Chapter 2

Mathematical Tools of Quantum Mechanics

2.1 Introduction

We deal here with the mathematical machinery needed to study quantum mechanics. Although this chapter is mathematical in scope, no attempt is made to be mathematically complete or rigorous. We limit ourselves to those practical issues that are relevant to the formalism of quantum mechanics.

The Schrödinger equation is one of the cornerstones of the theory of quantum mechanics; it has the structure of a *linear* equation. The formalism of quantum mechanics deals with operators that are linear and wave functions that belong to an abstract Hilbert space. The mathematical properties and structure of Hilbert spaces are essential for a proper understanding of the formalism of quantum mechanics. For this, we are going to review briefly the properties of Hilbert spaces and those of linear operators. We will then consider Dirac's *bra-ket* notation.

Quantum mechanics was formulated in two different ways by Schrödinger and Heisenberg. Schrödinger's wave mechanics and Heisenberg's matrix mechanics are the representations of the general formalism of quantum mechanics in *continuous* and *discrete* basis systems, respectively. For this, we will also examine the mathematics involved in representing kets, bras, bra-kets, and operators in discrete and continuous bases.

2.2 The Hilbert Space and Wave Functions

2.2.1 The Linear Vector Space

A linear vector space consists of two sets of elements and two algebraic rules:

- a set of *vectors* ψ, ϕ, χ, ... and a set of *scalars* $a, b, c, \ldots$;
- a rule for vector *addition* and a rule for scalar *multiplication*.

(a) Addition rule
The addition rule has the properties and structure of an *abelian* group:

- If ψ and ϕ are vectors (elements) of a space, their sum, $\psi + \phi$, is also a vector of the same space.
- Commutativity: $\psi + \phi = \phi + \psi$.
- Associativity: $(\psi + \phi) + \chi = \psi + (\phi + \chi)$.
- Existence of a zero or neutral vector: for each vector ψ, there must exist a zero vector O such that: $O + \psi = \psi + O = \psi$.
- Existence of a symmetric or inverse vector: each vector ψ must have a symmetric vector $(-\psi)$ such that $\psi + (-\psi) = (-\psi) + \psi = O$.

(b) Multiplication rule
The multiplication of vectors by scalars (scalars can be real or complex numbers) has these properties:

- The product of a scalar with a vector gives another vector. In general, if ψ and ϕ are two vectors of the space, any linear combination $a\psi + b\phi$ is also a vector of the space, a and b being scalars.
- Distributivity with respect to addition:

$$a(\psi + \phi) = a\psi + a\phi, \qquad (a + b)\psi = a\psi + b\psi, \tag{2.1}$$

- Associativity with respect to multiplication of scalars:

$$a(b\psi) = (ab)\psi \tag{2.2}$$

- For each element ψ there must exist a unitary scalar I and a zero scalar "o" such that

$$I\psi = \psi I = \psi \quad \text{and} \quad o\psi = \psi o = o. \tag{2.3}$$

2.2.2 The Hilbert Space

A Hilbert space $\mathcal{H}$ consists of a set of vectors $\psi, \phi, \chi, \ldots$ and a set of *scalars* $a, b, c, \ldots$ which satisfy the following *four* properties:

(a) $\mathcal{H}$ is a linear space

The properties of a linear space were considered in the previous section.

(b) $\mathcal{H}$ has a defined scalar product that is strictly positive

The scalar product of an element ψ with another element ϕ is in general a complex number, denoted by (ψ, ϕ), where (ψ, ϕ) = complex number. **Note:** Watch out for the order! Since the scalar product is a complex number, the quantity (ψ, ϕ) is generally not equal to (ϕ, ψ): $(\psi, \phi) = \psi^*\phi$ while $(\phi, \psi) = \phi^*\psi$. The scalar product satisfies the following properties:

- The scalar product of ψ with ϕ is equal to the complex conjugate of the scalar product of ϕ with ψ:

$$(\psi, \phi) = (\phi, \psi)^*. \tag{2.4}$$

- The scalar product of ϕ with ψ is linear with respect to the second factor if $\psi = a\psi_1 + b\psi_2$:

$$(\phi, a\psi_1 + b\psi_2) = a(\phi, \psi_1) + b(\phi, \psi_2), \tag{2.5}$$

and antilinear with respect to the first factor if $\phi = a\phi_1 + b\phi_2$:

$$(a\phi_1 + b\phi_2, \psi) = a^*(\phi_1, \psi) + b^*(\phi_2, \psi). \tag{2.6}$$

- The scalar product of a vector ψ with itself is a positive real number:

$$(\psi, \psi) = \| \psi \|^2 \geq 0, \tag{2.7}$$

where the equality holds only for $\psi = O$.

