Epilogue

The guiding principle in the presentation of quantum physics was the symmetry of the specially chosen systems, for which experimental data existed. This led us to the introduction of the basic concepts of quantum mechanics, including the notion of a state, an observable (linear operator in the vector space of the states) and the expectation value of an observable. By the same method, we have also discussed the time evolution of the physical systems. Our discussion introduced all mathematical concepts of quantum physics in an elementary way, while preserving the mathematical precision. We hope that a reader or a student, after studying our book will understand what quantum physics is, how it can be applied to the description of physical systems and above all, that he/she will understand the role which the symmetry plays in the description of the physical systems. This volume provides the conceptual basis of the forthcoming book, in which we will discuss further developments of the theory. A large part of our study will be devoted to the discussion of the scattering theory, theory of resonances and the description of unstable physical systems. We will also analyze the behavior of quantum systems in the slowly changing environment and the role of the quantum phase factors in such a description. As seen in this volume, our presentation will emphasize the simple description of complicated physical systems, using mathematically precise tools.

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Appendix: Mathematical Preliminaries

A.1 Introduction

A major new development in physics usually necessitates a corresponding development in mathematics. For example, differential and integral calculus were developed for classical mechanics to provide precise definitions for notions such as velocity and acceleration. It is true that special situations in mechanics can be treated without calculus, but the understanding remains vague without using calculus.

Quantum mechanics also has its own mathematical language, which was developed for the specific requirements of quantum physics—the physics of atoms, molecules, nuclei, and subatomic particles. The mathematical developments went hand-in-hand with the development of these areas of physics.

The mathematics of quantum mechanics uses vectors in linear, scalar-product spaces; linear operators; and algebras of operators in these spaces. Without the use of this mathematics, it is still possible to discuss some of the experimental data and to understand certain aspects of quantum mechanics. But the understanding is restricted in scope: a comprehensive understanding of the new ideas of quantum physics requires the use of its own mathematical language, which was discovered and developed for this very purpose.

Some of the key ideas of the mathematics of quantum mechanics as well as the notation are presented here without giving mathematical proofs. The treatment here is elementary, yet sufficiently detailed that it is possible to begin discussing quantum physics in its most general form with the mathematical tools presented here. Later, as required by the physics, additional mathematical concepts are introduced.

The mathematics that will be discussed here may be considered abstract as compared with differential operators or matrices. However, this is actually not the case. The one is as real as the other or, more precisely, as abstract as the other. A mathematical structure is a structure that exists in our minds. It is obtained by taking a set of mathematical objects and equipping this set with a structure by defining relations among these objects. Only familiarity makes some aspects of mathematics seem more real than others. Here in this introductory chapter, rather than treating

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the mathematics of quantum mechanics abstractly, each operation in a general linear space is motivated by first examining the corresponding operation in the familiar three-dimensional vector space. Also, when the properties of scalar-product spaces are discussed, each property is first shown to exist both for the scalar product in three-dimensional vector space and for the scalar product expressed as an integral.

The mathematical language of quantum mechanics was created so that quantum mechanics could be expressed in its general form. In 1926 P. Jordan and F. London started from the classical canonical transformations and recognized that these were coordinate transformations of a linear space. Physical quantities such as the intensity of radiation as an electron in an atom drops to a lower state were found to be represented by matrices. These matrices turned out to be matrices of operators in this linear space. First, Jordan and London considered only matrices and basis systems with discrete indices. The extension of the transformation theory to objects with continuous indices was done by Jordan and in particular by P.A.M. Dirac (1926–1927). Dirac's formalism was simple and beautiful but did not satisfy the requirement of mathematical rigor. The first rigorous mathematical formulation was given by D. Hilbert, L. Nordheim, and in particular by John von Neumann (1927) who associated the notions of quantum mechanical states and observables with vectors and operators, respectively, in the Hilbert space. Von Neumann's Hilbert space formulation could not accommodate objects with continuous indices and continuous eigenvalues. The mathematically rigorous formulation of quantum mechanics that includes the Dirac formalism, upon which our presentation here is based, was only possible after L. Schwartz (1950) had developed his distribution theory, and I.M. Gelfand and collaborators (1960) had introduced the rigged Hilbert space.

A.2 Linear, Scalar-Product Spaces

Linear spaces and linear operators are a generalization of certain aspects of three-dimensional space. The usual three-dimensional space consists of vectors that can be multiplied by real numbers and acted on by transformations or tensors. Mathematical objects such as vectors in three-dimensional space obey certain rules. To formulate the rules for a general, linear space, the rules from three-dimensional space are taken as the defining relations for a set of mathematical objects.

The linear spaces that are needed for quantum theory are, in general, not three-dimensional. They can have any dimension N, often infinite; the numbers are not real, but usually complex; the transformations are not orthogonal, but unitary; and the second rank tensors are not finite, but operators that can be represented by infinite matrices. In what follows, the rules for linear spaces are formulated in analogy with the usual rules for three-dimensional space.

Properties of the three -dimensional space $\Re_3$

Under addition, two vectors $\mathbf{a}, \mathbf{b} \in \Re_3$ (i.e. $\mathbf{a}, \mathbf{b}$ in the space $\Re_3$) satisfy

$$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}. \tag{A.2.1a}$$

Addition is associative.

$$(\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c}). \tag{A.2.2a}$$

There exists a zero vector with the property

$$\mathbf{0} + \mathbf{a} = \mathbf{a}. \tag{A.2.3a}$$

A vector can be multiplied with a real number b.

$$b(\mathbf{a}) = b\mathbf{a} \in \Re_3 \tag{A.2.4a}$$

Multiplication of a vector by real numbers a and b has the following properties:

$$a(b\mathbf{a}) = (ab)\mathbf{a} \tag{A.2.5a}$$

$$1\mathbf{a} = \mathbf{a} \tag{A.2.6a}$$

$$0\mathbf{a} = 0 \tag{A.2.7a}$$

Multiplication by real numbers satisfy

$$b(\mathbf{a} + \mathbf{b}) = b\mathbf{a} + b\mathbf{b}\,, \tag{A.2.8a}$$

$$(a + b)\mathbf{a} = a\mathbf{a} + b\mathbf{a}\,. \tag{A.2.9a}$$

The negative of a vector is defined by

$$(-1)\mathbf{a} = -\mathbf{a}\,. \tag{A.2.10a}$$

Defining relations for the general linear space Φ

The addition of two elements $\varphi, \psi \in \Phi$ is defined to satisfy

$$\varphi + \psi = \psi + \varphi. \tag{A.2.1b}$$

Addition is defined to be associative.

$$(\varphi + \psi) + \chi = \varphi + (\psi + \chi). \tag{A.2.2b}$$

There exists an element $0 \in \Phi$ with the property

$$0 + \psi = \psi\,. \tag{A.2.3b}$$

If $\psi \in \Phi$ and $b \in \mathbb{C}$ (b is a complex number), then

$$b(\psi) = b\psi \in \Phi\,. \tag{A.2.4b}$$

Multiplication of a vector by complex numbers a and b has, by definition, the following properties:

$$a(b\psi) = (ab)\psi \tag{A.2.5b}$$

$$1\psi = \psi \tag{A.2.6b}$$

$$0\psi = 0 \tag{A.2.7b}$$

On the left 0 is the number zero and on the right 0 is the element 0 of (A.2.7b).

Multiplication by complex numbers satisfy

$$b(\varphi + \psi) = b\varphi + b\psi\,, \tag{A.2.8b}$$

$$(a + b)\psi = a\psi + b\psi\,. \tag{A.2.9b}$$

The negative of a vector is defined by

$$-1\psi = -\psi\,. \tag{A.2.10b}$$

Since **a**, **b**, and **c** are called vectors, the elements $\varphi, \psi \in \Phi$ are also called vectors. The set of mathematical objects φ, ψ, etc. that obey rules or axioms (A.2.1b)–(A.2.10b) is called a linear space; therefore, a linear space is defined by these rules alone. There are, of course, linear spaces whose objects have more properties than those stated above, but those additional properties are not necessary for them to be elements of a linear space.

One realization of an N-dimensional linear space would be by N-dimensional column matrices whose entries are complex. Another realization of a linear space is provided by complex, continuous, rapidly decreasing functions for which the functions themselves as well as all derivatives are square integrable. Because some people have spent more time studying functions as opposed to, say, matrices, one person may be more comfortable with one realization than another. Ultimately it is important to free oneself from all realizations and consider the linear space simply as a set of thought objects defined by (A.2.1b)–(A.2.10b). In physics the vectors of the linear space are realized by pure physical states. That is, these thought objects are used as mathematical images of physical states.

A linear space does not have enough structure to be of much use. To equip it with more structure, a scalar product is defined. Linear spaces with scalar products are called linear, scalar-product spaces, Euclidean spaces, or Pre-Hilbert spaces. In the usual three-dimensional space $\Re_3$, the scalar product of the vectors **a** and **b** is denoted by $\mathbf{a} \cdot \mathbf{b}$ and can be calculated using the formula

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z \,. \tag{A.2.11}$$

In a general linear space, the scalar product of two vectors φ and ψ will be denoted by either (φ, ψ) or $\langle \varphi | \psi \rangle$. Since there are some features of a scalar-product space that are not present in $\Re_3$, in addition to $\Re_3$, a realization of a scalar-product space by a space of "well behaved" functions will also be used. "Well behaved" means that all operations performed with the functions are well-defined. For such well-behaved functions $f(x)$ and $g(x)$, their scalar product is defined by

$$(f, g) \equiv \int_{-\infty}^{\infty} f^*(x) g(x) \mathrm{d}x \,. \tag{A.2.12}$$

Note that in contrast to (A.2.11), the scalar product (A.2.12) is, in general, complex. In formulating the rules for scalar-product spaces, the rule will first be examined in $\Re_3$ and then the corresponding rule will be considered for the complex, continuous functions just mentioned with a scalar product defined in (A.2.12). Finally, a general rule will be formulated. The scalar product is required to have the following properties:

