}$$

where the Kronecker $\delta$ is defined by

$$\delta_{nm} = \delta_{E_n E_m} = \begin{cases} 1 & \text{for } n = m; \quad E_n = E_m, \\ 0 & \text{for } n \neq m; \quad E_n \neq E_m. \end{cases} \tag{4.8}$$

So these eigenvectors of the self-adjoint operator $H$ have the property (4.2) as required of orthonormal basis vectors. Inserting (4.7d) into (4.6d) one obtains:

$$(|E_m), \phi) = \sum_{n=0}^{\infty} \delta_{mn}(E_n|\phi) = (E_m|\phi). \tag{4.5}$$

This is the expected identity (4.5d).

The spectral theorem (4.4d) can be written in different forms: one can omit the arbitrary vector $\phi \in \Phi$ on both sides of (4.4d) and obtain the *spectral resolution of the identity operator* $I$:†

$$I = \sum_{n=0}^{\infty} |E_n)(E_n|. \tag{4.9d}$$

One can multiply both sides of (4.4d) with the operator $H$,

$$H\phi = \sum_{n=0}^{\infty} H|E_n)(E_n|\phi) = \sum_{n=0}^{\infty} E_n|E_n)(E_n|\phi),$$

and then omit the arbitrary vector $\phi$ on both sides to obtain:

$$H = \sum_{n=0}^{\infty} E_n|E_n)(E_n|. \tag{4.10d}$$

This identity between the operator $H$ and the weighted sum of operators $|E_n)(E_n|$ is called the *spectral resolution of the self-adjoint operator H with discrete spectrum.*

One can take the scalar product of (4.4d) with another $\psi \in \Phi$, then one obtains

$$(\psi, \phi) = \sum_{n=0}^{\infty} (\psi|E_n)(E_n|\phi) = \sum_{n=0}^{\infty} (E_n|\psi)^*(E_n|\phi). \tag{4.11d}$$

In particular if one chooses $\psi = \phi$ one obtains

$$\|\phi\|^2 = (\phi, \phi) = \sum_{n=0}^{\infty} (\phi|E_n)(E_n|\phi) = \sum_{n=0}^{\infty} |(E_n|\phi)|^2. \tag{4.12d}$$

Equation (4.11d) is the analogue of the formula

$$\mathbf{v} \cdot \mathbf{x} = \sum_{i,j=1}^{3} v_i \mathbf{e}_i \cdot \mathbf{e}_j x_j = \sum_{i=1}^{3} v_i x_i$$

for the ordinary scalar product in $\mathbb{R}^3$.

† The quantities $\Lambda_n = |E_n)(E_n|$ are projection operators as defined in the mathematical insert on p. 58.

As in the three-dimensional space $\mathbb{R}^3$, a vector $\phi$ is completely specified by its components $(E_n|\phi)$ with respect to a given basis $|E_n)$. But unlike the three-dimensional space $\mathbb{R}^3$, where any sequence of three real numbers $(x_1, x_2, x_3)$ defines a vector **x**, or unlike the $N$-dimensional complex space $\mathbb{C}^N$ where any sequence of $N$ complex numbers $(\xi_1, \xi_2, \ldots, \xi_N)$ defines a vector **x**, an arbitrary infinite sequence of complex numbers

$$(\phi_1, \phi_2, \phi_3, \ldots, \phi_n, \ldots)$$

does not in general define a vector in $\Phi$. As can be seen from (4.12d), in order that the scalar product be defined, the infinite sequence that defines a vector must at least fulfill the condition

$$\sum_{i=1}^{\infty} |\phi_i|^2 < \infty, \tag{4.12d'}$$

i.e., it must be *square summable*. If one further wants to demand that every operator $A$ of the set of operators which represents physical observables be defined in the whole space $\Phi$, one has to require that all $A\phi$ are well defined in $\Phi$, which means that $(A\phi, A\phi)$ must be finite. Choosing $A = H^p$ where $p = 0, 1, 2 \ldots$ is any power, one obtains for this requirement the following condition:

$$(H^p\phi, H^p\phi) = \sum_{n=0}^{\infty} (\phi|H^p|E_n)(E_n|H^p|\phi)$$
$$= \sum_{n=0}^{\infty} E_n^{2p}|(E_n|\phi)|^2 < \infty \quad \text{for any} \quad p = 0, 1, 2, \ldots. \tag{4.13d}$$

Thus not only will $\{(E_n|\phi)|n = 0, 1, 2, \ldots\}$ have to be square summable, but also $\{E^p(E_n|\phi)\}$ has to be a square summable sequence for any $p = 0, 1, 2, \ldots$.

Fortunately these (topological) questions of what happens at infinity are not very relevant for physics as only a finite number of the $|(E_n|\phi)|$ can be determined experimentally.

We now turn to the continuous spectrum and repeat the above considerations for the continuous case. We calculate the scalar product of $\phi$ with the generalized eigenvector $|x\rangle$[6] using Equation (4.4c):

$$(|x\rangle, \phi) = \int dy\, (|x\rangle, |y\rangle)\langle y|\phi\rangle.$$

This we rewrite with the following definition of the new symbol

$$\langle x|y\rangle \equiv (|x\rangle, |y\rangle)$$

[6] More precisely, using the notions that will be introduced in Section I.7, we should say that we calculate the value $(|x\rangle, \phi)$ of the functional $|x\rangle$ at the vector $\phi \in \Phi$, $(|x\rangle, \phi) = \langle x|\phi\rangle$ is a generalization of the usual scalar product.



as

$$(|x\rangle, \phi) = \int dy\, \langle x|y\rangle\langle y|\phi\rangle. \tag{4.6c}$$

$\langle x|\phi\rangle$ is the coordinate of the vector $\phi$ along the direction of the basis vector $|x\rangle$. $(|x\rangle, \phi)$ is the scalar product of $\phi$ with the basis vector $|x\rangle$. These two quantities should be the same, as stated by (4.5). Therefore (4.6c) has the form

$$\langle x|\phi\rangle = \int_{-\infty}^{\infty} dy\, \langle x|y\rangle\langle y|\phi\rangle. \tag{4.6c'}$$

The scalar products $\langle y|\phi\rangle$ are functions of the continuous variable $y$ in the same way as the scalar products $(E_n|\phi)$ are functions of the discrete variable $E_n$. Equation (4.6c') therefore says that the mathematical quantity $\langle x|y\rangle$ has the property that it maps the function $\phi(y) = \langle y|\phi\rangle$ by integration into its value at the point $x$: $\phi(x) = \langle x|\phi\rangle$. There exist no well-behaved and not even a locally integrable function which has this property.

Such a quantity is called a distribution or a generalized function. The distribution $\langle x|y\rangle$ *defined* by (4.6c') for a class of well-behaved functions $\phi(x) = \langle x|\phi\rangle$ is called the Dirac $\delta$-function and is denoted in analogy to (4.7d) as

$$\langle x|y\rangle = \delta(x - y). \tag{4.7c}$$

$\delta(x - y)$ is a generalization of the Kronecker $\delta_{E_n E_m}$ which is usually defined by (4.8) but which could as well have been defined by

$$(E_m, \phi) = \sum_{n=0}^{\infty} \delta_{E_m E_n}(E_n|\phi) \tag{4.6d'}$$

for a class of infinite sequences $\{(E_n|\phi)\}$. When we will use function sequences of the $\delta$-type in Section II.8, we will see in which sense $\delta(x - y)$ can be considered as a generalization of the right-hand side of (4.8).

The eigenvectors $|E_n)$ are normalized to 1 by (4.7''); the generalized eigenvectors $|x\rangle$ fulfilling (4.7c) are called $\delta$-function normalized. They are not dimensionless, but have the dimension $1/\sqrt{\dim dx}$. For example, if $dx$ has the dimension cm, then $\langle x'|x\rangle$ has the dimension $\text{cm}^{-1}$, and $|x\rangle$ has the dimension $\text{cm}^{-1/2}$.

Instead of the generalized eigenvectors with $\delta$-function normalization (4.7c) one could also choose generalized eigenvectors of $Q$ with a different normalization. Instead of (4.4c) one writes

$$\phi = \int d\mu(x)\, |x\}_{\rho\mu}\{x|\phi\rangle, \tag{4.4c$_\mu$}$$

where the $|x\}_\mu$ are again eigenvectors of $Q$:

$$Q|x\}_\mu = x|x\}_\mu, \tag{4.3c$_\mu$}$$

and $\rho(x) = d\mu(x)/dx$ is a real nonnegative and integrable function.

In order that the new components of $\phi$, the ${}_\rho\{x|\phi\rangle$, be the scalar product of $\phi$ with the new eigenvectors $|x\}_\rho$, i.e., in order that

$${}_\rho\{x|\phi\rangle = \int \rho(y)\, dy\, {}_\rho\{x|y\}_{\rho\rho}\{y|\phi\rangle, \qquad (4.6c'_\rho)$$

one has to demand

$$d\mu(y)\, {}_\rho\{x|y\}_\rho = dy\, \langle x|y\rangle = dy\, \delta(x-y).$$

So the normalization of the new generalized eigenvectors is

$${}_\rho\{x|y\}_\rho = \left(\frac{d\mu(y)}{dy}\right)^{-1} \delta(x-y) = \rho^{-1}(y)\,\delta(x-y). \qquad (4.7c_\rho)$$

Thus when the integration contains the weight function $\rho(x)$, the generalized eigenvector normalization contains the factor $\rho^{-1}(x)$.

The transformation between the two basis systems is

$$|x\}_\rho = |x\rangle \frac{1}{\sqrt{\rho(x)}}. \qquad (4.14)$$

The most appropriate choice for $\rho(x)$ depends upon the property of the operator $Q$ and its relation to the other operators of the problem.[7]

As in the case of the discrete spectrum the spectral theorem (4.4c) can be written in different forms. Omitting the arbitrary vector $\phi$ one obtains the resolution of the identity:

$$I = \int dx\, |x\rangle\langle x| = \int \rho(x)\, dx\, |x\}_{\rho\rho}\{x|. \qquad (4.9c)$$

Multiplying both sides of (4.4c) with the operator $Q$ and then omitting the arbitrary vector $\phi$ one obtains after (4.3c) has been used

$$Q = \int dx\, x\, |x\rangle\langle x| \qquad (4.10c)$$

which we call the spectral resolution of the self-adjoint operator $Q$ with (absolutely[7]) continuous spectrum.