(c) $\mathcal{H}$ is separable

There exists a Cauchy sequence $\psi_n \in \mathcal{H}$ $(n = 1, 2, \ldots)$ such that for every ψ of $\mathcal{H}$ and $\varepsilon > 0$, there exists at least one ψ_n of the sequence for which

$$\| \psi - \psi_n \| < \varepsilon. \tag{2.8}$$

(d) $\mathcal{H}$ is complete

Every Cauchy sequence $\psi_n \in \mathcal{H}$ converges to an element of $\mathcal{H}$. That is, for any ψ_n, the relation

$$\lim_{n,m\to\infty} \| \psi_n - \psi_m \| = 0, \tag{2.9}$$

defines a unique limit ψ of $\mathcal{H}$ such that

$$\lim_{n\to\infty} \| \psi - \psi_n \| = 0. \tag{2.10}$$

Remark

We should note that in a scalar product (ϕ, ψ), the second factor, ψ, belongs to the Hilbert space $\mathcal{H}$, while the first factor, ϕ, belongs to its dual Hilbert space $\mathcal{H}_d$. The distinction between $\mathcal{H}$ and $\mathcal{H}_d$ is due to the fact that, as mentioned above, the scalar product is not commutative: $(\phi, \psi) \neq (\psi, \phi)$; the order matters! From linear algebra, we know that every vector space can be associated with a dual vector space.

2.2.3 Dimension and Basis of a Vector Space

A set of N nonzero vectors $\phi_1, \phi_2, \ldots, \phi_N$ is said to be *linearly independent* if and only if the solution of the equation

$$\sum_{i=1}^{N} a_i \phi_i = 0 \tag{2.11}$$

is $a_1 = a_2 = \cdots = a_N = 0$. But if there exists a set of scalars, which are not all zero, so that one of the vectors (say ϕ_n) can be expressed as a linear combination of the others,

$$\phi_n = \sum_{i=1}^{n-1} a_i \phi_i + \sum_{i=n+1}^{N} a_i \phi_i, \tag{2.12}$$

the set $\{\phi_i\}$ is said to be *linearly dependent*.

Dimension: The *dimension* of a vector space is given by the *maximum number* of linearly independent vectors the space can have. For instance, if the maximum number of linearly independent vectors a space has is N (i.e., $\phi_1, \phi_2, \ldots, \phi_N$), this space is said to be N-dimensional. In this N-dimensional vector space, any vector ψ can be expanded as a linear combination:

$$\psi = \sum_{i=1}^{N} a_i \phi_i. \tag{2.13}$$

Basis: The *basis* of a vector space consists of a set of the maximum possible number of linearly independent vectors belonging to that space. This set of vectors, $\phi_1, \phi_2, \ldots, \phi_N$, to be denoted in short by $\{\phi_i\}$, is called the basis of the vector space, while the vectors $\phi_1, \phi_2, \ldots, \phi_N$ are called the base vectors. Although the set of these linearly independent vectors is arbitrary, it is convenient to choose them *orthonormal*; that is, their scalar products satisfy the relation $(\phi_i, \phi_j) = \delta_{ij}$ (we may recall that $\delta_{ij} = 1$ whenever $i = j$ and zero otherwise). The basis is said to be *orthonormal* if it consists of a set of orthonormal vectors. Moreover, the basis is said to be *complete* if it spans the entire space; that is, there is no need to introduce any additional base vector. The expansion coefficients a_i in (2.13) are called the *components* of the vector ψ in the basis. Each component is given by the scalar product of ψ with the corresponding base vector, $a_j = (\phi_j, \psi)$.

Examples of linear vector spaces

Let us give two examples of linear spaces that are Hilbert spaces: one having a *finite (discrete)* set of base vectors, the other an *infinite (continuous)* basis.