Three-dimensional space $\Re_3$	Space of complex, continuous functions that, along with all derivatives are square integrable	General scalar-product space Φ
The scalar product of a vector with itself is positive definite,	The scalar product of a function with itself is positive definite,	In a linear space Φ, the scalar product of a vector with itself is positive definite.
$\mathbf{a}\cdot\mathbf{a}\geq 0.$ (A.2.13a)	$\int_{-\infty}^{\infty} f^*(x)f(x)\mathrm{d}x \geq 0.$ (A.2.13b)	$(\psi,\psi)\geq 0.$ (A.2.13c)
$\mathbf{a}\cdot\mathbf{a}=0$ iff (if and only if) $\mathbf{a}=0$.	$\int_{-\infty}^{\infty} f^*(x)f(x)\mathrm{d}x = 0$ iff $f(x)=0$.	For any $\psi\in\Phi$ $(\psi,\psi)=0$ iff $\psi=0$.
Since the scalar product is real, it trivially satisfies $\mathbf{a}\cdot\mathbf{b}=(\mathbf{b}\cdot\mathbf{a})^*.$ (A.2.14a)	The scalar product satisfies $(f,g)=\int_{-\infty}^{\infty} f^*(x)g(x)\mathrm{d}x = \left[\int_{-\infty}^{\infty} g^*(x)f(x)\mathrm{d}x\right]^* = (g,f)^*.$ (A.2.14b)	Any two vectors $\psi,\varphi\in\Phi$ must satisfy $(\psi,\varphi)=(\varphi,\psi)^*.$ (A.2.14c)
Multiplication by a real scalar a satisfies $a(\mathbf{a}\cdot\mathbf{b})=\mathbf{a}\cdot(a\mathbf{b})$ $=(a\mathbf{a})\cdot\mathbf{b}.$ (A.2.15a)	Multiplication by a complex scalar satisfies $a(f,g)=\int_{-\infty}^{\infty} f^*(x)[ag(x)]\mathrm{d}x$ $=(f,ag)=\int_{-\infty}^{\infty}[a^*f(x)]^*g(x)\mathrm{d}x$ $=(a^*f,g)$ (A.2.15b)	For any $\psi,\varphi\in\Phi$ and any $a\in\mathbb{C}$, $a(\psi,\varphi)=(\psi,a\varphi)$ $=(a^*\psi,\varphi).$ (A.2.15c)

Note that while the convention (A.2.15c) for scalar products is standard in physics, it is not standard in the mathematical literature where one often finds $a(\psi,\varphi)=(\psi,a^*\varphi)=(a\varphi,\psi)$. That is, the scalar product in mathematical literature is often defined as the complex conjugate of the definition that is standard in the physics literature.

The scalar product of a sum of vectors is the sum of the scalar products.

$$(\mathbf{a}+\mathbf{b})\cdot\mathbf{c} = \mathbf{a}\cdot\mathbf{c}+\mathbf{b}\cdot\mathbf{c} \qquad \text{(A.2.16a)}$$

The scalar product of a sum satisfies

$$(f+g,h) = \int_{-\infty}^{\infty}[f(x)+g(x)]^{*}h(x)\mathrm{d}x = \int_{-\infty}^{\infty} f^{*}(x)h(x)\mathrm{d}x + \int_{-\infty}^{\infty} g^{*}(x)h(x)\mathrm{d}x\ . \qquad \text{(A.2.16b)}$$

For any $\psi, \varphi, \chi \in \Phi$ satisfies

$$(\psi+\varphi,\chi) = (\psi,\chi)+(\varphi,\chi) \qquad \text{(A.2.16c)}$$

The length or norm of a vector is

$$\|\mathbf{a}\| \equiv (\mathbf{a}\cdot\mathbf{a})^{\frac{1}{2}}. \qquad \text{(A.2.17a)}$$

The norm is defined by

$$\|f\| \equiv [\int_{-\infty}^{\infty} f^{*}(x)f(x)\mathrm{d}x]^{\frac{1}{2}}\ . \qquad \text{(A.2.17b)}$$

(φ,ψ) is called the scalar product of the vectors φ and ψ in the linear space Φ, and the space Φ is called a linear, scalar-product space or Euclidean space. In a scalar-product space the norm is defined by the scalar product

$$\|\psi\| \equiv (\psi,\psi)^{\frac{1}{2}}\ . \qquad \text{(A.2.17c)}$$

A vector is said to be normalized if $\|\psi\| = 1$.

Two vectors $\mathbf{a}$ and $\mathbf{b}$ are orthogonal if

$$\mathbf{a}\cdot\mathbf{b} = 0\ . \qquad \text{(A.2.18a)}$$

Two functions $f(x)$ and $g(x)$ are said to be orthogonal if

$$\int_{-\infty}^{\infty} f^{*}(x)g(x)\mathrm{d}x = 0\ . \qquad \text{(A.2.18b)}$$

Two vectors ψ and φ are defined to be orthogonal if

$$(\psi,\varphi) = 0\ . \qquad \text{(A.2.18c)}$$

Example A.2.1 Consider the following two functions on the interval $-\infty < x < \infty$:

$$f_1(x) = A_1 e^{-x^2/2} \qquad f_2(x) = A_2 x e^{-x^2/2}$$

Determine the constants $|A_1|$ and $|A_2|$ such that $f_1(x)$ and $f_2(x)$ are normalized. Are f_1(x) and f_2(x) orthogonal?

Solution The normalization conditions for the $f_i(x)$ are

$$1 = (f_i, f_i) = \int_{-\infty}^{\infty} f_i^{*}(x)f_i(x)\mathrm{d}x\ .$$

For $f_1(x)$, the above integral becomes

$$1 = |A_1|^2 \int_{-\infty}^{\infty} e^{-x^2} \mathrm{d}x = |A_1|^2 \sqrt{\pi},$$

where the integral was evaluated with the aid of a table of integrals. Thus,

$$|A_1| = \pi^{-\frac{1}{4}}.$$

Similarly,

$$1 = |A_2|^2 \int_{-\infty}^{\infty} x^2 e^{-x^2} \mathrm{d}x = \frac{\sqrt{\pi}}{2},$$

or

$$|A_2| = \sqrt{2}\pi^{-\frac{1}{4}}$$

To determine if $f_1(x)$ and $f_2(x)$ are orthogonal, their scalar product is calculated:

$$(f_1, f_2) = \int_{-\infty}^{\infty} f_1^*(x) f_2(x) \mathrm{d}x = A_1^* A_2 \int_{-\infty}^{\infty} x e^{-x^2} \mathrm{d}x = 0. \tag{A.2.19}$$

The above integral is zero from symmetry: By changing to the integration variable to $y = -x$, the integral is found to equal the negative of itself and is, therefore, zero. Since $(f_1, f_2) = 0$, the functions are orthogonal.

Example A.2.2 Using (A.2.14c), show that the relation $a(\psi, \varphi) = (\psi, a\varphi)$ implies the relation $a(\psi, \varphi) = (a^*\psi, \varphi)$ for $a \in \mathbb{C}$.

Solution Taking the complex number to be a^* instead of a, the first equality in (A.2.15c) immediately yields

$$a^*(\varphi, \psi) = (\varphi, a^*\psi).$$

Taking the complex conjugate of both sides of the above equation

$$a(\varphi, \psi)^* = (\varphi, a^*\psi)^*.$$

Using (A.2.14c) immediately yields the desired equality.

A.3 Linear Operators

The rules or axioms for linear operators in linear spaces are formulated here in analogy with operators in three-dimensional space.

Three-dimensional space $\Re_3$

Vectors in $\Re_3$ can be transformed into other vectors. One example is the rotation R, which rotates a vector $\mathbf{a}$ into a new vector $\mathbf{b} = R\mathbf{a}$. There are also other transformations such as the moment of inertia tensor I that transforms one vector into another according to $\mathbf{j} = I\boldsymbol{\omega}$. These transformations have the following properties:

$$R(\mathbf{a}+\mathbf{b}) = R\mathbf{a} + R\mathbf{b}, \tag{A.3.1a}$$

$$R(a\mathbf{b}) = a(R\mathbf{b}), \tag{A.3.2a}$$

where a is a real number.

Transformations (tensors) in $\Re_3$ can be added, multiplied by a real number, and multiplied by each other.

$$(R_1 + R_2)\mathbf{a} = R_1\mathbf{a} + R_2\mathbf{a}\,, \tag{A.3.3a}$$

$$(aR_1)\mathbf{a} = a(R_1\mathbf{a})\,, \tag{A.3.4a}$$

$$R_1R_2\mathbf{a} = R_1(R_2\mathbf{a})\,. \tag{A.3.5a}$$

The zero transformation 0 and the identity transformation 1 exist in $\Re_3$ and are defined, respectively, by

$$0\mathbf{a} = 0\,, \tag{A.3.6a}$$

$$1\,\mathbf{a} = \mathbf{a}\,, \tag{A.3.7a}$$

for all $\mathbf{a} \in \Re_3$.

General scalar-product space Φ

In a linear, scalar-product space transformations or linear operators are defined as follows: A function or operator A that maps each vector $\psi \in \Phi$ into a vector $\varphi \in \Phi$,

$$\varphi = A(\psi) \equiv A\psi,$$

is called a linear operator if it obeys the rules (A.3.1b) and (A.3.2b) listed below. Thus, by definition, linear operators have the following properties:

$$A(\psi + \varphi) = A\psi + A\varphi, \tag{A.3.1b}$$

$$A(a\psi) = a(A\psi), \tag{A.3.2b}$$

where $a \in \mathbb{C}$.

Linear operators A and B can be added, multiplied by a complex number, and multiplied by each other. Then $A + B$, $a\,A$, and $A\,B$ are also linear operators that satisfy

$$(A + B)\psi = A\psi + B\psi \tag{A.3.3b}$$

$$(aA)\psi = a(A\psi) \tag{A.3.4b}$$

$$(A\,B)\psi = A(B\psi)\,. \tag{A.3.5b}$$

Operators of special interest are the zero operator 0 and the unit or identity operator $\mathbb{1}$ defined, respectively, by

$$0\,\psi = 0, \quad 0 \in \Phi\,, \tag{A.3.6b}$$

$$\mathbb{1}\,\psi = \psi\,, \tag{A.3.7b}$$

for all $\psi \in \Phi$.

For every hermitian operator R defined for all vectors in $\Re_3$, there exists a non-zero vector $\mathbf{b}$ such that

$$R\mathbf{b} = \lambda \mathbf{b}\,, \quad \lambda \in \mathbb{R}\,. \tag{A.3.8a}$$

The vector $\mathbf{b}$ is called an eigenvector of R and λ is a (real) eigenvalue of R.

If there exists a non-zero vector ψ such that

$$A\psi = \lambda \psi\,, \quad \lambda \in \mathbb{C}\,, \tag{A.3.8b}$$

then ψ is called an eigenvector of A and λ is called an eigenvalue of A.