The scalar product of two vectors $\phi, \psi \in \Phi$, obtained from (4.4c), is

$$(\psi, \phi) = \int dx\, \langle\psi|x\rangle\langle x|\phi\rangle. \qquad (4.11c)$$

[7] The nuclear spectral theorem for an arbitrary self-adjoint operator does in fact not assert (4.4g) but (4.4$c_\mu$) with a general measure $d\mu(x)$, and it does not say anything about the spectral measure $d\mu(x)$ in addition to the assertion of its existence. However, all operators used in physics are of the special kind for which either $d\mu(x) = \rho(x)\, dx$ with $\rho(x)$ as described above (such operators are said to have an absolutely continuous spectrum and for them one can always make the transformation (4.14) from $|x\}_\rho$ to $|x\rangle$), or they have the property that $d\mu(x) = \sum_{x_i} \delta(x - x_i)\, dx$ (these are the operators with discrete spectrum), or they have both an absolutely continuous and a discrete spectrum. So (4.4g) is the most general form needed for physics.



From $(\psi, \phi) = (\phi, \psi)^*$ and from $(\phi, \psi) = \int dx\, \langle\phi|x\rangle\langle x|\psi\rangle$ for any $\phi, \psi \in \Phi$ one concludes that for the generalized scalar product one has the same relation as for the scalar product:

$$\langle\psi|x\rangle = \langle x|\psi\rangle^*.$$

Using the notation

$$\langle x|\phi\rangle = \phi(x), \qquad \langle x|\psi\rangle^* = \psi^*(x),$$

one can write (4.11c) in the form

$$(\psi, \phi) = \int dx\, \psi^*(x)\phi(x). \qquad (4.11c')$$

In particular, if one chooses $\psi = \phi$ one obtains

$$\|\phi\|^2 = (\phi, \phi) = \int dx\, \phi^*(x)\phi(x) = \int dx\, |\phi(x)|^2. \qquad (4.12c)$$

From this we see that not any arbitrary function $\phi(x)$ can give the components of a vector $\phi \in \Phi$ with respect to the continuous basis system $|x\rangle$, but only those functions for which the integral on the right-hand side of Equation (4.12c) exists, i.e., the square integrable functions.[8]

If one demands of the space $\Phi$ that on all its elements the operator $Q$ and any arbitrary power thereof, $Q^p$ $(p = 0, 1, 2, \ldots)$, be well defined, then one must have that

$$\|Q^p\phi\|^2 = (Q^p\phi, Q^p\phi) = \int dx\, x^{2p}|\phi(x)|^2 < \infty. \qquad (4.13c)$$

Thus $\phi(x)$ must decrease faster than any power of $x$. If other operators are also to be defined everywhere in $\Phi$ further conditions will have to be imposed on the components $\langle x|\phi\rangle$ of $\phi \in \Phi$. Thus the realization of $\Phi$ must be much better than $L^2$. An example of a realization of $\Phi$ is the *Schwartz-space* $S$. $S$ is defined as the space of infinitely differentiable complex-valued functions which together with their derivatives vanish at infinitely more rapidly than any power of $1/x$. We call those functions well behaved.

It can be that the space $\Phi$ is such that the components of all vectors $\psi \in \Phi$ with respect to the continuous basis $|x\rangle$, $\psi(x) = \langle x|\psi\rangle$, are boundary values of analytic functions $\psi(z)$ on the complex plane or a domain of the complex

[8] The scalar product space in which the scalar product is realized by the integral (4.11c') is called the space of square integrable functions $L^2$. If the scalar product space is complete then it is called a Hilbert space. For this reason a scalar product space is also called a pre-Hilbert space. The space of square (Lebesgue) integrable functions is one realization of the Hilbert space. Another realization of the Hilbert space is the space of square summable infinite sequences, cf. (4.12d').

plane, e.g., the lower half plane. Then the contour of integration in (4.11c') can be deformed and one obtains

$$(\psi, \phi) = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\phi(x) = \int_{\mathscr{C}} dz\, \psi^*(z)\phi(z)$$
$$= \int_{\mathscr{C}} dz\, \langle \psi | z \rangle \langle z | \phi \rangle. \tag{4.15}$$

$\mathscr{C}$ can be any contour which is obtained from the contour along the real axis by deforming it into the domain of analyticity without passing over a singularity. This defines the generalized eigenvectors $|z\rangle$ of the self-adjoint operator $Q$:

$$Q|z\rangle = z|z\rangle \tag{4.16}$$

with complex eigenvalue $z$. These generalized eigenvectors $|z\rangle$ can also be used in a generalized basis vector expansion. This is obtained from (4.15) by omitting the arbitrary vector $\psi \in \Phi$

$$\phi = \int_{\mathscr{C}} dz\, |z\rangle\langle z|\phi\rangle. \tag{4.4cc}$$

Thus instead of using the generalized basis vector expansion (4.4c) with respect to the generalized eigenvectors $|x\rangle$ with $x \in \mathbb{R}$, one can in this case as well use the generalized basis vector expansion (4.4cc) with respect to the generalized eigenvectors $|z\rangle$ with complex eigenvalues $z \in \mathbb{C}$. This possibility will be used in the description of decaying states.

## I.5 Realizations of Operators and of Linear Spaces

We have already mentioned that the components of all vectors $\phi \in \Phi$ with respect to a basis system constitute a realization of the space $\Phi$. A three-dimensional vector $\mathbf{x}$ in $R^3$ is thus realized by the sequence $(x_1, x_2, x_3)$ of its components $x_i = \mathbf{e}_i \cdot \mathbf{x}$. The components, of course, depend upon the basis system chosen. If one takes another basis system $\mathbf{e}'_i$ the components of the same vector $\mathbf{x}$ change: $x'_i = \mathbf{e}'_i \cdot \mathbf{x}$.

In a finite-dimensional linear scalar product space the components are finite sequences of complex numbers (4.5). In an infinite-dimensional space they are either infinite sequences $\phi_i = (E_i|\phi) \equiv (i|\phi)$ which fulfill certain conditions such as (4.12d') and (4.13d), or continuous infinite sequences $\phi(x) = \langle x|\phi\rangle$, i.e., functions of a continuous variable $x$, which also fulfill additional conditions like (4.12c) and (4.13c).

As in the three-dimensional case, if one changes the basis system of the space, the components of a given vector $\phi$ change too. Thus, if we take in addition to $H$ of (4.3d) another operator $A$ which has, like $H$, a discrete spectrum

$$A|a_i\rangle = a_i|a_i\rangle, \qquad a_i = a_0, a_1, a_2, \ldots, \tag{5.1}$$



then the same vector $\phi$ of (4.4d) can also be expanded as

$$\phi = \sum_{i=0}^{\infty} |a_i\rangle\langle a_i|\phi\rangle \equiv \sum_i |i\rangle\langle i|\phi\rangle, \tag{5.2}$$

where we defined for writing convenience: $|i\rangle \equiv |a_i\rangle$.

If $A$ and $H$ do not commute, then the components $\langle a_i|\phi\rangle$ and $(E_n|\phi)$ are entirely different. The components can be written as a column matrix

$$\phi \leftrightarrow (E_n|\phi) = \begin{pmatrix} (E_0|\phi) \\ (E_1|\phi) \\ \vdots \end{pmatrix}, \tag{5.3}$$

$$\phi \leftrightarrow \langle a_i|\phi\rangle = \begin{pmatrix} \langle a_0|\phi\rangle \\ \langle a_1|\phi\rangle \\ \langle a_2|\phi\rangle \\ \vdots \end{pmatrix}. \tag{5.4}$$

Column matrices can be added, by adding each of their components, they can be multiplied by a number by multiplying each component and a scalar product between column matrices can be defined as by the expression furthest to the right in Equation (4.11d). With these definitions it is easy to see that the set of column matrices: $\langle i|\phi\rangle, \langle i|\psi\rangle, \langle i|\chi\rangle, \ldots, i = 1, 2, 3, \ldots$ form a linear scalar product space $\mathbb{C}^{\infty}_{(i)}$ (cf. also Problem 1). In the same way the set of column matrices of components with respect to the basis system $\{|E_n) : E_n = E_1, E_2, \ldots\}$, the $(E_n|\phi), (E_n|\psi), (E_n, \chi), \ldots$, form a linear scalar product space $\mathbb{C}^{\infty}_{(E_n)}$. It is easy to see that $\mathbb{C}^{\infty}_{(E_n)}$ and $\mathbb{C}^{\infty}_{(i)}$ are isomorphic to each other and isomorphic to the space $\Phi$:

$$(\langle i|\phi\rangle) \leftrightarrow ((E_n|\phi)) \leftrightarrow \phi,$$
$$(\langle i|\psi\rangle) \leftrightarrow ((E_n|\psi)) \leftrightarrow \psi.$$

Therewith we can define the space $\Phi$ by specifying the set of all infinite column matrices. For instance we shall define $\mathbb{C}^{\infty}_{(E_n)}$ as the space of all $(E_n|\phi)$ which fulfill (4.13d) with $E_n = (n + \frac{1}{2}), n = 0, 1, 2, \ldots$. $\Phi$ can then be defined as the space isomorphic to it.[9] Thus the same vector can be represented by entirely different column matrices.

When vectors are realized by column matrices, operators are realized by quadratic matrices. We obtain these matrices of an operator $B$ in the following way:

Calculate

$$B\phi = \sum_i B|i\rangle\langle i|\phi\rangle, \tag{5.5}$$

[9] $\mathbb{C}^{\infty}_{(E_n)}$ has a natural topological structure which $\Phi$ then inherits. $\Phi$ is then the largest space in which all the operators $H^p$, $p = 0, 1, 2, \ldots$ are continuous operators, and its topological structure could have been defined by this requirement.

and take the scalar product of this equation with $|a_j\rangle$

$$\langle j|B\phi\rangle = \sum_i \langle j|B|i\rangle\langle i|\phi\rangle. \tag{5.6}$$

This can be written in matrix notation as

$$\begin{pmatrix} \langle 1|B\phi\rangle \\ \langle 2|B\phi\rangle \\ \langle 3|B\phi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 1|B|1\rangle & \langle 1|B|2\rangle & \langle 1|B|3\rangle & \cdots \\ \langle 2|B|1\rangle & \langle 2|B|2\rangle & \langle 2|B|3\rangle & \\ \langle 3|B|1\rangle & \langle 3|B|2\rangle & \cdots & \cdots \\ \vdots & \vdots & & \end{pmatrix} \begin{pmatrix} \langle 1|\phi\rangle \\ \langle 2|\phi\rangle \\ \langle 3|\phi\rangle \\ \vdots \end{pmatrix}. \tag{5.7}$$

The right-hand side of (5.6) gives the definition of multiplication of a quadratic matrix with the column matrix on the right-hand side of (5.7). Thus we see that the linear operator $B$ is realized by the infinite matrix

$$B \leftrightarrow \langle j|B|i\rangle = \begin{pmatrix} \langle 1|B|1\rangle & \langle 1|B|2\rangle & \cdots \\ \langle 2|B|1\rangle & \langle 2|B|2\rangle & \cdots \\ \langle 3|B|1\rangle & \cdots & \\ \vdots & & \end{pmatrix}, \tag{5.8}$$

which is called the matrix of the operator $B$ with respect to the basis system $\{|i\rangle | i = 1, 2, 3, \ldots\}$.