- The first one is the three-dimensional Euclidean vector space; the basis of this space consists of three linearly independent vectors, usually denoted by $\vec{i}, \vec{j}, \vec{k}$. Any vector of the Euclidean space can be written in terms of the base vectors as $\vec{A} = a_1\vec{i} + a_2\vec{j} + a_3\vec{k}$, where a_1, a_2, and a_3 are the components of $\vec{A}$ in the basis; each component can be determined by taking the scalar product of $\vec{A}$ with the corresponding base vector: $a_1 = \vec{i} \cdot \vec{A}$, $a_2 = \vec{j} \cdot \vec{A}$, and $a_3 = \vec{k} \cdot \vec{A}$. Note that the scalar product in the Euclidean space is real and hence symmetric. The norm in this space is the usual length of vectors $\parallel \vec{A} \parallel = A$. Note also that whenever $a_1\vec{i} + a_2\vec{j} + a_3\vec{k} = 0$ we have $a_1 = a_2 = a_3 = 0$ and that none of the unit vectors $\vec{i}, \vec{j}, \vec{k}$ can be expressed as a linear combination of the other two.

- The second example is the space of the entire complex functions $\psi(x)$; the dimension of this space is infinite for it has an infinite number of linearly independent basis vectors.

Example 2.1

Check whether the following sets of functions are linearly independent or dependent on the real x-axis.

(a) $f(x) = 4$, $g(x) = x^2$, $h(x) = e^{2x}$
(b) $f(x) = x$, $g(x) = x^2$, $h(x) = x^3$
(c) $f(x) = x$, $g(x) = 5x$, $h(x) = x^2$
(d) $f(x) = 2 + x^2$, $g(x) = 3 - x + 4x^3$, $h(x) = 2x + 3x^2 - 8x^3$

Solution

(a) The first set is clearly linearly independent since $a_1 f(x) + a_2 g(x) + a_3 h(x) = 4a_1 + a_2 x^2 + a_3 e^{2x} = 0$ implies that $a_1 = a_2 = a_3 = 0$ for any value of x.

(b) The functions $f(x) = x$, $g(x) = x^2$, $h(x) = x^3$ are also linearly independent since $a_1 x + a_2 x^2 + a_3 x^3 = 0$ implies that $a_1 = a_2 = a_3 = 0$ no matter what the value of x. For instance, taking $x = -1, 1, 3$, the following system of three equations

$$-a_1 + a_2 - a_3 = 0, \qquad a_1 + a_2 + a_3 = 0, \qquad 3a_1 + 9a_2 + 27a_3 = 0 \tag{2.14}$$

yields $a_1 = a_2 = a_3 = 0$.

(c) The functions $f(x) = x$, $g(x) = 5x$, $h(x) = x^2$ are not linearly independent, since $g(x) = 5f(x) + 0 \times h(x)$.

(d) The functions $f(x) = 2 + x^2$, $g(x) = 3 - x + 4x^3$, $h(x) = 2x + 3x^2 - 8x^3$ are not linearly independent since $h(x) = 3f(x) - 2g(x)$.

Example 2.2
Are the following sets of vectors (in the three-dimensional Euclidean space) linearly independent or dependent?

(a) $\vec{A} = (3, 0, 0)$, $\vec{B} = (0, -2, 0)$, $\vec{C} = (0, 0, -1)$
(b) $\vec{A} = (6, -9, 0)$, $\vec{B} = (-2, 3, 0)$
(c) $\vec{A} = (2, 3, -1)$, $\vec{B} = (0, 1, 2)$, $\vec{C} = (0, 0, -5)$
(d) $\vec{A} = (1, -2, 3)$, $\vec{B} = (-4, 1, 7)$, $\vec{C} = (0, 10, 11)$, and $\vec{D} = (14, 3, -4)$

Solution

(a) The three vectors $\vec{A} = (3, 0, 0)$, $\vec{B} = (0, -2, 0)$, $\vec{C} = (0, 0, -1)$ are linearly independent, since

$$a_1\vec{A} + a_2\vec{B} + a_3\vec{C} = 0 \Longrightarrow 3a_1\vec{i} - 2a_2\vec{j} - a_3\vec{k} = 0 \tag{2.15}$$

leads to

$$3a_1 = 0, \qquad -2a_2 = 0, \qquad -a_3 = 0, \tag{2.16}$$

which yields $a_1 = a_2 = a_3 = 0$.

(b) The vectors $\vec{A} = (6, -9, 0)$, $\vec{B} = (-2, 3, 0)$ are linearly dependent, since the solution to

$$a_1\vec{A} + a_2\vec{B} = 0 \quad \Longrightarrow \quad (6a_1 - 2a_2)\vec{i} + (-9a_1 + 3a_2)\vec{j} = 0 \tag{2.17}$$

is $a_1 = a_2/3$. The first vector is equal to -3 times the second one: $\vec{A} = -3\vec{B}$.