For every operator R defined for all vectors, the transpose operator R^T has the following property: Writing the scalar product in components

$$\begin{aligned}\mathbf{a}\cdot(R\mathbf{b}) &= \sum_{i=1}^{3}\sum_{j=1}^{3} a_i R_{ij} b_j \\ &= \sum_{i=1}^{3}\sum_{j=1}^{3} a_i R^T_{ji} b_j \\ &= \sum_{i=1}^{3}\sum_{j=1}^{3} (R^T_{ji} a_i) b_j = (R^T\mathbf{a})\cdot\mathbf{b}\end{aligned} \tag{A.3.9a}$$

A linear operator B in the space Φ is called the adjoint of the operator A if

$$(\psi, A\varphi) = (B\psi, \varphi)\,,$$

for all $\varphi, \psi \in \Phi$. The operator B is denoted $B = A^\dagger$. The operator A is called self-adjoint or hermitian[1] if

$$(\psi, A\varphi) = (A\psi, \varphi)\,, \tag{A.3.9b}$$

for all $\varphi, \psi \in \Phi$.

Example A.3.1 Find the adjoint of the operator $R = a\frac{d}{dx}$, $a \in \mathbb{C}$, for the space of complex, continuous functions which, along with all derivatives, are square integrable.

Solution Integrating by parts,

$$\begin{aligned}(f, R\,g) &= \int_{-\infty}^{\infty} f^*(x)\, a \frac{\mathrm{d}g(x)}{\mathrm{d}x}\mathrm{d}x, \\ &= af^*(x)g(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left[a\frac{\mathrm{d}f^*(x)}{\mathrm{d}x}\right] g(x)\mathrm{d}x.\end{aligned}$$

Since $f(\pm\infty) = g(\pm\infty) = 0$, the surface term vanishes. Therefore,

$$(f, R\,g) = \int_{-\infty}^{\infty}\left[-a^*\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right]^* g(x)\mathrm{d}x.$$

From the definition of the adjoint operator, $R^\dagger = -a^*\frac{\mathrm{d}}{\mathrm{d}x}$.

[1] For unbounded operators, if (A.3.9b) is fulfilled in a mathematically vague way without specifying the domain, the operator is often said to be hermitian. When (A.3.9b) is defined precisely mathematically, the operator is said to be selfadjoint.

Example A.3.2 Show that the scalar product $(A\psi, \psi)$ is real if $A^\dagger = A$.

Solution Using (A.2.14c),

$$(A\,\psi, \psi)^* = (\psi, A\,\psi).$$

But from the definition (A.3.6b) for the adjoint of an operator,

$$(\psi, A\,\psi) = (A^\dagger\psi, \psi).$$

Combining the above two equations,

$$(A\,\psi, \psi)^* = (A^\dagger\psi, \psi).$$

Thus if $A^\dagger = A$, the complex conjugate of the scalar product $(A\psi, \psi)$ equals itself and is therefore real.

If ψ is an eigenvector of the operator A, an immediate consequence of Example A.3.2 is that all eigenvalues of a hermitian operator are real. For this reason, hermitian operators are often called real operators.

Example A.3.3 Show that any two eigenvectors ψ, ϕ of a hermitian operator A satisfying

$$A\,\psi = a_1\psi, \qquad A\,\phi = a_2\phi; \qquad a_1 \neq a_2,$$

have the property

$$(\psi, \phi) = 0.$$

Solution Since ϕ is an eigenstate of A,

$$(\psi, A\,\phi) = (\psi, a_2\phi) = a_2(\psi, \phi).$$

Using the Hermiticity of the operator A as given in (A.3.6b),

$$(\psi, A\,\phi) = (A\,\psi, \phi) = (a_1\psi, \phi) = a_1^*(\psi, \phi).$$

Remembering that the eigenvalues of a hermitian operator are real, subtracting the above two expressions for $(\psi, A\phi)$ yields

$$0 = (a_2 - a_1)(\psi, \phi).$$

Thus if $a_1 \neq a_2$, $(\psi, \phi) = 0$.

For any two vectors $\psi, \phi \in \Phi$ and an operator A, the scalar product of $A\,\psi$ with ϕ, namely $(\phi, A\,\psi)$, plays an important role in physics and is called the matrix element of the operator A between the vectors ϕ and ψ .

Example A.3.4 Calculate the four matrix elements $(f_i(x), xf_j(x))$ where $f_1(x)$ and $f_2(x)$, respectively, are the normalized functions

$$f_1(x) = \pi^{-\frac{1}{4}} e^{-x^2/2} \quad \text{and} \quad f_2(x) = \sqrt{2}\,\pi^{-\frac{1}{4}} x e^{-x^2/2}$$

first discussed in Example A.3.1 on page 321.

Solution From the definition of a matrix element,

$$(f_i(x), xf_j(x)) = \int_{-\infty}^{\infty} f_i^*(x) x f_j(x)\,\mathrm{d}x.$$

Since $f_1(x)$ and $f_2(x)$ are real,

$$(f_1(x), xf_2(x)) = (f_2(x), xf_1(x)) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} e^{-x^2} x^2 \mathrm{d}x = \frac{1}{\sqrt{2}}.$$

Using the procedure mentioned in Example A.2.1 on page 318, the diagonal matrix elements are found to equal zero,

$$(f_1(x), xf_1(x)) = (f_2(x), xf_2(x)) = 0.$$

The results can be summarized by the single matrix

$$(f_i(x), xf_j(x)) = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

where the first index labels the row and the second labels the column of each matrix element.

All observables such as position, momentum, and energy are represented by linear operators in a linear, scalar-product space, and states are represented by vectors in this same space.

A.4 Basis Systems and Eigenvector Decompositions

A.4.1 Discrete Basis Vectors in Real, Three-Dimensional Space

Three basis vectors are introduced in the three-dimensional space $\Re_3$,

$$\mathbf{e}_i, \quad i = 1, 2, 3, \tag{A.4.1}$$

that span the space and are usually normalized to unity,

$$\mathbf{e}_i \cdot \mathbf{e}_i = 1. \tag{A.4.2}$$

These basis vectors are also usually chosen so that they are orthogonal to one another,

$$\mathbf{e}_i \cdot \mathbf{e}_j = 0 \text{ if } i \neq j. \tag{A.4.3}$$

Instead of labeling the vectors by $i = 1, 2, 3$, they could also be denoted by $\mathbf{e}_1 = \mathbf{e}_x$, $\mathbf{e}_2 = \mathbf{e}_y$, $\mathbf{e}_3 = \mathbf{e}_z$. Relations (A.4.2) and (A.4.3) can be written as the single equation

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}, \quad i, j = 1, 2, 3, \tag{A.4.4}$$

where δ_{ij} is the Kronecker-δ. The set of orthogonal, normalized vectors is called an orthonormal set.

A basis system may be chosen arbitrarily provided it spans the space although, for a specific physical problem, one basis system may be much easier to work with than others. For example, for a rigid body with an inertia tensor I, it is helpful to choose the basis system such that the inertia tensor is diagonal. Therefore, the $\mathbf{e}_i$ are chosen such that

$$\mathbf{e}_i \cdot I \cdot \mathbf{e}_j = I(j)\,\delta_{ij} \quad \text{or} \quad I \cdot \mathbf{e}_j = I(j)\,\mathbf{e}_j. \tag{A.4.5}$$

The $\mathbf{e}_j$ are the eigenvectors of the tensor I and the $I(j)$ are the eigenvalues.

In $\Re_3$ every vector $\mathbf{x}$ can be expanded in terms of the basis system,

$$\mathbf{x} = \sum_{i=1}^{3} x_i \mathbf{e}_i = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3. \tag{A.4.6}$$

The numbers x_i are the coordinates or components of $\mathbf{x}$ with respect to the $\mathbf{e_i}$. As shown in Fig. A.1 on the facing page, the x_1, x_2, and x_3 are, respectively, the x, y, and z-components of the vector $\mathbf{x}$.

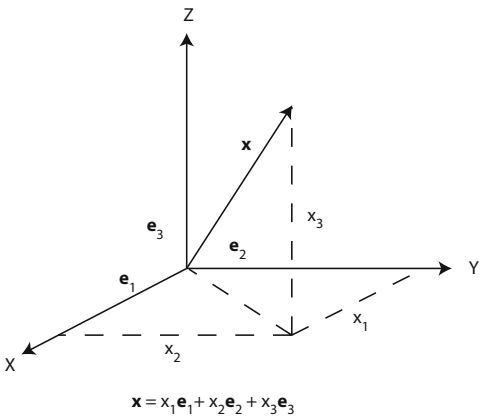

Fig. A.1 The three-dimensional vector **x** expressed in terms of the normalized (unit) vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$

Taking the scalar product of both sides of (A.4.6) with $\mathbf{e}_j$,

$$\mathbf{e}_j \cdot \mathbf{x} = \sum_{i=1}^{3} \mathbf{e}_j \cdot \mathbf{e}_i x_i = \sum_{i=1}^{3} \delta_{ij} x_i = x_j, \tag{A.4.7}$$

where the orthogonality relation (A.4.4) has been used. Clearly the x_i determine the vector **x** uniquely. Using the expression for x_j in (A.4.7), (A.4.6) can be written in the form

$$\mathbf{x} = \sum_{i=1}^{3} \mathbf{e}_i (\mathbf{e}_i \cdot \mathbf{x}) \,. \tag{A.4.8}$$

Example A.4.1 Consider the two-dimensional vector **V** shown in Fig. A.2 on the next page, which has a magnitude $|\mathbf{V}|$, makes an angle θ with the $\tilde{x}$-axis, and makes an angle θ' with the $\mathbf{e_1}$-axis. From geometrical considerations, express **V** in terms of the unit vectors $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$ and then in terms of $\mathbf{e}_1$ and $\mathbf{e}_2$. Show that the second formula agrees with (A.4.7).