Now, let $D$ be a second operator and apply $D + B$ to the basis vector $|i\rangle$ using (3.4)

$$(B + D)|i\rangle = B|i\rangle + D|i\rangle.$$

Taking the scalar product of both sides of this equation with the basis vector $|j\rangle$ one obtains (using (2.2d)):

$$\langle j|(B + D)|i\rangle = \langle j|B|i\rangle + \langle j|D|i\rangle. \tag{5.9}$$

Thus the matrix of the sum of two linear operators is equal to the sum of the matrices, as defined by the right-hand side of (5.9). Let us now consider the matrix element of $DB$ and use the resolution of the identity (4.9d) for the basis system (5.1):

$$\langle j|DB|i\rangle = \sum_{n=0}^{\infty} \langle j|D|n\rangle\langle n|B|i\rangle. \tag{5.10}$$

Written in matrix notation this has the form:

$$\begin{pmatrix} \langle 1|DB|1\rangle & \langle 1|DB|2\rangle & \langle 1|DB|3\rangle & \cdots \\ \langle 2|DB|1\rangle & \langle 2|DB|2\rangle & \langle 2|DB|3\rangle & \cdots \\ & \cdots\cdots\cdots & & \end{pmatrix} = \begin{pmatrix} \langle 1|D|1\rangle & \langle 1|D|2\rangle & \langle 1|D|3\rangle & \cdots \\ \langle 2|D|1\rangle & \langle 2|D|2\rangle & \langle 2|D|3\rangle & \cdots \\ & \cdots\cdots\cdots & & \end{pmatrix} \begin{pmatrix} \langle 1|B|1\rangle & \langle 1|B|2\rangle & \cdots \\ \langle 2|B|1\rangle & \langle 2|B|2\rangle & \cdots \\ \langle 3|B|1\rangle & \langle 3|B|2\rangle & \cdots \end{pmatrix} \tag{5.10'}$$



where the right-hand side of (5.10) gives the definition of the multiplication of two (infinite-dimensional) quadratic matrices.

Thus in the realization of the space $\Phi$ by the space of column vectors, the operators are realized by matrices in such a way that the sum of two operators corresponds to the sum of their matrices and the product of two operators corresponds to the product of their matrices.

If the basis system is chosen to be a system of eigenvectors of the operator $A$ as in (5.1), then the matrix of $A$ with respect to this basis system is diagonal as from (5.1) follows

$$\langle j|A|i\rangle = a_i\langle j|i\rangle = a_i\delta_{ij}, \tag{5.11}$$

or, written as a matrix,

$$\begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \langle 1|A|3\rangle & \cdots \\ \langle 2|A|1\rangle & \langle 2|A|2\rangle & \cdots & \\ \langle 3|A|1\rangle & \cdots & & \\ \vdots & \vdots & & \end{pmatrix} = \begin{pmatrix} a_1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & a_3 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}. \tag{5.11'}$$

The matrix elements with respect to the basis system of eigenvectors of $A$ of all other operators that do not commute with $A$ have nonzero off-diagonal matrix elements.

As the proper eigenvectors of $H$ are also elements of $\Phi$ one can use (4.4d) and expand them with respect to the basis system $|i\rangle$ of (5.1) and vice versa

$$|E_n\rangle = \sum_{i=1}^{\infty} |i\rangle\langle i|E_n\rangle; \tag{5.12}$$

$$|i\rangle = \sum_{n=1}^{\infty} |E_n\rangle\langle E_n|i\rangle. \tag{5.12'}$$

Taking the scalar product of this equation with $\phi$ and then taking the complex conjugate one obtains

$$\langle E_n|\phi\rangle = \sum_{i=1}^{\infty} \langle E_n|i\rangle\langle i|\phi\rangle. \tag{5.13}$$

Thus $\langle E_n|i\rangle$ are the matrix elements of a matrix that transforms the infinite-column matrix (5.4) into the infinite-column matrix (5.3). It is called the transition matrix (or transformation matrix) between the two basis systems $\{|i\rangle | i = 1, 2, \ldots$ and $\{|E_n\rangle | n = 1, 2, \ldots\}$. Its elements $\langle E_n|i\rangle$ are also called transition coefficients. Taking the scalar product of (5.12') with $|j\rangle$ gives

$$\langle j|i\rangle = \delta_{ij} = \sum_{n=1,2,\ldots}^{\infty} \langle j|E_n\rangle\langle E_n|i\rangle = \sum_n \langle E_n|j\rangle^*\langle E_n|i\rangle. \tag{5.14'}$$

Similarly one obtains

$$\langle E_m|E_n\rangle = \delta_{mn} = \sum_{j=1}^{\infty} \langle E_m|j\rangle\langle j|E_n\rangle = \sum_j \langle E_m|j\rangle\langle E_n|j\rangle^*. \tag{5.14}$$

A matrix whose matrix elements fulfill the condition (5.14) is called a unitary matrix. If the matrix elements are also real, which happens sometimes in $\Phi$ (and always in a real linear space), then the matrix is called orthogonal.

If the matrix elements of the operator $A$ in the basis $|E_n\rangle$ are given, $(E_n|A|E_m)$, then one can obtain the matrix elements $\langle i|A|j\rangle$ by using the transformation (5.12'):

$$a_j\delta_{ij} = \langle i|A|j\rangle = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\langle i|E_n)(E_n|A|E_m)(E_m|j\rangle. \qquad (5.15)$$

One says, the transition matrix transforms the matrix $(E_n|A|E_m)$ into its diagonal form. Multiplying both sides of (5.15) by $\langle E_r|i\rangle$, summing over $i$ and using (5.14') one obtains:

$$\sum_{m=1}^{\infty}(E_r|A|E_m)(E_m|j\rangle = a_j(E_r|j\rangle. \qquad (5.16)$$

If the eigenvalues $a_j$ are unknown, then this is the eigenvalue problem in matrix notation. For the case that the space is $N$-dimensional (instead of $\infty$-dimensional) this is a system of $N$ linear homogeneous equations[10] for the $N$ unknown $(E_m|j\rangle$:

$$\sum_{m=1}^{N}[(E_n|A|E_m) - a\delta_{nm}](E_m|j\rangle = 0. \qquad (5.17)$$

It has nonzero solutions for $(E_m|j\rangle$ if and only if

$$\det[(E_n|A|E_m) - a\delta_{nm}] = 0. \qquad (5.18)$$

The eigenvalues of the matrix $(E_n|A|E_m)$ are the $N$ solutions of this equation. These solutions are not necessarily distinct. Equation (5.18) is a polynomial of degree $N$ and, by a famous theorem of algebra,[10] every polynomial of degree $N$ has $N$ (in general complex but if $A$ is Hermitian then real) solutions.

We now turn to the case that one of the basis systems,

$$\{|x\rangle \mid -\infty < x < +\infty\}, \qquad (5.19)$$

is continuous. Then the vector $\phi$ is realized by a function of a continuous variable $x$, rather than by a function of a discrete variable as in (5.3) and (5.4):

$$\phi \leftrightarrow \langle x|\phi\rangle = \phi(x). \qquad (5.20)$$

As in the discrete case, the space $\Phi$ can be defined by its isomorphism (5.20) to a space of functions. We want to consider the particular case where $\Phi$ is the space of vectors whose components $\langle x|\phi\rangle$ are elements of the function space $S$.

[10] See, e.g., A Lichnerowicz (1967).



The eigenvector $|E_n)$ is a particular vector of the space $\Phi$; so one can use the continuous basis system expansion (4.4c) for it:

$$|E_n) = \int dx\,|x\rangle\langle x|E_n). \qquad (5.21)$$

The $\langle x|E_n)$ are the analogue of the transition matrix elements $\langle i|E_n)$ between two discrete basis systems. They are the transition coefficients between the discrete basis system $|E_n)$ and the continuous basis system $|x\rangle$. For fixed value of $x$ the $\langle x|E_n\rangle$ are functions of the discrete variable $E_n$ and for fixed value of $E_n$ they are functions of the continuous variable $x$. They also occur if one takes the scalar product of the basis vector expansion (4.4d) with the continuous basis vector $|x\rangle$:

$$\langle x|\phi\rangle = \sum_{n=0}^{\infty}\langle x|E_n)(E_n|\phi). \qquad (5.22)$$

The $\langle x|E_n)$ constitute a particular set of functions in the space $S$, which, as a consequence of (4.3d), have the property:

$$\langle x|H|E_n) = E_n\langle x|E_n). \qquad (5.23)$$

Because of this property they are called eigenfunctions of the operator $H$. Equation (5.22), which is an immediate consequence of the eigenvector expansion (4.4d), is called the eigenfunction expansion of the function $\langle x|\phi\rangle \in S$.

We want to illustrate this on a well-known example. We choose for the space of functions the subspace $K(a) \subset S$ of all functions $\phi(x) = \langle x|\phi\rangle$ which are identically zero outside the domain $|x| < a$.

Let the operator $Q$ have the continuous spectrum $\{x \mid -a < x < +a\}$. So the spectral representation of an arbitrary vector $\phi \in \Phi$ is

$$\phi = \int_{-a}^{+a} dx\,|x\rangle\langle x|\phi\rangle. \qquad (5.24)$$

Let the self-adjoint operator $H = P^2$ be defined by

$$\langle x|H|\phi\rangle = -\frac{d^2}{dx^2}\langle x|\phi\rangle \qquad (5.25)$$

for every component $\langle x|\phi\rangle$ of any $\phi \in \Phi$. In order that $Q$, $P$ and any power of these operators be defined in $\Phi$, the space of components $\langle x|\phi\rangle$ must be the space of continuous infinitely differentiable functions for which

$$\int_{-a}^{+a} dx\left|x^n\frac{d^m}{dx^m}\langle x|\phi\rangle\right|^2 < \infty.$$

Further

$$\langle x \geq a|\phi\rangle = \langle x \leq -a|\phi\rangle = 0. \qquad (5.26)$$

(This boundary condition is important to establish the self-adjointness of $H$, cf. Problem 14.) Let the eigenvector of $H$ be denoted by $|n\rangle$:

$$H|n\rangle = E_n|n\rangle. \tag{5.27}$$

We want to find all eigenvalues $E_n$ and the transition coefficients $\langle x|n\rangle$. From (5.25) and (5.27) follows

$$-\frac{d^2}{dx^2}\langle x|n\rangle = E_n\langle x|n\rangle. \tag{5.28}$$

The solutions of this differential equation which fulfill the boundary condition (5.26) are

$$\begin{aligned}\langle x|n\rangle &= \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right) \quad \text{for } n = 1, 3, 5, 7, \ldots, \\ \langle x|n\rangle &= \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right) \quad \text{for } n = 2, 4, 6, \ldots.\end{aligned} \tag{5.29}$$