(c) The vectors $\vec{A} = (2, 3, -1)$, $\vec{B} = (0, 1, 2)$, $\vec{C} = (0, 0, -5)$ are linearly independent, since

$$a_1\vec{A} + a_2\vec{B} + a_3\vec{C} = 0 \Longrightarrow 2a_1\vec{i} + (3a_1 + a_2)\vec{j} + (-a_1 + 2a_2 - 5a_3)\vec{k} = 0 \tag{2.18}$$

leads to

$$2a_1 = 0, \qquad 3a_1 + a_2 = 0, \qquad -a_1 + 2a_2 - 5a_3 = 0. \tag{2.19}$$

The only solution of this system is $a_1 = a_2 = a_3 = 0$.

(d) The vectors $\vec{A} = (1, -2, 3)$, $\vec{B} = (-4, 1, 7)$, $\vec{C} = (0, 10, 11)$, and $\vec{D} = (14, 3, -4)$ are not linearly independent, because $\vec{D}$ can be expressed in terms of the other vectors:

$$\vec{D} = 2\vec{A} - 3\vec{B} + \vec{C}. \tag{2.20}$$

2.2.4 Square-Integrable Functions: Wave Functions

In the case of function spaces, a "vector" element is given by a *complex function* and the *scalar product* by *integrals*. That is, the scalar product of two functions $\psi(x)$ and $\phi(x)$ is given by

$$(\psi, \phi) = \int \psi^*(x)\phi(x)\, dx. \tag{2.21}$$

If this integral *diverges*, the scalar product *does not exist*. As a result, if we want the function space to possess a scalar product, we must select only those functions for which (ψ, ϕ) is *finite*. In particular, a function $\psi(x)$ is said to be *square integrable* if the scalar product of ψ with itself,

$$(\psi, \psi) = \int |\psi(x)|^2\, dx, \tag{2.22}$$

is *finite*.

It is easy to verify that the space of square-integrable functions possesses the properties of a Hilbert space. For instance, any linear combination of square-integrable functions is also a square-integrable function and (2.21) satisfies all the properties of the scalar product of a Hilbert space.

Note that the dimension of the Hilbert space of square-integrable functions is infinite, since each wave function can be expanded in terms of an infinite number of linearly independent functions. The dimension of a space is given by the maximum number of linearly independent basis vectors required to span that space.

A good example of square-integrable functions is the *wave function* of quantum mechanics, $\psi(\vec{r}, t)$. We have seen in Chapter 1 that, according to Born's probabilistic interpretation of $\psi(\vec{r}, t)$, the quantity $|\ \psi(\vec{r}, t)\ |^2\, d^3r$ represents the probability of finding, at time t, the particle in a volume d^3r, centered around the point $\vec{r}$. The probability of finding the particle somewhere in space must then be equal to 1:

$$\int |\ \psi(\vec{r}, t)\ |^2\, d^3r = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} |\ \psi(\vec{r}, t)\ |^2\, dz = 1; \tag{2.23}$$

hence the wave functions of quantum mechanics are square-integrable. Wave functions satisfying (2.23) are said to be normalized or square-integrable. As wave mechanics deals with square-integrable functions, any wave function which is not square-integrable has no physical meaning in quantum mechanics.

2.3 Dirac Notation

The physical state of a system is represented in quantum mechanics by elements of a Hilbert space; these elements are called state vectors. We can represent the state vectors in different bases by means of function expansions. This is analogous to specifying an ordinary (Euclidean) vector by its components in various coordinate systems. For instance, we can represent equivalently a vector by its components in a Cartesian coordinate system, in a spherical coordinate system, or in a cylindrical coordinate system. *The meaning of a vector is, of course, independent of the coordinate system chosen to represent its components*. Similarly, the state of a microscopic system has a meaning independent of the basis in which it is expanded.

To free state vectors from coordinate meaning, Dirac introduced what was to become an invaluable notation in quantum mechanics; it allows one to manipulate the formalism of quantum mechanics with ease and clarity. He introduced the concepts of kets, bras, and bra-kets, which will be explained below.

Kets: elements of a vector space
Dirac denoted the state vector ψ by the symbol $\mid \psi\rangle$, which he called a *ket* vector, or simply a ket. Kets belong to the Hilbert (vector) space $\mathcal{H}$, or, in short, to the ket-space.