Solution The $\tilde{x}$ and $\tilde{y}$-components of **V** are clearly $|\mathbf{V}| \cos\theta$ and $|\mathbf{V}| \sin\theta$, respectively. Therefore,

$$\mathbf{V} = |\mathbf{V}| \cos\theta \; \tilde{\mathbf{x}} + |\mathbf{V}| \sin\theta \; \tilde{\mathbf{y}}.$$

Using similar logic, in terms of the orthonormal basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$,

$$\mathbf{V} = |\mathbf{V}| \cos\theta' \mathbf{e}_1 + |\mathbf{V}| \sin\theta' \mathbf{e}_2.$$

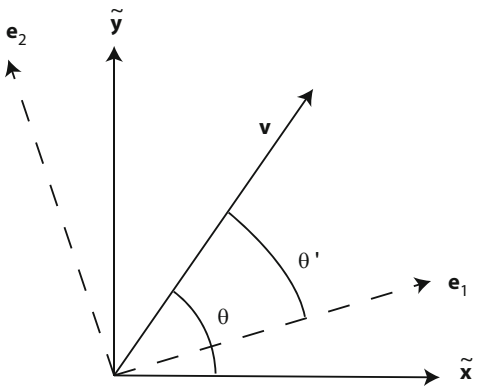

Fig. A.2 The two-dimensional vector **V** shown with respect to the $\tilde{\mathbf{x}}$, $\tilde{\mathbf{y}}$ basis and the $\mathbf{e}_1$, $\mathbf{e}_2$ basis

Now from the definition of the dot product,

$$\mathbf{e}_1 \cdot \mathbf{V} = |\mathbf{e}_1||\mathbf{V}| \cos\theta' = |\mathbf{V}| \cos\theta',$$

and

$$\mathbf{e}_2 \cdot \mathbf{V} = |\mathbf{e}_2||\mathbf{V}| \cos(90 - \theta'\rangle = |\mathbf{V}| \sin\theta'.$$

Combining the above three equations,

$$\mathbf{V} = \mathbf{e}_1(\mathbf{e}_1 \cdot \mathbf{V}) + \mathbf{e}_2(\mathbf{e}_2 \cdot \mathbf{V}),$$

which, for two-dimensional vectors **V**, agrees with (A.4.8).

In $\Re_3$, the scalar product of the vectors

$$\mathbf{x} = \sum_{i=1}^{3} \mathbf{e}_i x_i \quad \text{and} \quad \mathbf{y} = \sum_{j=1}^{3} \mathbf{e}_j y_j$$

is calculated as follows:

$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{3} \sum_{j=1}^{3} \mathbf{e}_i x_i \cdot \mathbf{e}_j y_j$$

Using (A.4.4),

$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{3} \sum_{j=1}^{3} x_i \ \delta_{ij} \ y_j ,$$
$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{3} x_i \ y_i . \tag{A.4.9}$$

The square of the norm (square of the length) of the vector $\mathbf{x}$ is given by

$$\|\mathbf{x}\|^2 = \mathbf{x} \cdot \mathbf{x} = \sum_{i=1}^{3} x_i \ x_i . \tag{A.4.10}$$

A.4.2 Discrete Basis Vectors in Infinite-Dimensional, Complex Space

In a linear, scalar-product space over the complex numbers, it is possible to introduce, in analogy to Fig. A.1 on page 325, a basis system in a three-dimensional, complex linear space for which the coordinates x_i of a vector ψ are in general complex numbers. Without any difficulties this three-dimensional space can be generalized to an N-dimensional space. To go from N dimensions to infinite dimensions is more difficult: the meaning of convergence of infinite sequences must be defined, which means that the topology of the linear space Φ must be defined. This can be done in many different ways, two of which result in the Hilbert space and the Schwartz space.

In an N-dimensional (or infinite-dimensional) space the basis vectors are denoted

$$e_n = |n) \quad \text{or} \quad e_n = |n\rangle \quad n = 1, 2, 3, \ldots N \ \text{ or } \ \infty . \tag{A.4.11}$$

These vectors are again chosen to be orthonormal,

$$(e_i, e_j) = \langle i | j \rangle = \delta_{ij} . \tag{A.4.12}$$

In an N-dimensional (or infinite-dimensional), complex, linear, scalar-product space Φ, there exists an orthonormal basis system. That is, every vector $\psi \in \Phi$ can be expressed as

$$\psi = \sum_{n=1}^{N \text{ or } \infty} |e_n\rangle c_n = \sum_{n=1}^{N \text{ or } \infty} |e_n\rangle \langle e_n | \psi \rangle , \tag{A.4.13}$$

where the coordinates or components $c_n = \langle e_n|\psi\rangle$ are complex numbers. To make the expansions (A.4.13) mathematically rigorous, theorems are required that are not proved here. Instead the expansions are simply constructed in analogy to (A.4.8).

In analogy with the vectors $\mathbf{e}_i$ in the three dimensional space $\Re^3$ that satisfy (A.4.5), it is often convenient to choose the basis vectors $|e_n\rangle$ to be eigenvectors of a self-adjoint operator $A = A^\dagger$ that is of particular physical significance. The eigenvectors in the N-dimensional (or infinite-dimensional), linear, scalar-product space, are solutions of the eigenvalue equation

$$A|e_n\rangle = a_n|e_n\rangle, \quad |e_n\rangle \in \Phi, \quad n = 1, 2, 3 \ldots . \tag{A.4.14}$$

In Examples A.3.2 and A.3.3 on page 322 it was established that the eigenvalues a_i of a self-adjoint operator A are real and that two eigenvectors $|e_i\rangle$ and $|e_j\rangle$ with different eigenvalues $a_i \neq a_j$ are orthogonal. Thus it is possible to normalize[2] the eigenvalues in (A.4.14) such that (A.4.12) is fulfilled.

If $|e_i\rangle$ is a normalized eigenvector with eigenvalue a_i then

$$|e'_n\rangle = e^{i\omega}|e_n\rangle, \qquad \omega \in \Re\,, \tag{A.4.15}$$

is also a normalized eigenvector with the same eigenvalue a_i (See Problem A.10.) so the solutions of (A.4.14) are only determined up to a phase factor $e^{i\omega}$.

Since only the combination $|e_n\rangle\langle e_n|$ appears in (A.4.13) and

$$|e'_n\rangle\langle e'_n| = e^{i\omega}|e_n\rangle\langle e_n|e^{-i\omega} = |e_n\rangle\langle e_n|\,, \tag{A.4.16}$$

the choice of phase (A.4.15) is of no consequence. The important mathematical quantities are the projection operators $\Lambda_n = |e_n\rangle\langle e_n|$ that project onto orthogonal subspaces,

$$\Lambda_n \Lambda_m = \delta_{nm} \Lambda_n\,, \tag{A.4.17}$$

and are independent of the phase. The projection operators have the property that $\Lambda_n \mathbf{V} = |e_n\rangle\langle e_n|\mathbf{V}) = v_n|e_n\rangle$, implying that the projection operator Λ_n projects out the component v_n of the vector $\mathbf{V}$ along the $\mathbf{e}_n$ axis as shown in Fig. A.3 on the facing page.

Two cases are now distinguished:

1. There is only one normalized eigenvector (up to a phase) for each eigenvalue of the chosen operator A. The eigenvalues are said to be nondegenerate, and the projection operator Λ_n projects onto a one-dimensional subspace.
2. There is more than one normalized eigenvector (up to the phase) for at least one eigenvalue of the operator A. The eigenvalues are said to be degenerate. A

[2] If $|e_i\rangle$ is not normalized and $\| |e_i\rangle\| \neq 0$, the new vector $|e'_i\rangle = |e_i\rangle/\| |e_i\rangle\|$ } is a normalized eigenvector with the same eigenvalue.

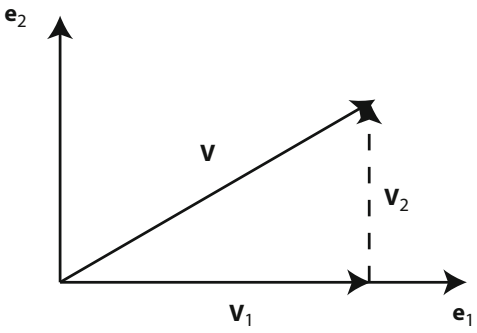

Fig. A.3 The two-dimensional vector **V** with components v_1 and v_2 along the respective basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$

discussion of Case 2 will be postponed until it is needed to describe physical problems.

Example A.4.2 Show that the functions

$$f_1(x, y) = xe^{-x^2/2}\, e^{-y^2/2} \quad \text{and} \quad f_2(x, y) = ye^{-x^2/2}\, e^{-y^2/2}$$

both satisfy

$$Af_i(x, y) = af_i(x, y), \quad i = 1, 2,$$

where the constant a is the eigenvalue of the operator

$$A = \frac{\mathrm{d}^2}{\mathrm{d}x^2} - x^2 + \frac{\mathrm{d}^2}{\mathrm{d}y^2} - y^2.$$

The coordinates x and y range from $-\infty$ to ∞ .

Solution Allowing the differential operator A to act on $f_1(x, y)$ and $f_2(x, y)$,

$$Af_1(x, y) = -4f_1(x, y), \quad Af_2(x, y) = -4f_2(x, y).$$

If the functions $f_1(x, y)$ and $f_2(x, y)$ are labeled only by their eigenvalue a,

$$f_{a=-4}(x, y) = f_1(x, y) \quad \text{and} \quad f_{a=-4}(x, y) = f_2(x, y).$$

Since there are two different eigenfunctions $f_{a=-4}(x, y)$, the eigenfunctions of A are not uniquely specified by the eigenvalue a.

For Case 1 the eigenvector $|e_n\rangle$ in (A.4.11) is uniquely determined (up to a phase) by its eigenvalue a_n. Therefore, the vector $|e_n\rangle$ can be labeled by the value a_n,

$$|e_n\rangle \equiv |a_n\rangle \quad n = 1, 2, 3, \ldots N\,. \tag{A.4.18}$$

The eigenvalue equation (A.4.14) then becomes

$$A|a_n\rangle = a_n|a_n\rangle, \quad |a_n\rangle \in \Phi, \quad n = 1, 2, 3\ldots, \tag{A.4.19a}$$

$$\langle a_n|a_m\rangle = \delta_{nm}\,, \tag{A.4.19b}$$

and the basis vector expansion (A.4.13) becomes the eigenvector expansion

$$\psi = \sum_{n=1}^{N \text{ or } \infty} |a_n\rangle c_n = \sum_{n=1}^{N \text{ or } \infty} |a_n\rangle\langle a_n|\psi\rangle\,, \tag{A.4.20}$$

A complete system of eigenvectors possesses the property that every vector $\psi \in \Phi$ can be expanded in terms of the $|a_n\rangle$ according to the eigenvector expansion (A.4.20). Is it possible to find a complete system of eigenvectors $|a_n\rangle$ for every self-adjoint operator A in a linear scalar product space Φ? When Φ is finite-dimensional, the answer is "yes," and when Φ is infinite-dimensional, as is the case for the Hilbert space, the answer is "no."