The eigenvalues are

$$E_n = \frac{n^2\pi^2}{4a^2}. \tag{5.30}$$

The normalization factor $1/\sqrt{a}$ in (5.29) has been chosen so that $\langle n|n\rangle = 1$, which according to (5.24) is given by

$$\begin{aligned}\langle n|n\rangle &= \int_{-a}^{+a} dx\,\langle n|x\rangle\langle x|n\rangle \\ &= \frac{1}{a}\int_{-a}^{+a} dx\cos\left(\frac{n\pi}{2a}x\right)\cos\left(\frac{n\pi}{2a}x\right) = 1,\end{aligned} \tag{5.31e}$$

or

$$\langle n|n\rangle = \frac{1}{a}\int_{-a}^{+a} dx\sin\left(\frac{n\pi}{2a}x\right)\sin\left(\frac{n\pi}{2a}x\right) = 1. \tag{5.31o}$$

In the last equalities of (5.31e) and (5.31o) properties of integrals over the trigonometric functions have been used. For $n' \neq n$ one should have as a consequence of the orthogonality of eigenvectors of self-adjoint operators

$$\langle n'|n\rangle = \int_{-a}^{+a} dx\,\langle n'|x\rangle\langle x|n\rangle = 0. \tag{5.32}$$

But this can also be obtained by inserting (5.29) into (5.32) and calculating the integrals over the trigonometric functions. Because of (5.32), one says that the eigenfunctions $\langle n'|x\rangle$ and $\langle n|x\rangle$ are orthogonal.

The eigenfunction expansion (5.22) for this particular case is

$$\begin{aligned}\langle x|\phi\rangle = \phi(x) &= \sum_{n=1,3,5}^{\infty} a_n\cos\left(\frac{n\pi}{2a}x\right) + \sum_{n=2,4,6}^{\infty} b_n\sin\left(\frac{n\pi}{2a}x\right) \quad \text{for } |x| < a, \\ \phi(x) &= 0 \quad \text{for } |x| \geq 0.\end{aligned} \tag{5.33}$$



The coordinates of the vector $\phi$ are given by:

$$\begin{aligned}\sqrt{a}b_n = \langle n|\phi\rangle &= \int_{-a}^{+a} dx\,\langle n|x\rangle\langle x|\phi\rangle \\ &= \frac{1}{\sqrt{a}}\int_{-a}^{+a} dx\sin\left(\frac{n\pi}{2a}x\right)\phi(x); \quad n = 2, 4, 6\ldots\end{aligned}$$

and

$$\begin{aligned}\sqrt{a}a_n = \langle n|\phi\rangle &= \int_{-a}^{+a} dx\,\langle n|x\rangle\langle x|\phi\rangle \\ &= \frac{1}{\sqrt{a}}\int_{-a}^{+a} dx\cos\left(\frac{n\pi}{2a}x\right)\phi(x); \quad n = 1, 3, 5, \ldots.\end{aligned}$$

Equation (5.33) is called a Fourier series representation of the arbitrary function $\phi(x) \in K(a)$. The coordinates of the vector $\phi$ with respect to the basis system $|n\rangle$, $a_n$ and $b_n$, are called the Fourier coefficients of the function $\phi(x) = \langle x|\phi\rangle$. Because (5.22) is just a generalization of a classical Fourier series (5.33) one also calls (5.22) and even (4.4d) often a Fourier series representation or Fourier expansion. In general the eigenfunctions $\langle x|E_n\rangle$ will not be trigonometric functions, however (5.32) must always be fulfilled, i.e., the $\langle x|E_n\rangle$ always form an orthogonal system of basis functions. Well-known examples of orthogonal basis functions are the Hermite Polynomials, the Legendre Polynomials, and the Laguerre Polynomials. In particular, for the space $S$, when the spectrum of $Q$ is the entire real line $\Re$, the Hermite polynomials are an appropriate choice of basis functions.

So far we have considered transition coefficients between two discrete basis systems $\langle i|E_n\rangle$, and the transition coefficients $\langle x|E_n\rangle$ between a discrete and a continuous basis system. Now we want to go one step further and consider transition coefficients between two continuous basis systems. We choose for $\Phi$ the space realized by $S$ and consider the operator $P$ defined by (cf. Problem 7)

$$\langle x|P|\phi\rangle = \frac{1}{i}\frac{d}{dx}\langle x|\phi\rangle \quad \text{for every} \quad \phi \in \Phi, \quad \text{i.e.,} \quad \langle x|\phi\rangle \in S. \tag{5.34}$$

We want to consider (5.34) also for the case that $\phi$ is an eigenvector of the operator $P$ (extending the definition of $P$ if this eigenvector is not in $\Phi$):

$$P|p\rangle = p|p\rangle. \tag{5.35}$$

Equation (5.34) then reads

$$\langle x|P|p\rangle = p\langle x|p\rangle = \frac{1}{i}\frac{d}{dx}\langle x|p\rangle. \tag{5.36}$$

It is well known that this differential equation has solutions for any complex value of $p$ given by

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ixp}, \quad p \in \mathbb{C}. \tag{5.37}$$

None of these solutions, however, is square integrable so that $|p\rangle \notin \Phi$ (cf. Problem 9).

We can expand any $\phi \in \Phi$ with respect to the basis system $|p\rangle$ of eigenvectors of $P$:

$$\phi = \int_{\text{Spectr.}\,P} dp\,|p\rangle\langle p|\phi\rangle, \tag{5.38}$$

where the integral has to extend over the spectrum of the operator $P$. We want to determine the spectrum of $P$. It is contained in the set of generalized eigenvalues which is identical with all of $\mathbb{C}$. We take the scalar product[11] of (5.38) with $|x\rangle$

$$\langle x|\phi\rangle = \int_{\text{Spectr.}\,P} dp\,\langle x|p\rangle\langle p|\phi\rangle = \frac{1}{\sqrt{2\pi}}\int dp\, e^{ixp}\langle p|\phi\rangle. \tag{5.39}$$

If the $p$ integration in (5.39) extends over the real line, $-\infty < p < +\infty$, then (5.39) says that $\phi(x) = \langle x|\phi\rangle$ is the Fourier transform of the function $\tilde{\phi}(p) = \langle p|\varphi\rangle$. We therefore want to give a brief review of the properties of the Fourier transform.[12]

Let $\phi(x)$ be an element of the space $S$, then the (inverse) Fourier transform,† which we denote by $F_p^{-1}[\phi(x)] \equiv \tilde{\phi}(p)$, is defined by

$$F_p^{-1}[\phi(x)] \equiv \tilde{\phi}(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dx\, e^{-ixp}\phi(x). \tag{5.40a}$$

The Fourier transform has the following properties:

(a) $F^{-1}$ maps $S$ onto itself; that means $\tilde{\phi}(p)$ also belongs, as a function of $p$, to the space $S$.

(b) The Fourier transform which we denote by $F_x[\tilde{\phi}(p)]$ and which is defined by

$$\phi(x) \equiv F_x[\tilde{\phi}(p)] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\, e^{ixp}\tilde{\phi}(p) \tag{5.40b}$$

also belongs to the space $S$ if $\tilde{\phi}(p) \in S$.

(c)

$$\left(\frac{1}{i}\frac{d}{dx}\right)^n \phi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\, p^n e^{ixp}\tilde{\phi}(p) = F_x[p^n\tilde{\phi}(p)] \tag{5.40c}$$

for any power $n = 0, 1, 2, 3, \ldots$, which we also write as

$$\left(\frac{1}{i}\frac{d}{dx}\right)^n F_x[\tilde{\phi}(p)] = F_x[p^n\tilde{\phi}(p)],$$

[11] Section I.4, footnote 6.

[12] For the proofs and details see I. M. Gelfand *et al.* (1964), Vol. 2, Chapter III, or E. J. Beltrami and M. R. Wohlers, *Distributions and the Boundary Values of Analytic Functions*, Academic Press, New York, 1966.

† One sometimes calls inverse Fourier transform what we call Fourier transform here and vice versa; we may do the same.



(d)

$$\left(-\frac{1}{i}\frac{d}{dp}\right)^n \tilde{\phi}(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dx\, x^n e^{-ixp}\phi(x) = F_p^{-1}[x^n\phi(x)] \tag{5.40d}$$

for any power $n = 0, 1, 2, 3, \ldots$, which we also write as

$$\left(-\frac{1}{i}\frac{d}{dp}\right)^n F_p^{-1}[\phi(x)] = F_p^{-1}[x^n\phi(x)],$$

(e)

$$\int dx\, \psi^*(x)\phi(x) = \int dp\, \tilde{\psi}^*(p)\tilde{\phi}(p), \tag{5.40e}$$

where $\tilde{\psi}(p), \tilde{\phi}(p) \in S$ are the Fourier transforms of $\psi(x), \phi(x) \in S$.

Thus the Fourier transform $F$ and its inverse $F^{-1}$ establish two reciprocal isomorphisms between the Schwartz space functions $S_x$ of the variable $x$ and the Schwartz space functions $S_p$ of the variable $p$.

We can now return to the problem of the spectrum of $P$. As every $\langle x|\phi\rangle = \phi(x) \in S$ can be written according to (5.40b) and (5.37) in the form (5.39) with the integration extending over the real axis $-\infty < p < +\infty$ with $\langle p|\phi\rangle$ being again an element of $S$, we conclude that

$$\text{Spectr.}\,P = \{p \mid -\infty < p < \infty\},$$

i.e., the real axis $\mathbb{R}$. Thus we have found the spectral resolution (5.38) of $\phi$ with respect to the basis system of eigenvectors of $P$. The spectrum of $P$ is continuous and the $|p\rangle$ are generalized eigenvectors (not elements of $\Phi$). The transition coefficients between the generalized basis systems $\{|x\rangle\}$ and $\{|p\rangle\}$ are given by (5.37) with $p \in \mathbb{R}$ and $x \in \mathbb{R}$. For fixed value of $x$ they are functions of the continuous variable $p$, and for fixed value of $p$ they are functions of the continuous variable $x$. They satisfy the differential equation (5.36), but they are not well-behaved functions, i.e., elements of the function space $S$. Therefore they are called generalized eigenfunctions or distributions. It is easily seen by exchanging $x$ and $p$ in the preceding arguments and using (5.40a) in place of (5.40b) that

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-ipx}. \tag{5.41}$$

Consequently we have shown that for this special case of transition coefficients between two continuous basis systems the following relation holds:

$$\langle p|x\rangle = \langle x|p\rangle^*. \tag{5.42}$$

The exponential function is just one example of transition coefficients between two continuous basis systems. Other examples that we will meet in the second part of the book are the spherical Bessel functions.