Bras: elements of a dual space
As mentioned above, we know from linear algebra that a dual space can be associated with every vector space. Dirac denoted the elements of a dual space by the symbol $\langle \mid$, which he called a bra vector, or simply a bra; for instance, the element $\langle\psi \mid$ represents a bra. *Note: For every ket* $\mid \psi\rangle$ *there exists a unique bra* $\langle\psi \mid$ *and vice versa.* Again, while kets belong to the Hilbert space $\mathcal{H}$, the corresponding bras belong to its dual (Hilbert) space $\mathcal{H}_d$.

Bra-ket: Dirac notation for the scalar product
Dirac denoted the scalar (inner) product by the symbol $\langle \mid \rangle$, which he called a a *bra-ket*. For instance, the scalar product (ϕ, ψ) is denoted by the bra-ket $\langle\phi \mid \psi\rangle$:

$$(\phi, \psi) \quad \longrightarrow \quad \langle\phi \mid \psi\rangle. \tag{2.24}$$

Note: When a ket (or bra) is multiplied by a complex number, we also get a ket (or bra).

Remark: In wave mechanics we deal with wave functions $\psi(\vec{r}, t)$, but in the more general formalism of quantum mechanics we deal with abstract kets $\mid \psi\rangle$. Wave functions, like kets, are elements of a Hilbert space. We should note that, like a wave function, a ket represents the system completely, and hence knowing $\mid \psi\rangle$ means knowing all its amplitudes in all possible representations. As mentioned above, kets are independent of any particular representation. There is no reason to single out a particular representation basis such as the representation in the position space. Of course, if we want to know the probability of finding the particle at some position in space, we need to work out the formalism within the coordinate representation. The state vector of this particle at time t will be given by the spatial wave function $\langle\vec{r}, t \mid \psi\rangle = \psi(\vec{r}, t)$. In the coordinate representation, the scalar product $\langle\phi \mid \psi\rangle$ is given by

$$\langle\phi \mid \psi\rangle = \int \phi^*(\vec{r}, t)\psi(\vec{r}, t)\, d^3r. \tag{2.25}$$

Similarly, if we are considering the three-dimensional momentum of a particle, the ket $\mid \psi\rangle$ will have to be expressed in momentum space. In this case the state of the particle will be described by a wave function $\psi(\vec{p}, t)$, where $\vec{p}$ is the momentum of the particle.

Properties of kets, bras, and bra-kets

- **Every ket has a corresponding bra**

  To every *ket* $\mid \psi\rangle$, there corresponds a unique *bra* $\langle\psi \mid$ and vice versa:

$$\mid \psi\rangle \quad \longleftrightarrow \quad \langle\psi \mid . \tag{2.26}$$

  There is a one-to-one correspondence between bras and kets:

$$a \mid \psi\rangle + b \mid \phi\rangle \quad \longleftrightarrow \quad a^*\langle\psi \mid + b^*\langle\phi \mid, \tag{2.27}$$

  where a and b are complex numbers. The following is a common notation:

$$\mid a\psi\rangle = a \mid \psi\rangle, \qquad \langle a\psi \mid = a^*\langle\psi \mid . \tag{2.28}$$

- **Properties of the scalar product**

  In quantum mechanics, since the scalar product is a complex number, the ordering matters a lot. We must be careful to distinguish a scalar product from its complex conjugate; $\langle\psi \mid \phi\rangle$ is not the same thing as $\langle\phi \mid \psi\rangle$:

$$\langle\phi \mid \psi\rangle^* = \langle\psi \mid \phi\rangle. \tag{2.29}$$

  This property becomes clearer if we apply it to (2.21):

$$\langle\phi \mid \psi\rangle^* = \left(\int \phi^*(\vec{r}, t)\psi(\vec{r}, t)\, d^3r\right)^* = \int \psi^*(\vec{r}, t)\phi(\vec{r}, t)\, d^3r = \langle\psi \mid \phi\rangle. \tag{2.30}$$

  When $\mid \psi\rangle$ and $\mid \phi\rangle$ are real, we would have $\langle\psi \mid \phi\rangle = \langle\phi \mid \psi\rangle$. Let us list some additional properties of the scalar product:

$$\langle\psi \mid a_1\psi_1 + a_2\psi_2\rangle = a_1\langle\psi \mid \psi_1\rangle + a_2\langle\psi \mid \psi_2\rangle, \tag{2.31}$$

$$\langle a_1\phi_1 + a_2\phi_2 \mid \psi\rangle = a_1^*\langle\phi_1 \mid \psi\rangle + a_2^*\langle\phi_2 \mid \psi\rangle, \tag{2.32}$$

$$\begin{aligned}\langle a_1\phi_1 + a_2\phi_2 \mid b_1\psi_1 + b_2\psi_2\rangle &= a_1^*b_1\langle\phi_1 \mid \psi_1\rangle + a_1^*b_2\langle\phi_1 \mid \psi_2\rangle \\ &\quad + a_2^*b_1\langle\phi_2 \mid \psi_1\rangle + a_2^*b_2\langle\phi_2 \mid \psi_2\rangle.\end{aligned} \tag{2.33}$$