A.4.3 Continuous Basis Systems of a Linear Space

Some properties of physical systems can be described by operators with a complete set of discrete eigenvectors $|a_n\rangle$, $n = 1, 2, 3, \ldots$. The eigenvalues a_n represent the values observed in experiments on quantum physical systems. For example, if the operator A is the energy operator of the hydrogen atom, the eigenvalues a_n are the discrete energy values $E_n = -2\pi \mathrm{R}\hbar\mathrm{c}/n^2$, $n = 1, 2, 3, \ldots$, where R is the Rydberg constant.

On the other hand it is impossible to describe all physical systems with operators that have discrete spectra. In addition to the discrete eigenvalues E_n corresponding to the electron-proton bound states of the hydrogen atom, an electron interacting with a proton also has continuous values of energy when there is no binding and the electron is scattered by the proton. The electron's motion corresponds to the hyperbolic orbits of the corresponding classical Kepler system. Another operator with a continuous eigenvalue spectrum is the momentum operator P of electrons in cathode rays. The operator P can have any of a continuous set of values depending on the accelerating potential. The position x must similarly be described by an operator with a continuous eigenvalue spectrum.

Thus in addition to the set of discrete eigenvectors $H|E_n\rangle = E_n|E_n\rangle$, eigenvectors of energy H, momentum P, position Q, as well as many other operators can

have continuous eigenvalues:

$$H|E\rangle = E|E\rangle\,, \qquad 0 \le E < \infty\,, \tag{A.4.21a}$$

$$P|p\rangle = p|p\rangle\,, \qquad -\infty \le p \le +\infty\,, \tag{A.4.21b}$$

$$Q|x\rangle = x|x\rangle\,, \qquad -\infty \le x < +\infty \quad \text{or} \quad M \le x \le N. \tag{A.4.21c}$$

These are the eigenkets first introduced by Dirac. They are called generalized eigenvectors and, as in (A.4.21), are denoted by the symbol $|\ \rangle$ to indicate that the spectrum of the eigenvalue is continuous.

Since the eigenvalue x of the position operator Q is continuous, it is not possible to choose eigenvectors such that their (generalized) scalar product is a Kronecker-δ (A.4.19b) because a Kronecker-δ only involves discrete indices. In spite of this mathematical complication, it is possible to discuss generalized eigenvectors of operators with a continuous spectrum in analogy to the discrete case. The starting point is the eigenvector expansion, which was postulated by Dirac as the continuous analogue of (A.4.20).

There are spaces, an example of which is the Schwartz space Φ, for which any vector $\psi \in \Phi$ can be expanded in terms of the generalized eigenvectors $|x\rangle$ of Q according to

$$\psi = \int \mathrm{d}x\,|x\rangle\langle x|\psi\rangle \equiv \int \mathrm{d}x|x\rangle\psi(x)\,, \qquad \psi(x) \equiv \langle x|\psi\rangle\,. \tag{A.4.22a}$$

The above equation implies that

$$\langle\phi|\psi\rangle = \int \mathrm{d}x\ \langle\phi|x\rangle\langle x|\psi\rangle = \int \mathrm{d}x\,\phi(x)^*\psi(x)\,, \tag{A.4.22b}$$

where the integral extends over the continuous set of eigenvalues M< x< N where often $M = -\infty$ and $N = +\infty$.

To make the transition from (A.4.20) to (A.4.22a), the sum over the discrete variable n is replaced by a continuous sum (integral) over the continuous variable x, and the eigenvectors $|n\rangle$ are replaced by the generalized eigenvectors $|x\rangle$. Equation (A.4.22a) is called the generalized basis system expansion and was justified mathematically by the Nuclear Spectral Theorem.[3]

The coordinates or components $\psi(x) \equiv \langle x|\psi\rangle = (|x\rangle, |\psi\rangle)$ of the vector ψ with respect to the basis system $|x\rangle$ are the (generalized) "scalar product" between the vector ψ and the generalized eigenvector $|x\rangle$ and are complex numbers just as the coordinates $\langle a_n|\psi\rangle$ are complex numbers in the discrete case (A.4.20). For the continuous case the coordinates $\langle x|\psi\rangle$are continuous, well-behaved (infinitely

[3]After Dirac introduced (A.4.22a), approximately 30 years elapsed until Distribution Theory (L. Schwartz (1950–1951)) and the Rigged Hilbert Space (Gelfand et al., K. Maurin (1955–1959)) provided the mathematics for its justification.

differentiable, rapidly decreasing) functions of the continuous variable x whereas in (A.4.20) they are functions of the discrete variable a_n.

The progression from (A.4.8) to (A.4.22) can be taken as a justification of the mathematics underlying Dirac's eigenvector expansion (A.4.22); however, the mathematical proof is provided by the Nuclear Spectral Theorem and is required to make the mathematics rigorous.[4]

For the discrete case, taking the scalar product of ψ as given in (A.4.20) with the vector $|a_m\rangle$ gives,

$$(|a_m\rangle, \psi) \equiv \langle a_m|\psi\rangle = \sum_n \langle a_m|a_n\rangle\langle a_n|\psi\rangle\,, \tag{A.4.23}$$

which implies $\langle a_m|a_n\rangle = \delta_{mn} = \delta_{a_m a_n}$.

In analogy to (A.4.23) the (generalized) scalar product of ψ, as given in (A.4.22a), with the generalized eigenvector $|x'\rangle$ is written as

$$(|x'\rangle, \psi) \equiv \langle x'|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, \langle x'|x\rangle\langle x|\psi\rangle. \tag{A.4.24}$$

The quantity $\langle x'|x\rangle$ is thus the analog of $\langle a_m|a_n\rangle$ in (A.4.23). Since $\langle a_m|a_n\rangle = \delta_{mn}$, where δ_{mn} is the Kronecker-δ, the generalized scalar product $\langle x'|x\rangle$ was also written by Dirac as

$$\langle x'|x\rangle = \delta(x - x), \tag{A.4.25}$$

where $\delta(x - x')$ is called the Dirac-δ functional, which is continuous. The Dirac-δ, $\delta(x' - x)$, is not a (locally integrable) function. Instead it is a new mathematical quantity called a functional that is defined by (A.4.24). Defining the function $\psi(x) \equiv \langle x|\psi\rangle$, (A.4.24) is then written as

$$\psi(x') = \int \mathrm{d}x\, \delta(x' - x)\, \psi(x). \tag{A.4.26}$$

This functional is defined as the mathematical object with the property that it gives the value of the well-behaved function at x'. That is, integrating from $-\infty < x < +\infty$ over the product of a Dirac-δ and a "well-behaved" function is the the mathematical procedure that maps $\psi(x)$ into $\psi(x')$, the value of the function at the position x'.

The generalized eigenvectors $|x\rangle$ are not vectors in the space Φ. The generalization $\langle x'|\psi\rangle$ is not an ordinary scalar product of a vector ψ with a vector $|x'\rangle$. The generalized scalar product can be made mathematically precise as an anti-linear functional on the space Φ: $F_x(\psi) \equiv \langle\psi|x\rangle$. The function F_x assigns a

[4] Ibid.

number $F_x(\psi)$ to every $\psi \in \Phi$. This function fulfills the relation $F_x(a\psi + b\phi) = \bar{a}F_x(\psi) + \bar{b}F_x(\phi)$ for all $\psi, \phi \in \Phi$ and for all complex numbers $a, b \in \mathbb{C}$, which is the defining property of an anti-linear functional. But for calculations here, generalized eigenvectors can be treated as if they were proper eigenvectors, and $\langle\psi|x\rangle$ can be treated as if it were a scalar product $\langle\psi|x\rangle$. The distinction between eigenvectors $|a_n\rangle$ and generalized eigenvectors $|x\rangle$ is that the sums over $|a_n\rangle$ in (A.4.23) must be replaced by integrals as in (A.4.24).

The generalized basis expansion (A.4.22a) does not hold for all vectors ψ for which the discrete basis vector expansion (A.4.20) is correct. Instead it is valid only for a subset of the Hilbert space which here is chosen as the Schwartz space Φ. This is due to the fact that (A.4.26) does not hold for all (Lebesgue square integrable) functions but only for "well-behaved" functions $\psi(x)$. An example of such functions are the Schwartz-space functions that are continuous, infinitely differentiable and have derivatives of any order that decrease faster than any inverse power of x.

Although the above discussion has focused on the eigenket $|x\rangle$, where x usually represents position, the statements apply equally well to the eigenkets $|E\rangle$ and $|p\rangle$ etc. in (A.4.21a) and (A.4.21b).

The components $\psi(x) = \langle x|\psi\rangle$, $\psi(p) = \langle p|\psi\rangle$, and $\psi(E) = \langle E|\psi\rangle$, which are also called wave functions, must satisfy certain conditions in quantum mechanics.

A.4.4 Working with Eigenvectors and Basis Vector Expansions

The eigenvector expansion

$$\psi = \sum_{n=1}^{\infty} |a_n\rangle\langle a_n|\psi\rangle\,, \tag{A.4.27}$$

associates with every vector ψ an infinite sequence of numbers $\{\langle a_n|\psi\rangle\,, n = 1, 2, 3\ldots\}$. The coordinates $c_n = \langle a_n|\psi\rangle$ are, in general, complex numbers and are a function of the discrete variable n. The vector $\psi = 0$ iff all of its coordinates are zero. Equivalently, the vectors ϕ and ψ are equal if all their coordinates are equal. The set of eigenvectors $|a_n\rangle$ in (A.4.27) is thus a complete system of eigenvectors. The set of eigenvalues $\{a_n, n = 1, 2, \ldots\}$ is called the spectrum of the operator A.

In analogy with (A.4.10), the square of the norm of a vector ψ is given by

$$\|\psi\|^2 \equiv (\psi, \psi) = \sum_{n=1}^{\infty} |c_n|^2 = \sum_{n=1}^{\infty} |\langle a_n|\psi\rangle|^2 = \sum_{n=1}^{\infty} \langle a_n|\psi\rangle^* \langle a_n|\psi\rangle\,. \tag{A.4.28}$$

If the vector has a finite norm (finite length) then

$$\sum_{n=1}^{\infty} |c_n|^2 = \sum_{n=1}^{\infty} |\langle a_n|\psi\rangle|^2 < \infty\,. \tag{A.4.29}$$

The space of square summable sequences, which is the space of all vectors ψ with components that fulfill (A.4.29), is the Hilbert space $\mathscr{H}$.