Finally, in this section we want to consider the realization of operators in terms of a continuous basis system. This is again done in analogy to the discrete case. To obtain the analogue of (5.5) we apply the operator $B$ to the continuous basis system expansion (4.4c)

$$B\phi = \int dx\, B|x\rangle\langle x|\phi\rangle. \tag{5.43}$$

Taking the scalar product[13] with the basis vector $|y\rangle \in \{|x\rangle \mid \infty < x < \infty\}$ we obtain

$$\langle y|B\phi\rangle = \int dx\, \langle y|B|x\rangle\langle x|\phi\rangle \tag{5.44}$$

which is the continuous analogue of (5.6). This is an integral transform transforming the function $\langle x|\phi\rangle$ into the function $\langle y|\psi\rangle = \langle y|B\phi\rangle$. The continuous analogue of the matrix element (5.8), $\langle y|B|x\rangle$, is called the kernel of the integral transform. Choosing for $B = A$ and for $\phi = i\rangle$, the eigenvector (5.1) of $A$ we obtain from (5.44)

$$\int dx\, \langle y|A|x\rangle\langle x|i\rangle = a_i\langle y|i\rangle. \tag{5.45}$$

This is the analogue of (5.16). If the eigenvalues $a_i$ and eigenfunctions $\langle y|i\rangle$ are unknown this is a homogeneous integral equation for the determination of these values.

## I.6 Hermite Polynomials as an Example of Orthonormal Basis Functions

We start with the operator $Q$ realized by the multiplication operator and the operator $P$ realized by the differential operator (Equation (5.34)) on the space of functions $S$:

$$\langle x|Q|\phi\rangle = x\langle x|\phi\rangle, \qquad -\infty < x < +\infty, \tag{6.1}$$

$$\langle x|P|\phi\rangle = \frac{1}{i}\frac{\partial}{\partial x}\langle x|\phi\rangle, \qquad \langle x|\phi\rangle \in S. \tag{6.2}$$

Another operator $H$ is defined by

$$H = \tfrac{1}{2}(P^2 + Q^2), \tag{6.3}$$

and its eigenvectors are denoted by $|n\rangle$:

$$H|n\rangle = E_n|n\rangle. \tag{6.4}$$

We denote the space in which $Q$, $P$, $H$ and any element of the algebra generated by them act by $\Phi$. Thus $\phi \in \Phi \Leftrightarrow \langle x|\phi\rangle \in S$.[14]

[13] Section I.4, footnote 6.

[14] One can also construct $\Phi$ in the following manner (cf. Chapter II): Start from the algebra of operators $P$, $Q$, and $H$ which fulfills in addition to (6.3) the relation $PQ - QP = (1/i)I$, and construct the space $\Phi$ as the largest space in which this algebra is given (represented) as an algebra of (continuous) operators and in which there exists at least one eigenvector of $H$.



The discreteness of the spectrum of $H$, which is implied by (6.4), is in fact a consequence of the assumption that the eigenvectors $|n\rangle$ of $H$ lie in the space $\Phi$ or that $\langle x|n\rangle \in S$, as will be shown below.

The transition coefficients between the $Q$-eigenvectors and the $H$-eigenvectors, $\langle x|n\rangle$, are orthonormal basis functions of the space $S$ in the sense of (5.22). We want to determine $\langle x|n\rangle$ and the eigenvalues $E_n$ explicitly.

We denote

$$\lambda = 2E_n. \tag{6.5}$$

Using (6.3) in (6.4) we obtain with (6.2) and (6.1):

$$2\langle x|H|n\rangle = \left(-\frac{d^2}{dx^2} + x^2\right)\langle x|n\rangle = \lambda\langle x|n\rangle. \tag{6.6}$$

Thus we have to find the solutions

$$\psi(x) = \langle x|n\rangle \tag{6.7}$$

of the differential equation

$$\psi''(x) + (\lambda - x^2)\psi(x) = 0. \tag{6.8}$$

In addition we will demand that the $\psi(x) \in S$. Then they must in particular fulfill the boundary conditions:

$$\psi(x) \to 0 \quad \text{faster than any polynomial of } 1/x \text{ as } x \to \pm\infty \tag{6.9}$$

Equation (6.8) is highly singular at $|x| \to \infty$ and for large values of $|x|$ is given approximately by $\psi'' - x^2\psi = 0$, which has the solutions $\psi \sim e^{\mp x^2/2}$. One therefore makes the ansatz

$$\psi(x) = c_1 e^{-x^2/2} y(x) + c_2 e^{x^2/2} y_2(x) \tag{6.10}$$

with $y_2$ and $y$ expanded as power series in $x$:

$$y = \sum_{k=0}^{\infty} a_k x^k. \tag{6.11}$$

The second term in (6.10) increases rapidly and cannot lead to an element of $S$, therefore $c_2$ must be zero. Inserting

$$\psi(x) = c_1 e^{-x^2/2} y(x) \tag{6.12}$$

into (6.8) one obtains the differential equation

$$y'' - 2xy' + (\lambda - 1)y = 0. \tag{6.13}$$

Substituting (6.11) into (6.13) and collecting powers of $x$ one obtains

$$(k+2)(k+1)a_{k+2} - 2ka_k + (\lambda - 1)a_k = 0$$

which leads to the recurrence formula

$$a_{k+2} = \frac{2k - (\lambda - 1)}{(k+2)(k+1)} a_k. \tag{6.14}$$

This determines the coefficients of the higher powers in (6.11) from those of the lower powers. By comparing the ratio $a_{k+2}/a_k$ for large values of $k$ with the ratios $b_{k+2}/b_k$ in a power series expansion of $e^{x^2}$, we can show that the function (6.11) with (6.14) will be divergent like $e^{x^2}$, as $x \to \pm\infty$. Thus, the only way that we can construct solutions $y(x)$ of the form (6.12) which converge in the desired manner at $\pm\infty$ is to choose values for $\lambda$ such that the series (6.11) terminates. This we can accomplish by letting $\lambda - 1 = 2n$ for $n = 0, 1, 2, \ldots$, and we thus see that $\psi(x)$ can be an element of $S$ only if

$$\lambda = 2n + 1 \quad \text{or} \quad E_n = n + \tfrac{1}{2}, \quad n = 0, 1, 2, \ldots. \tag{6.15}$$

The solutions of the differential equation (6.13) corresponding to the eigenvalues (6.15) are also labelled by $n$ and denoted by $y(x) = H_n(x)$. Thus, we obtain a family of equations

$$H_n'' - 2xH_n' + 2nH_n = 0, \qquad n = 0, 1, 2, \ldots, \tag{6.16}$$

which are called the Hermite differential equations. Their solutions $H_n(x)$ are called the Hermite polynomials. It is easy to check that the polynomials defined by:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}) \tag{6.17}$$

fulfill (6.16). Equation (6.17) is called the Rodrigues formula for the Hermite polynomials.

Therewith we have found for the transition coefficient (6.7):

$$\langle x|n\rangle = \psi_n(x) = \frac{1}{N_n} e^{-x^2/2} H_n(x). \tag{6.18}$$

The factor $N_n$ will be chosen so that

$$(n|n) = \int dx\, (n|x\rangle\langle x|n) = \left|\frac{1}{N_n}\right|^2 \int dx\, e^{-x^2} H_n(x) H_n(x) = 1. \tag{6.19}$$

The orthogonality of the eigenvectors of the self-adjoint operator $H$ can now be written in the form

$$N_{n'}^* N_n (n'|n) = \int dx\, e^{-x^2} H_{n'}(x) H_n(x) = 0 \quad \text{for} \quad n \neq n'. \tag{6.20}$$

The second equality of (6.20), which we obtained as a consequence of the orthogonality of the $|n)$, is called the orthogonality relation for the Hermite polynomials. The normalization factor $N_n$ has to be calculated using the special properties of the Hermite polynomials defined by (6.17). This is done using standard methods in the Appendix to this section. From (A.12) one obtains

$$|N_n|^2 = \sqrt{\pi}\, n!\, 2^n. \tag{6.21}$$

$N_n$ and therewith the transition coefficients $\langle x|n)$ in (6.16) are only determined up to a phase factor, i.e., a factor $e^{i\alpha(n)}$ of modulus one, which can still vary with $n$. It is standard to choose these factors equal to $(+1)$. Thus we obtain



$$\langle x|n) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} e^{-x^2/2} H_n(x). \tag{6.22}$$

## Appendix to Section I.6

The normalization factor $N_n$ in (6.19) is calculated in the following way: We consider the function $f(t) = e^{-t^2+2tx}$. Considered as a function of the complex variable $t$, $f(t)$ is an entire function and can be expanded into a Taylor series of $t$:

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} a_n(x) t^n \quad \text{for all} \quad |t| < \infty, \tag{A.1}$$

where the expansion coefficients depend upon the parameter $x$. These coefficients are given by

$$a_n = \frac{1}{n!} \left.\frac{d^n f(t)}{dt^n}\right|_{t=0}. \tag{A.2}$$

As $f(t)$ is an analytic function for every value of the parameter $x$ we can use the Cauchy theorem which states that

$$\frac{d^n f(t)}{dt^n} = \frac{n!}{2\pi i} \oint \frac{f(z)}{(z-t)^{n+1}}\, dz, \tag{A.3}$$

where the integration is along a contour enclosing the point $z = t$. Applying this to $f(z) = e^{-z^2+2zx}$ and using (A.2) we obtain at $t = 0$

$$a_n = \frac{1}{2\pi i} \oint \frac{e^{-z^2+2zx}}{z^{n+1}}\, dz. \tag{A.4}$$

On the other hand, we can use (A.3) for the function $f(z) = e^{-z^2}$ and obtain

$$\frac{d^n}{dx^n} e^{-x^2} = \frac{n!}{2\pi i} \oint \frac{e^{-z^2}}{(z-x)^{n+1}}\, dz, \tag{A.5}$$

where the contour of integration encloses the point $z = x$, which can be in particular any point on the real axis.

On the left-hand side of (A.5) we use (6.17). On the right-hand side we perform a change of integration variable $z = x - t$, $dz = -dt$. Then (A.5) goes over into

$$e^{-x^2}(-1)^n H_n(x) = \frac{n!}{2\pi i} \oint \frac{1}{(-1)^n} \frac{e^{-(x-t)^2}}{t^{n+1}}\, dt, \tag{A.6}$$

where the contour of integration encloses the point $t = 0$. Dividing both sides by $e^{-x^2}(-1)^n$ one obtains

$$H_n(x) = \frac{n!}{2\pi i} \oint \frac{e^{-t^2+2tx}}{t^{n+1}}\, dt. \tag{A.7}$$

Comparison of (A.4) and (A.7) shows that the coefficients in (A.1) are given by

$$a_n(x) = \frac{1}{n!} H_n(x)$$

and (A.1) can be written

$$e^{-t^2+2tx} = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(x) t^n \quad \text{for} \quad |t| < \infty. \tag{A.8}$$

The function $f(t) = e^{-t^2+2tx}$ is called the generating function of the Hermite polynomials. Many properties of **orthogonal polynomials** are easily derived using their generating function.