Using the fact that the identity operator $\mathbb{1}$ satisfies $\psi = \mathbb{1}\,\psi$ and $|a_n\rangle = \mathbb{1}\,|a_n\rangle$, it is possible to omit the vector ψ from both sides of (A.4.27) because the equation is true for any $\psi \in \Phi$ and write it as an equation for operators,

$$\mathbb{1} = \sum_{n=1}^{\infty} |a_n\rangle\langle a_n|\,. \tag{A.4.30}$$

Equation (A.4.30) is called the completeness relation for the basis system $\{|a_n\rangle\}$ or the spectral resolution of the identity operator. Using (A.4.30) the scalar product of two vectors $\phi, \psi \in \Phi$ can be expressed as an infinite sum,

$$(\phi, \psi) = (\phi, \mathbb{1}\,\psi) = \sum_{n=1}^{\infty} \langle \phi, |a_n\rangle\langle a_n|\psi\rangle, = \sum_{n=1}^{\infty} \langle\phi|a_n\rangle\langle a_n|\psi\rangle = \sum_{n=1}^{\infty} \langle a_n|\phi\rangle^*\langle a_n|\psi\rangle. \tag{A.4.31}$$

Equation (A.4.31) is the analogue of (A.4.9) in $\Re_3$. Here, since the space is complex, the scalar product is the sum of the products of the components of one vector with complex conjugate of the components of the other.

Equation (A.4.31) makes sense only if the sum converges. It is possible to show that if (A.4.29) is fulfilled for all vectors, in particular for the two vectors φ and ψ in (A.4.31) then

$$|(\varphi, \psi)| = |\sum_{n=1}^{\infty} (a_n, \varphi)^*\langle a_n|\psi\rangle| < \infty\,. \tag{A.4.32}$$

All vectors ψ, φ for which (A.4.32) is fulfilled have finite scalar products with each other and form the space $\mathscr{H}$.

The linear operators $A, B, C, \ldots$, of (A.3.1b) and (A.3.2b) act in the space $\mathscr{H}$ and can be added and multiplied according to (A.3.3b)–(A.3.5b), forming an associative algebra. As is justified in the various chapters, the vectors $\varphi, \psi, \ldots, \in \mathscr{H}$ and the operators $A, B, \ldots, |\varphi\rangle\langle\varphi|, |\psi\rangle\langle\psi| \ldots$ represent quantum physical states and observables, respectively. Quantities such as $|(\varphi, \psi)|^2$, $|(\varphi, A\varphi)|$, $|(\varphi, A\psi)|$, and $|(\varphi, AB\psi)|$ are Born probabilities that describe the quantum physical quantities that are extracted from experiments. Since such quantities must be finite, it is necessary to require not only that (A.4.29) be finite, but also that $(\varphi, A^r\varphi)$, $(\varphi, B^s\varphi)$, $(\varphi, AB^r\varphi) \ldots, r, s = 1, 2, 3, \ldots$, have finite absolute values.

A space Φ that is "better" than a Hilbert space $\mathscr{H}$ is required because all operators $A, B, \ldots$ that represent observables for the quantum physical system under consideration and any arbitrary power r of the operators $A, B, \ldots$ must be well-defined in the space Φ. Thus the vector $A^r\psi$ must also have a finite norm. To determine the restriction this imposes, the square of the norm of $A^r\psi$, $B^s\psi$ is calculated.

Expressing the vector ψ in terms of the eigenvectors $|a_n\rangle$ of the operator A as given in (A.4.27) and then applying the operator A,

$$A\psi = A\sum_{n=1}^{\infty}|a_n\rangle\langle a_n|\psi\rangle = \sum_{n=1}^{\infty}a_n|a_n\rangle\langle a_n|\psi\rangle\,. \tag{A.4.33}$$

Since (A.4.33) is true for any $\psi \in \Phi$, ψ can be omitted in (A.4.33) just as was done in arriving at (A.4.30). Then (A.4.33) becomes the operator relation

$$A = \sum_{n=1}^{\infty}a_n|a_n\rangle\langle a_n| = \sum_{n=1}^{\infty}a_n\Lambda_n\,. \tag{A.4.34}$$

Thus a linear operator is the sum of projection operators $\Lambda_n = |a_n\rangle\langle a_n|$ multiplied by the respective eigenvalues a_n that are real if $A = A^\dagger$. Equation (A.4.34) is called the spectral resolution of the operator A.

An operator B that does not commute with A (i.e. for which $BA - AB \neq 0$) cannot be written in terms of the eigenvectors $|a_n\rangle$ of the operator A in the form (A.4.34) because $B|a_n\rangle \neq b_n|a_n\rangle$. However, if B is self-adjoint and has a discrete spectrum, then it can be expressed in terms of its eigenvectors $|b_n\rangle$ that satisfy $B|b_n\rangle = b_n|b_n\rangle$. Results analogous to (A.4.30) and (A.4.34) are then immediately obtained:

$$\mathbb{1} = \sum_{n=1}^{\infty}|b_n\rangle\langle b_n|, \qquad B = \sum_{n=1}^{\infty}b_n|b_n\rangle\langle b_n| \tag{A.4.35}$$

Using the eigenvectors of B as a basis system, every $\psi \in \Phi$ can as well be written as

$$\psi = \sum_{n=1}^{\infty}|b_n\rangle\langle b_n|\psi\rangle \tag{A.4.36}$$

which, of course, is just (A.4.27) in a different basis system $\{|b_n\rangle, n = 1, 2, \ldots\}$. In general the $|b_i\rangle$ and $|a_i\rangle$ are completely different vectors. Replacing ψ by $|a_i\rangle$ in (A.4.36), each basis vector $|a_i\rangle$ can be expressed as an infinite sum of basis vectors $|b_n\rangle$,

$$|a_i\rangle = \sum_{n=1}^{\infty}|b_n\rangle\langle b_n|a_i\rangle. \tag{A.4.37}$$

Using (A.4.33) it is possible to calculates $A^r\psi$ and $B^s\psi$ for any ψ and for $r, s = 1, 2, 3, \ldots$. Using the fact that A and, as a consequence A^r, is self-adjoint,

$$\|A^r\psi\|^2 = (A^r\psi, A^r\psi) = (\psi, A^{2r}\psi)\,. \tag{A.4.38}$$

Expressing ψ as an infinite sum of eigenstates of the operator A as given in (A.4.27),

$$\|A^r\psi\|^2 = \sum_{n=1}^{\infty}(\psi, A^{2r}|a_n\rangle\langle a_n|\psi\rangle, = \sum_{n=1}^{\infty} a_n^{2r}\langle\psi|a_n\rangle\langle a_n|\psi\rangle, \tag{A.4.39}$$

Thus the vector $A^r\psi$ is defined if the sum

$$\sum_{n=1}^{\infty} a_n^{2r}|\langle\psi|a_n\rangle|^2 < \infty \quad \text{for every } r = 1, 2, \ldots\,. \tag{A.4.40}$$

The norm of the vector $B^s\psi$ is calculated similarly.

From the preceding discussion it follows that the space of vectors on which all powers of operators A^r, $B^s, \ldots$ are defined is the space of vectors with components $|\langle\psi|a_n\rangle|$, $|\langle\varphi|b_n\rangle|$ that are rapidly decreasing. These are the vectors of the space $\mathscr{H}$ for which not only (A.4.29) holds, but also for which the more stringent condition (A.4.40) is fulfilled for all operators $A, B, \ldots$, thereby ensuring that matrix elements of the form $(\varphi, A^r B^s\psi)$ are also defined.

This smaller space

$$\Phi \subset \mathscr{H} \tag{A.4.41}$$

is by hypothesis the space of states and of observables of quantum physical systems. These spaces can be defined mathematically such that it is possible to prove Dirac's continuous basis vector expansion (A.4.22a) as a mathematical theorem, the "Nuclear Spectral Theorem." The kets $|a\rangle, |x\rangle, |E\rangle, \ldots$ are not vectors in Φ or in $\mathscr{H}$, they are instead continuous, anti-linear functionals on the space Φ. The space of continuous, anti-linear functionals, which is the space containing these kets, is denoted by $\Phi^\times$. That is, the space of all anti-linear, continuous functionals on the space Φ (with respect to the convergence in Φ) are denoted by $\Phi^\times$. Since the space of continuous, anti-linear functionals $\mathscr{H}^\times$ on the Hilbert space $\mathscr{H}$ is again a Hilbert space, $\mathscr{H}^\times = \mathscr{H}$. From (A.4.41) the following triplet of spaces is obtained:

$$\Phi \subset \mathscr{H} \subset \Phi^\times\,. \tag{A.4.42}$$

This is called the Gelfand triplet or Rigged Hilbert Space. The vectors $\psi, \phi \in \Phi$ are called "well-behaved," and the Dirac kets $|x\rangle, |p\rangle, |E\rangle, \ldots$ are elements of $\Phi^\times$.

For practical calculations in physics, the underlying mathematics is not so important. But it is important to know that these mathematical objects are rigorously defined and to know their limitations and properties. The most important property

of the Rigged Hilbert Space is the Nuclear Spectral Theorem that justifies the basis vector expansion (A.4.22) as Dirac foresaw.

The continuous analogue of (A.4.34), the spectral resolution of the operator Q, can be obtained by first operating on both sides of (A.4.22) with Q,

$$Q\psi = \int \mathrm{d}x\, Q|x\rangle\langle x|\psi\rangle \int \mathrm{d}x\, x|x\rangle\langle x|\psi\rangle\,,$$

and then omitting the arbitrary vector $\psi \in \Phi$:

$$Q = \int \mathrm{d}x\, x|x\rangle\langle x|\,. \tag{A.4.43}$$

Because (A.4.22) is true for any $\psi \in \Phi$, it is possible to omit ψ from the equation,

$$\mathbb{1} = \int \mathrm{d}x|x\rangle\langle x|\,. \tag{A.4.44}$$

Equation (A.4.44) is the continuous analogue of the discrete relation (A.4.30) and is called the completeness relation of the generalized basis system $\{|x\rangle\}$.

The scalar product of two elements $\varphi, \psi \in \Phi$ is then obtained from (A.4.44),

$$(\varphi, \psi) \equiv \langle\varphi|\psi\rangle = \langle\varphi|\mathbb{1}\,\psi\rangle = \int \mathrm{d}x\langle\varphi|x\rangle\langle x|\psi\rangle. \tag{A.4.45}$$

In (A.4.45)

$$\langle\varphi|x\rangle \equiv \langle\varphi, |x\rangle) = (|x\rangle, \varphi)^* \equiv \langle x|\varphi\rangle^* \tag{A.4.46}$$

is the (generalized) scalar product of $\varphi \in \Phi$ with the generalized basis vector $|x\rangle$. Using the standard notation $\psi(x) = \langle x|\psi\rangle$ and $\varphi^*(x) = \langle\varphi|x\rangle$, (A.4.45) can be rewritten in the form

$$(\varphi, \psi) = \int \mathrm{d}x\, \varphi^*(x)\psi(x), \tag{A.4.47}$$

the familiar form of the scalar product in function spaces (A.2.12).

Just as there are conditions on the components $c_n = \langle a_n|\psi\rangle$ for the discrete case, there are also corresponding conditions on the components $\psi(x) = \langle x|\psi\rangle$ for the continuous case. From (A.4.45), it immediately follows that the square of the norm of ψ is given by

$$\|\psi\|^2 = (\psi, \psi\rangle = \int \mathrm{d}x\langle\psi|x\rangle\langle x|\psi\rangle = \int \mathrm{d}x|\psi(x)|^2. \tag{A.4.48}$$

The components $\psi(x)$ must therefore be square integrable functions for the norm to be finite. Furthermore, if the operator Q and an arbitrary power r of the operator Q are to be well-defined in the space Φ, the vector $Q^r\psi$ must also have a finite norm. Performing a calculation analogous to (A.4.39),

$$\|Q^r\psi\|^2 = (Q^r\psi, Q^r\psi\rangle = \int \mathrm{d}x\, x^{2r}|\psi(x)|^2. \tag{A.4.49}$$

If the norm $\|Q^r\psi\|$ is to be finite, from (A.4.39) it follows that $|\psi(x)|^2$ must decrease faster than any power of x.

Using (A.4.21c) the matrix elements of the self-adjoint operator Q with eigenkets $|x\rangle$ are

$$\langle x|Q|\psi\rangle = (Q|x\rangle, |\psi\rangle) = (x|x\rangle, |\psi\rangle) = x\langle x|\psi\rangle \quad \text{for all } \psi \in \Phi. \tag{A.4.50}$$

An operator P is now sought with matrix elements $\langle x|P|\psi\rangle$ between the continuous basis vector $|x\rangle$ and any $\psi \in \Phi$ that are given by

$$\langle x|P|\psi\rangle = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}\langle x|\psi\rangle = \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}\psi(x). \tag{A.4.51}$$

Since an arbitrary power Q^rP^s (or P^sQ^r) is to be a well-defined operator, their matrix elements must be finite. Thus the components $\langle x|\varphi\rangle$ and $\langle x|\psi\rangle$ must fulfill the condition that

$$\langle\varphi|Q^rP^s|\psi\rangle = \int \mathrm{d}x\langle\varphi|Q^r|x\rangle\langle x|P^s|\psi\rangle \tag{A.4.52}$$

exists. Using (A.4.50) and (A.4.51)

$$|\langle\varphi|Q^rP^s|\psi\rangle| = |\int \mathrm{d}x\varphi^*(x)\, x^r\frac{1}{i^s}\frac{\mathrm{d}^s}{\mathrm{d}x^s}\psi(x)| < \infty \tag{A.4.53}$$

for all $r = 1, 2, \ldots$ $s = 1, 2, \ldots$ and all φ, ψ.

Equation (A.4.53) reveals that the components in the $|x\rangle$-basis, called the position wave functions $\varphi(x)$ and $\psi(x)$, must fulfill the following condition: The products of the position wave functions and all their s derivatives must decrease faster than any power r of x. The infinitely differentiable, rapidly decreasing, smooth functions that fulfill these conditions are call Schwartz-space functions, and the space of these functions is called the Schwartz space.

It is possible to calculate the commutator of the operators Q and P defined by (A.4.50), (A.4.51) in the Schwartz space:

$$\begin{aligned}\langle x|[Q,\,P]|\psi\rangle &= \langle x|QP - PQ|\psi\rangle \\ &= x\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}\langle x|\psi\rangle - \frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}\langle x|Q|\psi\rangle = -\frac{1}{i}\langle x|\psi\rangle = i\langle x|\mathbb{1}|\psi\rangle. \end{aligned} \tag{A.4.54}$$

The above formula is valid for every function $\langle x|\psi\rangle$ in Schwartz space, which means it is valid for every $|x\rangle$ and for every vector $\psi \in \Phi$. Thus it is true as an operator equation in Φ,

$$[Q,\,P] = i\mathbb{1}. \tag{A.4.55}$$

The correspondence in the following table,

Space Φ		Schwartz Function Space of x
ψ	corresponds to	$\langle x\|\psi\rangle$
Q	corresponds to	operator that multiplies by x
P	corresponds to	differentiation operator $\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x}$

is called a realization of the space Φ.

It is important to emphasize that no proofs have been given in the above discussion . Formalism has been presented based on (A.4.27) and (A.4.43), which have been written in analogy to the basis vector expansion in $\Re_3$. But the statements (A.4.27) and (A.4.43), which are special cases of the Nuclear Spectral Theorem, are far from trivial and require proofs. In fact the Nuclear Spectral Theorem is one of the more important mathematical theorems, with much of this section being a consequence of it. But long before (A.4.43) was proved or even precisely formulated in terms of well-defined mathematical quantities, it was used successfully by Dirac in his formulation of quantum mechanics.

A.5 Realizations by Matrices and Functions

"Realizations" of linear, scalar-product spaces and linear operators are now briefly discussed. To illustrate what is meant by a "realization" it is convenient to return to the three-dimensional space $\Re_3$. There a vector $\mathbf{x}$ can be described by giving its magnitude and direction. Alternatively, it can be specified by its components

$x_i = \mathbf{e}_i \cdot \mathbf{V}$. Thus there are two alternate but equivalent descriptions which are written symbolically as

$$\mathbf{x} \leftrightarrow x_i = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix}. \tag{A.5.1}$$

The coordinates or components, of course, depend on the chosen basis system.

In the same way, instead of using the vector $\psi \in \Phi$, it is possible to use the components $\langle n|\psi\rangle$ with respect to a discrete basis, which can be written as a column matrix.

$$\psi \leftrightarrow \langle n|\psi\rangle = \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \\ \vdots \end{pmatrix} \tag{A.5.2}$$

Just as a vector in $\Re_3$ can be expressed in terms of coordinates or components with respect to different basis systems, it is possible to express ψ in terms of components with respect to a different basis. Instead of the basis $|n\rangle$, which are, say, eigenstates of the energy operator H, it is possible to use as a basis eigenvectors $|a_n\rangle$ of the operator A satisfying $A|a_n\rangle = a_n|a_n\rangle$. In terms of $|a_n\rangle$, the same vector is given by an entirely different column matrix.

$$\psi \leftrightarrow \langle a_n|\psi\rangle = \begin{pmatrix} \langle a_1|\psi\rangle \\ \langle a_2|\psi\rangle \\ \langle a_3|\psi\rangle \\ \vdots \end{pmatrix}. \tag{A.5.3}$$

The column matrices $\langle n|\psi\rangle$ and $\langle a_n|\psi\rangle$ are related by an infinite-dimensional transformation matrix, which is usually so complicated that it is of no practical value. (See Problem A.14.) If the infinite column matrix appears more real to someone than the abstract vector ψ, then that person will speak of a realization of ψ by a column matrix and a realization of the space Φ by the space of column matrices.

When vectors are realized by column matrices, operators are realized by quadratic matrices. To illustrate this concept, the action of an arbitrary operator B on the vector ψ is calculated using the expansion (A.4.13),

$$B\psi = \sum_{n=1}^{\infty} B|n\rangle\langle n|\psi\rangle. \tag{A.5.4}$$

Taking the scalar product of the above equation with the basis vector $|m\rangle$ yields

$$\langle m|B\psi\rangle = \sum_{n=1}^{\infty} \langle m\ |B|n\rangle\langle n|\psi\rangle. \tag{A.5.5}$$

The above relation can be written in matrix notation as follows:

$$\begin{pmatrix} \langle 1|B\psi\rangle \\ \langle 2|B\psi\rangle \\ \langle 3|B\psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 1|B|1\rangle & \langle 1|B|2\rangle & \langle 1|B|3\rangle & \dots \\ \langle 2|B|1\rangle & \langle 2|B|2\rangle & \langle 2|B|3\rangle & \dots \\ \langle 3|B|1\rangle & \langle 3|B|2\rangle & \langle 3|B|3\rangle & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \\ \vdots \end{pmatrix} \tag{A.5.6}$$

The numbers $\langle m|B|n\rangle$ form an infinite-dimensional quadratic matrix which is called the matrix of the operator B with respect to the basis $|n\rangle$. An orthonormal basis is almost always used in calculating the matrix of an operator.

For any two vectors $\psi, \varphi \in \Phi$ and an operator B, the scalar product of $B\psi$ with φ, namely $\langle\varphi|B\psi\rangle$, plays an important role in physics and is called the matrix element of the operator B between the vectors φ and ψ.

The vector $\psi \in \Phi$ can be expanded in terms of a continuous basis instead of a discrete basis. Then instead of the correspondence (A.5.2),

$$\psi \leftrightarrow \langle x|\psi\rangle. \tag{A.5.7}$$

The column matrix $\langle x|\psi\rangle$ has continuously infinite rows with one row for each value of x. With the association (A.5.7), the space Φ is realized by the space of "well-behaved" functions.

A.6 Summary

Quantum mechanics can be expressed in terms of differential operators using the Schrödinger equation. Equivalently, it can be expressed in terms of matrices using matrix mechanics. These two formulations of quantum mechanics are not distinct theories but are merely two different representations of quantum mechanics obtained from the general formulation by taking matrix elements with respect to different basis systems. In its most general form, quantum mechanics is formulated in terms of linear operators on a linear, scalar-product space.