We are now ready to calculate the normalization factor $N_n$. Using (A.8) we obtain

$$\int_{-\infty}^{+\infty} dx\, e^{-t^2+2tx} e^{-s^2+2sx} e^{-x^2} = \sum\sum_{n,m=0}^{\infty} \frac{t^n s^m}{n!\,m!} \int_{-\infty}^{+\infty} dx\, e^{-x^2} H_n(x) H_m(x). \tag{A.9}$$

The left-hand side of (A.9) can be written as

$$e^{2st} \int_{-\infty}^{+\infty} dx\, e^{-(x-(s+t))^2} = e^{2st} \int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2} = e^{2st}\sqrt{\pi}. \tag{A.10}$$

Expanding $e^{2st}$ into a power series one obtains

$$\text{left-hand side (A.9)} = \sqrt{\pi} \sum_{\nu=0}^{\infty} \frac{2^\nu (st)^\nu}{\nu!} \tag{A.11}$$

Equating equal powers of $s$ and $t$ on the right-hand side of (A.9) and (A.11) one obtains

$$\int_{-\infty}^{+\infty} dx\, e^{-x^2} H_n(x) H_n(x) = \sqrt{\pi}\, n!\, 2^n. \tag{A.12}$$

For $n \neq m$ one again obtains (6.20). Because of the property (6.20) and (A.12) the $H_n(x)$ are called orthonormal on the interval $-\infty < x < +\infty$ with respect to the weight function $(\sqrt{\pi n!\, 2^n})^{-1} e^{-x^2}$.

Other important properties obtained from the generating function are the recurrence relations. To obtain the recurrence relation for the Hermite polynomials we differentiate (A.8) with respect to $t$:

$$\sum_{n=0}^{\infty} \frac{2x}{n!} H_n(x) t^n - \sum_{n=0}^{\infty} \frac{2}{n!} H_n(x) t^{n+1} = \sum_{n=1}^{\infty} \frac{1}{(n-1)!} H_n(x) t^{n-1}.$$



Equating powers of $t^n$ one obtains:

$$2xH_n(x) = H_{n+1}(x) + 2nH_{n-1}(x). \tag{A.13}$$

This recurrence relation can be used to calculate the Hermite polynomials step by step starting from $H_0(x) = 1$, $H_1(x) = 2x$.

In Chapter II we will also need some properties of the Fourier transforms of the $H_n(x)$ which are easily derived from the generating function. Multiplying (A.8) by $e^{iyx - x^2/2}$, where $-\infty < y < +\infty$, and integrating we obtain:

$$\int_{-\infty}^{+\infty} e^{2xt - t^2 + iyx - x^2/2}\, dx = \int e^{iyx - x^2/2}\, dx \sum_n \frac{1}{n!} H_n(x) t^n$$
$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{+\infty} e^{iyx - x^2/2} H_n(x)\, dx. \tag{A.14}$$

The integral on the left-hand side is calculated using the substitution $\eta = x - 2t$ and gives (cf. Problem 11):

$$e^{t^2} e^{i2yt} \int e^{-\eta^2/2} e^{iy\eta}\, d\eta = e^{-(it)^2} e^{2y(it)} \sqrt{2\pi}\, e^{-y^2/2}. \tag{A.15}$$

For the right-hand side of this equality we use (A.8) with $t$ replaced by $(it)$. Then we obtain from (A.14):

$$\sqrt{2\pi}\, e^{-y^2/2} \sum_{n=0}^{\infty} \frac{(it)^n}{n!} H_n(y) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{+\infty} e^{iyx} e^{-x^2/2} H_n(x)\, dx. \tag{A.16}$$

Comparing coefficients of identical powers of $t$ we obtain

$$i^n e^{-y^2/2} H_n(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx\, e^{iyx} e^{-x^2/2} H_n(x). \tag{A.17}$$

## I.7 Continuous Functionals[15]

In the previous sections of this chapter we presented the mathematics of quantum mechanics as an algebraic structure. Generalized eigenvectors were introduced by analogy to the basis vectors of a three-dimensional space and it was asserted that they could be treated very much like ordinary vectors. However, they are not vectors of the space $\Phi$ but are in fact continuous functionals on the space. In this section we define them and explain their distinction from ordinary vectors.

Let $\Phi$ be a complex linear space. A functional on $\Phi$ is a mapping $F$ from the space $\Phi$ into the complex numbers $\mathbb{C}$, $F: \Phi \to \mathbb{C}$. (If $\Phi$ is a real space then

[15] This section can be omitted in first reading. It gives a mathematical explanation of notions used in Sections I.4 and I.5 and is not essential for an understanding of the following chapters except for Chapter XXI.

the mapping is into the real numbers $\mathbb{R}$.) It is thus the analog of a complex-valued function of a real variable $x \in \mathbb{R}$, $F: \mathbb{R} \to \mathbb{C}$, only now the variable is not a real number but a vector $\phi \in \Phi$. If $F$ satisfies

$$F(\alpha\phi + \beta\psi) = \alpha^* F(\phi) + \beta^* F(\psi) \quad \text{for all} \quad \phi, \psi \in \Phi \quad \text{and} \quad \alpha, \beta \in \mathbb{C}, \tag{7.1}$$

then $F$ is called an antilinear functional. If $F$ satisfies

$$F(\alpha\phi + \beta\psi) = \alpha F(\phi) + \beta F(\psi), \tag{7.1a}$$

then $F$ is called a linear functional. (If $\Phi$ is a real space there is no distinction between linear and antilinear mappings.) We will consider here antilinear functionals rather than linear ones (note that in the mathematical literature one usually considers linear functionals).

An example of an antilinear functional on a linear space is given by

$$F(\phi) = (\phi, \psi), \tag{7.2}$$

where $\psi$ is a *fixed* element $\psi \in \Phi$ and $(\phi, \psi)$ is the scalar product of $\psi$ with $\phi$ where $\phi$ varies over $\Phi$ (cf. Problem 12). Because of this example and because in the general case we want to consider a functional to be a generalization of the scalar product, one uses for the antilinear functional $F(\phi)$ the symbol

$$F(\phi) = \langle \phi | F \rangle. \tag{7.3}$$

Any two antilinear functionals, $F_1$ and $F_2$, on a linear space $\Phi$ may be added and multiplied by numbers according to

$$(\alpha F_1 + \beta F_2)(\phi) = \alpha F_1(\phi) + \beta F_2(\phi), \quad \alpha, \beta \in \mathbb{C}, \tag{7.4'}$$

or, using the notation (7.3),

$$\langle \phi | \alpha F_1 + \beta F_2 \rangle = \alpha \langle \phi | F_1 \rangle + \beta \langle \phi | F_2 \rangle. \tag{7.4}$$

The functional $\alpha F_1 + \beta F_2$ defined by (7.4) is again an antilinear functional over $\Phi$ (Problem 13). Thus the set of antilinear functionals on a linear space $\Phi$ forms a linear space.[16] This space is called the conjugate space or dual space (precisely, the algebraic dual or algebraic conjugate space) to the space $\Phi$ and is denoted by $\Phi^\times$.

Let $\Phi$ be finite-dimensional, $\dim \Phi = n$, and let $e_i, i = 1, 2, \ldots, n$ be a basis for $\Phi$; let $F$ be an arbitrary antilinear functional on $\Phi$. Let us denote by $f_i$ the complex numbers

$$f_i = F(e_i), \quad i = 1, 2, \ldots, n. \tag{7.5}$$

The functional $F$ at an arbitrary $\phi \in \Phi$, $\phi = \sum_{i=1}^n \phi^i e_i$, can then be written as

$$F(\phi) = \sum_{i=1}^n F(\phi^i e_i) = \sum_i \phi^{i*} F(e_i) = \sum_{i=1}^n \phi^{i*} f_i. \tag{7.6}$$

[16] This is the analog to the statement that the set of linear operators on a linear space forms an algebra (i.e., a linear space in which a multiplication is defined). (7.4) is the analog to the first two equations of (3.4).



One has thus a one-to-one correspondence between the set of antilinear functionals on a finite-dimensional space and the sequence of numbers $(f_1, f_2, \ldots, f_n)$. With these numbers one can now define a vector $f$ in $\Phi$ by

$$f = \sum_{i=1}^n f_i e_i. \tag{7.7}$$

Then the right-hand side of (7.6) is the scalar product of the vectors $\phi$ and $f$ and we have shown that in a finite-dimensional linear scalar product space there is a one-to-one correspondence between the functionals $F$ and the $f \in \Phi$:

$$F \leftrightarrow f \tag{7.8a}$$

such that the value of the functional $F(\phi)$ at the element $\phi \in \Phi$ is given by the scalar product:

$$F(\phi) = (\phi, f). \tag{7.8b}$$

This shows that in the finite-dimensional case the symbol (7.3) can always be identified with the scalar product[17]

$$\langle \phi | F \rangle = (\phi, f). \tag{7.8c}$$

When the identification (7.8) can be made, then $\Phi$ is said to be self-dual[17] and we write

$$\Phi^\times = \Phi. \tag{7.8d}$$

For infinite-dimensional scalar product spaces such an identification is in general not possible. As we have already seen that the scalar product always defines an antilinear functional, we can identify those antilinear functionals $F_f$, whose values at any $\phi \in \Phi$ can be written as the scalar product $F_f(\phi) = (\phi, f)$ with a fixed $f \in \Phi$, with the vectors $f$: $F_f \leftrightarrow f$. Then we have

$$\Phi^\times \supset \Phi. \tag{7.9}$$

For the understanding of functionals on infinite-dimensional spaces topological notions are of great importance. So far we have only discussed how algebraic structures are imposed upon a set. The linear scalar product space defined in Section I.2, which we want to call $\Psi$ if it has no other structure, is a purely algebraic notion. One can now impose upon it a topological structure. Topological structures are defined by giving a specific meaning to the notion of convergence of infinite sequences.[18]

The Hilbert space convergence of a sequence of vectors $\phi_1, \phi_2, \phi_3, \ldots, \phi_\nu, \ldots$ to the vector $\phi \in \mathscr{H}$, denoted by

$$\phi_\nu \xrightarrow{\mathscr{H}} \phi \quad \text{for} \quad \nu \to \infty, \tag{7.10'}$$

[17] This identification is not necessary and often it is useful not to identify the functionals with elements of $\Phi$.

[18] There are topological spaces for which the definition of convergence of sequences is not sufficient to define the topology. But for the spaces $\Phi$ which we shall consider here (with first axiom of countability) this definition is sufficient.

is defined as

$$\|\phi_\nu - \phi\| \to 0 \quad \text{for} \quad \nu \to \infty. \tag{7.10}$$

The $\Phi$-space convergence is defined with the help of the algebra of operators and is therefore dependent upon it. For the algebra generated by $P$, $Q$, $H$ of (6.3) and (6.4) it is defined by[19]

$$\phi_\nu \xrightarrow{\Phi} \phi \quad \text{for } \nu \to \infty \qquad \text{iff} \tag{7.11'}$$

$$\|H^p(\phi_\nu - \phi)\| \to 0 \quad \text{for } \nu \to \infty \quad \text{for every } p = 0, 1, 2, 3, \ldots. \tag{7.11}$$

As (7.11) includes (for $p = 0$) the property (7.10) it is clear that from

$$\phi_\nu \xrightarrow{\Phi} \phi \quad \text{follows} \quad \phi_\nu \xrightarrow{\mathscr{H}} \phi \tag{7.12}$$

but not vice versa. The convergence (a topology) defined by (7.11) is called *stronger* (finer) than the convergence (topology) defined by (7.10), and the convergence defined by (7.10) is called weaker (coarser) than the convergence defined by (7.11). $\mathscr{H}$ is the space which contains in addition to the elements of $\Psi$ all limit elements of $\xrightarrow{\mathscr{H}}$-convergent sequences. $\Phi$ is the space which contains in addition to the elements of $\Psi$ all limit elements of $\xrightarrow{\Phi}$-convergent sequences. As because of (7.12) every $\Phi$-convergent sequence is also $\mathscr{H}$-convergent but not vice versa, we have

$$\Phi \subset \mathscr{H}. \tag{7.13}$$

The antilinear functionals that we will consider in the case of infinite-dimensional spaces will always be *continuous* functionals. An antilinear functional is continuous iff from

$$\phi_\nu \to \phi \quad \text{follows} \quad F(\phi_\nu) \xrightarrow{\mathbb{C}} F(\phi) \quad \text{for} \quad \nu \to \infty, \tag{7.14}$$

where $\xrightarrow{\mathbb{C}}$ denotes convergence for complex numbers.[20] $\Phi^\times$, $\mathscr{H}^\times$, etc. will always denote spaces of continuous functionals.

We can now consider the set of continuous linear functionals on $\mathscr{H}$ and on $\Phi$.

$\Phi^\times$ is the set of all $F^\Phi$ with the property that

$$F^\Phi(\phi_\nu) \xrightarrow{\mathbb{C}} F^\Phi(\phi) \quad \text{for all} \quad \phi_\nu \xrightarrow{\Phi} \phi.$$

$\mathscr{H}^\times$ is the set of all $F^{\mathscr{H}}$ with the property that

$$F^{\mathscr{H}}(\phi_\nu) \xrightarrow{\mathbb{C}} F^{\mathscr{H}}(\phi) \quad \text{for all} \quad \phi_\nu \xrightarrow{\mathscr{H}} \phi.$$

The condition fulfilled by $F \in \mathscr{H}^\times$ is more stringent than the condition fulfilled by $F \in \Phi^\times$ because according to (7.12) there are more sequences for which $\phi_\nu \xrightarrow{\mathscr{H}} \phi$ than sequences for which $\phi_\nu \xrightarrow{\Phi} \phi$. Therefore

$$\mathscr{H}^\times \subset \Phi^\times. \tag{7.15}$$

[19] This is the weakest topology or convergence that makes all elements of the algebra continuous operators.

[20] A sequence $c_1, c_2, \ldots$ of $c_\nu \in \mathbb{C}$ converges to a number $c$ iff $|c_\nu - c| \to 0$ for $\nu \to \infty$.



As mentioned above, infinite-dimensional linear spaces do not in general have the property (7.8d). However, the infinite-dimensional Hilbert space has the following remarkable property expressed by the Fréchet–Riesz theorem: For every $\mathscr{H}$-continuous functional $F^{\mathscr{H}}$ there exists an $f \in \mathscr{H}$ which is uniquely determined, such that

$$F^{\mathscr{H}}(\phi) = \langle\phi|F^{\mathscr{H}}\rangle = (\phi, f). \tag{7.16}$$

Thus for $\mathscr{H}$ one can make the identification (7.8) as for finite-dimensional spaces and obtains from (7.13) and (7.15) the triplet of spaces:

$$\Phi \subset \mathscr{H} = \mathscr{H}^\times \subset \Phi^\times \tag{7.17}$$

called a *Gelfand triplet* or *rigged Hilbert space*. The symbol $\langle\phi|F\rangle$ is therefore an extension of the scalar product to those $F \in \Phi^\times$ which are not in $\mathscr{H}$.

One can now consider antilinear continuous functionals $\tilde{\phi}$ on $\Phi^\times$ and denote the space of all $\tilde{\phi}$ by $\Phi^{\times\times}$. For a large class of linear topological spaces $\Phi$ (called reflexive) there is a natural one-to-one correspondence between a $\phi \in \Phi$ and $\tilde{\phi} \in \Phi^{\times\times}$ given by

$$\tilde{\phi}(F) = \overline{F(\phi)} = \overline{\langle\phi|F\rangle}. \tag{7.18}$$

As $\overline{\langle\phi|F\rangle}$ is an extension of $(f, \phi) = \overline{(\phi, f)}$ we can consider the functional $\tilde{\phi}$ at the vector $F \in \Phi^\times$ as an extension of the scalar product $(f, \phi)$. It is therefore convenient to write $\tilde{\phi}(F) \equiv \langle F|\phi\rangle$, where $F \in \Phi^\times$ is now the variable, i.e., $\langle F|\phi\rangle$ is the value of the functional $\tilde{\phi}$ on the space $\Phi^\times$ at the vector $F$. With this definition of $\langle F|\phi\rangle$, (7.18) reads

$$\langle F|\phi\rangle = \overline{\langle\phi|F\rangle} \tag{7.18'}$$

giving an extension of the property (2.2b) of the scalar product.

In order to define the generalized eigenvectors which appear in the spectral resolution (4.4c) we will have to consider the linear operators on $\Phi$. We will only consider operators which are continuous on $\Phi$. In analogy to the definition of a continuous functional we say that an operator $A: \Phi \to \Phi$ is continuous iff for all convergent sequences

$$\phi_\nu \xrightarrow{\Phi} \phi \quad \text{follows that} \quad A\phi_\nu \xrightarrow{\Phi} A\phi.$$

The notion of continuity thus depends—like all topological notions—on the definition of convergence. An operator which is a continuous operator with respect to the $\Phi$-convergence need not be a continuous operator with respect to the $\mathscr{H}$-convergence. (Many physical observables cannot be represented by continuous operators on the Hilbert space $\mathscr{H}$ but they can still be continuous operators on $\Phi$.)

For every continuous linear operator $A$ on $\Phi$ one can define an adjoint operator $A^\times$ on $\Phi^\times$ by

$$\langle\phi|A^\times|F\rangle = \langle A\phi|F\rangle. \tag{7.19}$$

One can prove that $A^\times$ is a linear continuous operator on $\Phi^\times$. This is the extension of the Hilbert space-adjoint operator defined by (cf. Section I.3):

$$(\phi, A^\dagger f) = (A\phi, f) \quad \text{for all } \phi \in \Phi \tag{7.20}$$

(which in general is not defined for all $f \in \mathscr{H}$).

If one has two operators $A$ and $\bar{A}$ with $A$ defined on a subspace of the space on which $\bar{A}$ is defined and with the property $A\phi = \bar{A}\phi$ for all $\phi \in$ subspace, then one writes $A \subset \bar{A}$ and calls $\bar{A}$ an *extension of the operator A*.* For an operator $A$ on $\Phi$ which is self-adjoint and has a unique self-adjoint[21] extension $\bar{A}$ to $\mathscr{H}$ one has therefore the following triplet of operators:

$$A \subset \bar{A} = A^\dagger \subset A^\times \tag{7.21}$$

on the triplet of spaces

$$\Phi \subset \mathscr{H} \subset \Phi^\times.$$

A functional $F$ over $\Phi$ is called a generalized eigenvector of the operator $A$ on $\Phi$ with eigenvalue $\omega$ iff

$$\langle A\phi|F\rangle = \omega\langle\phi|F\rangle \quad \text{for all} \quad \phi \in \Phi. \tag{7.22}$$

The generalized eigenvector $F$ with eigenvalue $\omega$ is also denoted

$$|F\rangle = |\omega\rangle. \tag{7.23}$$

Another precise form of writing (7.22) is

$$A^\times|\omega\rangle = \omega|\omega\rangle, \tag{7.24}$$

which is often just written as

$$A|\omega\rangle = \omega|\omega\rangle. \tag{7.25}$$

If $F \leftrightarrow f \in \mathscr{H}$ then (7.22) becomes

$$(A\phi, f) = (\phi, A^\dagger f) = \omega(\phi, f) \quad \text{for all} \quad \phi \in \Phi, \tag{7.26}$$

which for $A$ self-adjoint (as $\Phi$ is dense in $\mathscr{H}$) is identical with the definition of an eigenvector (cf. (3.6b)):

$$Af = \omega f. \tag{7.27}$$

The definition (7.22) of a generalized eigenvector and its generalized eigenvalue is thus a generalization of the definition (7.27) of a proper eigenvector and its proper eigenvalue. This generalization need not have all the properties of ordinary eigenvectors and eigenvalues. In particular, $\omega$ in (7.22) need not be real even if $A$ is (essentially) self-adjoint.

The eigenvectors $|x\rangle$ that appear in the continuous eigenvector expansion are generalized eigenvectors in the sense of (7.22). The coordinate $\langle x|\phi\rangle = \phi(x)$ of the vector $\phi \in \Phi$ along the basis vector $|x\rangle$, or the value of the function $\phi$ at the number $x$, is thus the complex conjugate of the value of the functional $|x\rangle \in \Phi^\times$ at the vector $\phi \in \Phi$: $\langle x|\phi\rangle = \langle\phi|x\rangle^*$. Using (7.18), one can also say that $\langle x|\phi\rangle$ is the value of the functional $\phi \in \Phi^{\times\times} = \Phi$ at the vector $\langle x| \in \Phi^\times$.

[21] An operator which is defined on $\Phi$, is Hermitian on $\Phi$ as defined in Section I.3 and has a unique self-adjoint extension to $\mathscr{H}$ is called essentially self-adjoint.

* For operators the symbol $\subset$ does not mean inclusion as for spaces.