A linear space Φ possesses the following ten properties where φ, ψ, and χ are elements or vectors in Φ; $0 \in \Phi$ is the null element; and a, b are complex numbers:

1. $\varphi + \psi = \psi + \varphi$
2. Addition is associative: $(\varphi + \psi) + \chi = \varphi + (\psi + \chi)$

3. The null element satisfies $0 + \psi = \psi$
4. $b(\psi) = b\psi \in \Phi$
5. $a(b\psi) = (ab)\psi$
6. $\mathbb{1}\psi = \psi$
7. $0\psi = 0$
8. $b(\varphi + \psi) = b\varphi + b\psi$
9. $(a + b)\psi = a\psi + b\psi$
10. $-\mathbb{1}\psi = -\psi$

A linear, scalar-product space Φ possesses the ten properties that characterize a linear space plus the following four properties that define a scalar-product (ψ, φ) on a linear space:

1. $(\psi, \psi) \geq 0$, $(\psi, \psi) = 0$ if $\psi = 0$
2. $(\psi, \varphi) = (\varphi, \psi)^*$
3. $a(\psi, \varphi) = (\psi, a\varphi)$
4. $(\psi + \varphi, \chi) = (\psi, \chi) + (\varphi, \chi)$

Linear operators A and B on a linear, scalar-product space Φ possess the following nine properties:

1. $A(\psi) \equiv A\psi \in \Phi$
2. $A(\psi + \varphi) = A\psi + A\varphi$
3. $A(a\psi) = a(A\psi)$
4. $(A + B)\psi = A\psi + B\psi$
5. $(aA)\psi = a(A\psi)$
6. $(AB)\psi = A(B\psi)$
7. The zero operator 0 satisfies $0\psi = 0 \in \Phi$.
8. The identity operator $\mathbb{1}$ satisfies $\mathbb{1}\psi = \psi$.
9. The adjoint of the operator A, denoted $A^\dagger$, is defined by $(\psi, A\varphi) = (A^\dagger\psi, \varphi)$.

The basis vector expansion for quantum theory has been motivated by starting with the simplest case and then generalizing. First a vector in three-dimensional space is expanded in terms of its components,

$$\mathbf{x} = \sum_{i=1}^{3} \mathbf{e}_i x^i = \sum_{i=1}^{3} \mathbf{e}_i (\mathbf{e}_i | \mathbf{x}\rangle,$$

where x^i is real. Just as vectors in three-dimensional space can be expressed as components along various sets of three linearly independent axes, vectors in a linear, scalar-product space can also be expressed as components along various sets of linearly independent axes or vectors. In a complex, N-dimensional, linear, scalar-product space the above equation is generalized to

$$\psi = \sum_{i=1}^{N} |e_i\rangle c_i = \sum_{i=1}^{N} |e_i\rangle\langle e_i|\psi\rangle\,,$$

where c_i is complex. Finally, the above equation is generalized to infinite dimensions, $N \to \infty$,

$$\psi = \sum_{n=1}^{\infty} |e_n\rangle c_n = \sum_{n=1}^{\infty} |e_n\rangle\langle e_n|\psi\rangle\,, \tag{A.6.1}$$

where the c_n are complex. The set of all vectors with components c_n that are square summable,

$$\sum_{n=1}^{\infty} |c_n|^2 < \infty\,,$$

is called the Hilbert space $\mathscr{H}$.

For finite-dimensional spaces, a set of basis functions $\{|e_i\rangle\}$ can be formed from the eigenvectors of any self-adjacent operator A:

$$|e_i\rangle = |a_i\rangle \qquad \text{where} \qquad A|a_i\rangle = a_i|a_i\rangle.$$

For the infinite-dimensional spaces there are some operators that do not have a discrete set of eigenvectors (called discrete spectrum). Then there exists a continuous set of eigenvectors satisfying

$$A|a\rangle, = a|a\rangle, \qquad M \le a \le N.$$

The vector ψ can be expanded in terms of $|a\rangle$,

$$\psi = \int \mathrm{d}a|a\rangle\langle a|\psi\rangle,$$

which is justified mathematically by the Nuclear Spectral Theorem and is the continuous generalization of (A.6.1).

Problems

For Sect. A.2

A.1 Consider the two functions $g_1(x)$ and $g_2(x)$ on the interval $-\infty \le x < \infty$,

$$g_1(x) = A_1 e^{-|x|}, \qquad g_2(x) = A_2(a + x^2)e^{-|x|},$$

where the constants A_1 and A_2 are real.

(a) Determine the constant a such that $g_1(x)$ and $g_2(x)$ are orthogonal.
(b) Determine the constants A_1 and A_2 such that $g_1(x)$ and $g_2(x)$ are normalized.

A.2 Show that if the vectors $\psi, \varphi \in \Phi$ are represented by the respective column matrices

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_N \end{pmatrix}, \quad \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \vdots \\ \varphi_N \end{pmatrix},$$

where the ψ_i and ϕ_i are complex numbers, then the scalar product defined by

$$(\psi, \varphi) = \sum_{i=1}^{N} \psi_i^* \varphi_i$$

satisfies the rules (A.2.13c)–(A.2.16c).

For Sect. A.3

A.3 Show that rules (A.3.1b)–(A.3.5b) are satisfied if the vectors $\psi, \varphi \in \Phi$ are represented by column matrices as given in Problem A.2, and that an arbitrary linear operator A is represented by an $N \times N$ matrix A_{ij} such that the action of A on ψ is represented by

$$A\psi = \sum_{j=1}^{\infty} A_{ij} \psi_j \ .$$

The operator B is defined analogously.

A.4 If the vectors in a scalar-product space are represented by column matrices, and the operator A is represented by the matrix A_{ij} as given in Problems A.2 and A.3, by what is the operator $A^\dagger$ represented? Hint: Use a procedure similar to that employed in obtaining (A.3.6a).

A.5 Using (A.3.5b) and the definition (A.3.6b) of the adjoint of an operator, show that $(AB)^\dagger = B^\dagger A^\dagger$.

A.6 Let A and B be hermitian operators and c be an arbitrary, complex number. Under what conditions is each of the following operators hermitian?

(a) cA
(b) $cA + cB$
(c) cAB
(d) $c\{A, B\} = c(AB + BA)$
(e) $c[A, B] = c(AB - BA)$

A.7 Calculate the four possible matrix elements of the operator $-i\dfrac{\mathrm{d}}{\mathrm{d}x}$ between the functions

$$f_1(x) = \pi^{-1/4} e^{-x^2/2} \quad \text{and} \quad f_2(x) = \sqrt{2}\,\pi^{-1/4}\, x e^{-x^2/2},$$

where $-\infty < x < \infty$.

A.8 On the interval $-\infty < x < \infty$, consider the operator A, where

$$A = \frac{\mathrm{d}^2}{\mathrm{d}x^2} - x^2,$$

and the two functions

$$\psi_1(x) = e^{-x^2/2}, \qquad \psi_2(x) = x e^{\frac{2}{x}/2}.$$

(a) Show that $A = A^\dagger$.
(b) Show that

$$A\psi_i(x) = a_i \psi_i(x), \quad i = 1, 2\ .$$

The constant a_i is called the eigenvalue of the operator A when it acts on $\psi_i(x)$, and $\psi_i(x)$ is called an eigenfunction of the operator A. What are the values a_1 and a_2?

(c) Using only the facts that $A^\dagger = A$ and $a_1 \neq a_2$, explain why the scalar product of $\psi_1(x)$ and $\psi_2(x)$ must be zero. Explicitly calculate the scalar product and verify that it is indeed zero.

For Sect. A.4

A.9 Let $\psi \in \Phi$ be normalized to unity. If $|n\rangle$ is a basis system of eigenvectors of an observable with a discrete spectrum, show that the components of ψ with respect to this basis fulfill the condition

$$\sum_n |\langle n|\psi\rangle|^2 = 1 \,.$$

A.10 If $|e_i\rangle$ is a normalized eigenvector with eigenvalue a_i, show that

$$|e'_n\rangle = e^{i\omega}|e_n\rangle, \qquad \omega \in \Re \,,$$

is also a normalized eigenvector with the same eigenvalue a_i.

For Sect. A.5

A.11 Let A be a hermitian operator and $|n\rangle$ be a discrete basis system. Show that the matrix of A with respect to this basis system,

$$\begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \dots \\ \langle 2|A|1\rangle & \langle 2|A|2\rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix},$$

is a hermitian matrix. That is, show that $\langle m|A|n\rangle = \langle n|A|m\rangle^*$.

A.12 A matrix T is said to be orthogonal if $T^{\mathrm{t}} = T^{-1}$. Here T^{t} is the transposed matrix, $T^{\mathrm{t}}_{mn} = T_{nm}$, and T^{-1} is the inverse matrix defined by

$$\sum_r T_{nr}(T^{-1})_{rm} = \delta_{nm} \,.$$

(a) Show that the matrix

$$T = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

is orthogonal.

(b) Calculate the determinant of T.
(c) Apply the matrix T to the vector

$$\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

using the rules of matrix multiplication. Using a sketch, show that $T\mathbf{r}$ is the vector obtained by rotating the vector $\mathbf{r}$ around the z axis by an angle θ.

A.13 A matrix $\mathscr{P}$ is called a projection matrix if

$$\mathscr{P}^2 = \mathscr{P} \, .$$

(a) Show that the matrix

$$\mathscr{P}' = \begin{pmatrix} \sin^2\theta & -\sin\theta\cos\theta & 0 \\ -\sin\theta\cos\theta & \cos^2\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

is a projection matrix.
(b) Apply the projection matrix $\mathscr{P}'$ to the vector $\mathbf{r}' = T\mathbf{r}$ obtained in Problem A.11, and discuss the result.
(c) If the rotation T is applied to the vector $\mathbf{r}' = T\mathbf{r}$ calculated in Problem A.11, a simple result is found that suggests defining a new matrix

$$\mathscr{P} = T^{-1}\mathscr{P}'T \, .$$

Calculate $\mathscr{P}$ and verify that it is a projection matrix.
(d) Describe the geometrical meaning of the matrix $\mathscr{P}$. In particular, determine the subspace of the three-dimensional space on which $\mathscr{P}$ projects.
(e) Describe the geometrical meaning of the matrix $\mathscr{P}'$ and determine the subspace upon which it projects.

A.14 Let two basis systems of the linear, scalar-product space Φ be denoted by $|a_n\rangle$ and by $|b_\nu\rangle$. Show that the components of a vector $\varphi \in \Phi$ with respect to the basis system $|b_\nu\rangle$, the $(b_\nu|\phi\rangle$, can be obtained from the components $\langle a_n|\varphi\rangle$ with respect to the other basis system $|a_n\rangle$ by the matrix transformation

$$\langle b_\nu|\varphi\rangle = \sum_n \langle b_\nu|a_n\rangle\langle a_n|\varphi\rangle \, ,$$

where $\langle b_\nu|a_n\rangle$ is the scalar product of the basis vector $|b_\nu\rangle$ with the basis vector $|a_n\rangle$. To show this, use the fact that every vector $|a_n\rangle$ can be expanded with respect to the basis system $|b_\nu\rangle$.

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