## I.8 How the Mathematical Quantities Will Be Used

We conclude this chapter by a table which gives the correspondences between the mathematical objects introduced in this chapter and the physical quantities which they will represent. To establish, explain, and utilize this correspondence will be the subject of the following chapters of this book.

| Mathematical Image | Physical Quantity |
|---|---|
| vector $\phi \in \Phi$ (modulo a phase factor) | pure physical state |
| linear operator $A$ on $\Phi$ | physical observable |
| eigenvalues (spectrum) of $A$ | values obtained in a measurement of the observable $A$ |
| eigenvector $|\lambda\rangle$ of $A$ with eigenvalue $\lambda$ | state in which measurement of $A$ gives the value $\lambda$, eigenstate, bound state |
| generalized eigenvector $|\lambda\rangle$ of $A$ with real eigenvalue $\lambda$ | scattering state |
| generalized eigenvector $|\omega\rangle$ of $A$ with complex eigenvalue $\omega = E - i\Gamma/2$ | resonance state with resonance energy $E$ and width $\Gamma$ |
| scalar product $\langle\lambda|\phi\rangle$ with $|\lambda\rangle \in \Phi$, $\phi \in \Phi$ | probability amplitude |
| modulus squared of it $|\langle\lambda|\phi\rangle|^2$ | probability to obtain the value $\lambda$ in a measurement of the observable $A$ on a physical system in the state $\phi$ |
| functional $\langle\lambda|\phi\rangle$ | wave function |
| modulus squared of it $|\langle\lambda|\phi\rangle|^2$ | probability density for measuring the value $\lambda$ for the observable $A$ in the state $\phi$ |
| diagonal matrix element or expectation value $(\phi, A\phi)$ | average value for the measurement of $A$ in in the state $\phi$ |
| matrix element $(\psi, A\phi)$ | transition amplitude |
| its modulus square $|(\psi, A\phi)|^2$ | transition probability for transition caused by $A$ from state $\phi$ to state $\psi$ |

## Problems

1. Let $\mathbb{C}^n$ denote the set of all sequences $x = (\xi_1, \xi_2, \ldots, \xi_n)$ with $\xi_i \in \mathbb{C}$ (complex numbers). Define addition and multiplication with elements of $\mathbb{C}$ by the formulas

$$(\xi_1, \xi_2, \ldots, \xi_n) + (\eta_1, \eta_2, \ldots, \eta_n) = (\xi_1 + \eta_1, \xi_2 + \eta_2, \ldots, \xi_n + \eta_n).$$
$$\alpha(\xi_1, \xi_2, \ldots, \xi_n) = (\alpha\xi_1, \alpha\xi_2, \ldots, \alpha\xi_n).$$

(a) Show that $\mathbb{C}^n$ is a linear space.
(b) Let $x = (\xi_1, \ldots, \xi_n)$, $y = (\eta_1, \ldots, \eta_n)$ be two elements of $\mathbb{C}^n$. Show that $(x, y)$ defined by

$$(x, y) = \sum_{i=1}^{n} \bar{\xi}_i \eta_i$$

fulfills all conditions of a scalar product.

2. Let $\Phi$ be $\mathbb{C}^n$ of Problem 1 and let a map $A$ be defined by

$$A(\xi_1, \xi_2, \ldots, \xi_n) = (\xi'_1, \xi'_2, \ldots, \xi'_n),$$

where

$$\xi'_i = \sum_{k=1}^{n} a_{ik} \xi_k,$$

where $a_{ik}$ ($i, k = 1, 2, \ldots, n$) are fixed numbers.

$$a \equiv \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

is called the matrix of the map $A$. Define another map $B$ in the same way. Show that these maps $A$ and $B$ are linear operators on the space $\mathbb{C}^n$ (i.e., fulfill the relations for linear operators). Show that the set of operators form an algebra if multiplication and addition of their matrices and multiplication of their matrices by a number are defined by the usual rules for matrix multiplication.

3. Show that $af$ ($a \in \mathbb{C}$, $f \in \Phi$) is an eigenvector of a linear operator $A$ if $f$ is an eigenvector of $A$ with eigenvalue $\lambda$. What is the eigenvalue of the vector $af$?

4. Show that a Hermitian operator $A$ has the following properties:
(a) All eigenvalues are real.
(b) Two eigenvectors $\phi_1$ and $\phi_2$ of $A$ are orthogonal to each other if the eigenvalues corresponding to them are different from each other.

5. Show that two vectors $\phi$ and $\psi$ are equal iff all their components with respect to a basis system are equal.

6. Show that the Cauchy–Schwarz–Bunyakovski inequality, Equation (2.7), follows from the definition (2.5) of a positive Hermitian form.

7. Let $Q$ be the operator with continuous spectrum $\{x \mid -\infty < x < +\infty\}$ and let $|x\rangle$ denote its generalized eigenvector. Define another operator $P$ by:

$$\langle x|P|\psi\rangle = \frac{1}{i}\frac{d}{dx}\langle x|\psi\rangle \quad \text{for all} \quad \psi \in \Phi \qquad (i^2 = -1).$$

(a) Show that $P$ is a linear operator.
(b) Show that in order to have the operators $Q$ and $P$ well defined, i.e., $\|P\phi\|$ and $\|Q\phi\|$ be finite for all vectors $\phi \in \Phi$, the components of every vector $\langle x|\phi\rangle$ must be infinitely differentiable continuous functions which together with their derivatives vanish at infinity more rapidly than any polynomial of $x$ (i.e., $\langle x|\phi\rangle$ must be functions of the Schwartz space $S$).



(c) Show that the operators $P$ and $Q$ fulfill the commutation relation

$$PQ - QP = \frac{1}{i}1.$$

8. Let $\Phi$ be a linear scalar product space with elements $\phi, \psi, \chi, \ldots$. Let $|i\rangle$, $|E_n\rangle$, $i = 1, 2, \ldots, E_n = E_1, E_2, \ldots$, be two discrete basis systems in $\Phi$ and $|x\rangle$, $-\infty < x < +\infty$ a continuous basis system of $\Phi$. Show that the spaces of components $\mathbb{C}^\infty_{(i)}$ with elements $\langle i|\phi\rangle, \langle i|\psi\rangle, \langle i|\chi\rangle, \ldots$ and $\mathbb{C}^\infty_{(E_n)}$ with elements $(E_n|\phi), (E_n|\psi), (E_n|\chi), \ldots$ and $S_{(x)}$ with elements $\langle x|\phi\rangle, \langle x|\psi\rangle, \langle x|\chi\rangle, \ldots$ are all isomorphic to the space $\Phi$ and isomorphic to each other.

9. Show that the generalized function $\langle x|p\rangle = (1/\sqrt{2\pi})e^{ixp}$ is a generalized eigenfunction of the operator defined in Problem 7:

$$\langle x|P|p\rangle = \frac{1}{i}\frac{d}{dx}\langle x|p\rangle = p\langle x|p\rangle$$

if $p$ is real, but that it is not a well-behaved function, i.e., that $|p\rangle \notin \Phi$.

10. Show that the polynomials defined by

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}(e^{-\xi^2}), \qquad n = 0, 1, 2, \ldots$$

satisfy the differential equation

$$H''_n - 2\xi H'_n + 2nH_n = 0.$$

11. Calculate the Fourier transform

$$\phi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\, e^{ixp}\tilde{\phi}(p)$$

of the function $\tilde{\phi}(p) = e^{-ap^2} \in S$ $(a > 0)$.

12. Show that the scalar product $(\phi, \psi)$ with $\psi \in \Phi$ fixed and $\phi \in \Phi$ variable defines an antilinear functional $F_\psi(\phi) \equiv (\phi, \psi)$ on the space $\Phi$.

13. Let $F_1$ and $F_2$ be linear functions over $\Phi$, $\alpha, \beta$ be complex numbers, show that $(\alpha F_1 + \beta F_2)$ defined by

$$(\alpha F_1 + \beta F_2)(\phi) = \alpha F_1(\phi) + \beta F_2(\phi)$$

for all $\phi \in \Phi$ is again a linear functional over $\Phi$.

14. Let $P^2$ be the operator defined by Equation (5.25) and $P$ the operator defined by

$$\langle x|P|\phi\rangle = \frac{1}{i}\frac{d}{dx}\langle x|\phi\rangle$$

with the same requirements for the functions $\langle x|\phi\rangle$. Show that as a consequence of (5.26) $P$ and $P^2$ are self-adjoint operators. Are $P$ and $P^2$ self-adjoint operators if (5.26) is not fulfilled? *Hint:* Use integration by parts.

15. In Section I.7 it was shown that

$$\mathscr{H} \subset \Phi^\times \quad \text{by proving} \quad \mathscr{H}^\times \subset \Phi^\times$$

and using the Fréchet–Riesz theorem $\mathscr{H} = \mathscr{H}^\times$. Give an alternate proof of $\mathscr{H} \subset \Phi^\times$ without using $\mathscr{H} = \mathscr{H}^\times$ by proving the following:

(a) Show that from

$$h_n \xrightarrow{\mathscr{H}} h \quad \text{follows} \quad (h_n, f) \to (h, f)$$

for all $f \in \mathscr{H}$. *Hint*: Use the Cauchy–Schwarz–Bunyakowski inequality.

(b) Show that every $f \in \mathscr{H}$ defines an element of $F \in \Phi^\times$ by $F(\varphi) = (\varphi, f)$ for every $\varphi \in \Phi$. E.g., show that $F$, which is antilinear by Problem 12, is continuous.

*Hint*: Show that from $g_n \xrightarrow{\Phi} g$ follows $F(g_n) \to F(g)$ using the result of part (a).

CHAPTER II

# Foundations of Quantum Mechanics—The Harmonic Oscillator

This chapter, the longest in the book, introduces three of the basic assumptions of quantum mechanics and then illustrates them, using mainly the example of the harmonic oscillator. Though some historical remarks are included, neither the historical development nor any other heuristic way towards quantum mechanics is followed. The basic assumptions are formulated, explained, and applied. In Sections II.2, II.4, the basic assumptions are introduced; in Sections II.3, II.5, II.7 the harmonic oscillator is used to illustrate them. Section II.6 contains the derivations of some general consequences and might be omitted in first reading. The discussion for the continuous spectra, important for the description of the scattering and decay phenomena in the second part of the book, is given in Section II.8. Several remarks throughout this chapter emphasize the particular problems connected with generalized eigenvalues and eigenvectors and our unified treatment of continuous and discrete spectra. In Section II.9 we are ready to explain the physical meaning of the quantum-mechanical constant of nature, $\hbar$.

## II.1 Introduction

Physicists believe that there is something in nature, or in each restricted domain of it, that may be "understood"; that there is a structure in nature. To "understand" means to bring this structure into congruence with some structure in our mind, with a structure of thought objects, with a structure