- **The norm is real and positive**

  For any state vector $\mid \psi\rangle$ of the Hilbert space $\mathcal{H}$, the norm $\langle\psi \mid \psi\rangle$ is real and positive; $\langle\psi \mid \psi\rangle$ is equal to zero only for the case where $\mid \psi\rangle = O$, where O is the zero vector. If the state $\mid \psi\rangle$ is normalized then $\langle\psi \mid \psi\rangle = 1$.

- **Schwarz inequality**

  For any two states $\mid \psi\rangle$ and $\mid \phi\rangle$ of the Hilbert space, we can show that

$$|\langle\psi \mid \phi\rangle|^2 \le \langle\psi \mid \psi\rangle\langle\phi \mid \phi\rangle. \tag{2.34}$$

  If $\mid \psi\rangle$ and $\mid \phi\rangle$ are linearly dependent (i.e., proportional: $\mid \psi\rangle = \alpha \mid \phi\rangle$, where α is a scalar), this relation becomes an equality. The Schwarz inequality (2.34) is analogous to the following relation of the real Euclidean space

$$|\vec{A} \cdot \vec{B}|^2 \le |\vec{A}|^2 \, |\vec{B}|^2 . \tag{2.35}$$

- **Triangle inequality**

$$\sqrt{\langle\psi + \phi \mid \psi + \phi\rangle} \le \sqrt{\langle\psi \mid \psi\rangle} + \sqrt{\langle\phi \mid \phi\rangle}. \tag{2.36}$$

  If $\mid \psi\rangle$ and $\mid \phi\rangle$ are linearly dependent, $\mid \psi\rangle = \alpha \mid \phi\rangle$, and if the proportionality scalar α is real and positive, the triangle inequality becomes an equality. The counterpart of this inequality in Euclidean space is given by $|\vec{A} + \vec{B}| \le |\vec{A}| + |\vec{B}|$.

- **Orthogonal states**

  Two *kets*, $\mid \psi\rangle$ and $\mid \phi\rangle$, are said to be orthogonal if they have a vanishing scalar product:

$$\langle\psi \mid \phi\rangle = 0. \tag{2.37}$$

- **Orthonormal states**

  Two *kets*, $| \psi\rangle$ and $| \phi\rangle$, are said to be orthonormal if they are orthogonal and if each one of them has a unit norm:

$$\langle\psi \mid \phi\rangle = 0, \qquad \langle\psi \mid \psi\rangle = 1, \qquad \langle\phi \mid \phi\rangle = 1. \tag{2.38}$$

- **Forbidden quantities**

  If $| \psi\rangle$ and $| \phi\rangle$ belong to the same vector (Hilbert) space, products of the type $| \psi\rangle | \phi\rangle$ and $\langle\psi | \langle\phi |$ are forbidden. They are nonsensical, since $| \psi\rangle | \phi\rangle$ and $\langle\psi | \langle\phi |$ are neither kets nor bras (an explicit illustration of this will be carried out in the example below and later on when we discuss the representation in a discrete basis). If $| \psi\rangle$ and $| \phi\rangle$ belong, however, to different vector spaces (e.g., $| \psi\rangle$ belongs to a spin space and $| \phi\rangle$ to an orbital angular momentum space), then the product $| \psi\rangle | \phi\rangle$, written as $| \psi\rangle \otimes | \phi\rangle$, represents a tensor product of $| \psi\rangle$ and $| \phi\rangle$. Only in these typical cases are such products meaningful.

Example 2.3
(**Note:** We will see later in this chapter that kets are represented by column matrices and bras by row matrices; this example is offered earlier than it should because we need to show some concrete illustrations of the formalism.) Consider the following two kets:

$$| \psi\rangle = \begin{pmatrix} -3i \\ 2+i \\ 4 \end{pmatrix}, \qquad | \phi\rangle = \begin{pmatrix} 2 \\ -i \\ 2-3i \end{pmatrix}.$$

(a) Find the bra $\langle\phi |$.
(b) Evaluate the scalar product $\langle\phi \mid \psi\rangle$.
(c) Examine why the products $| \psi\rangle | \phi\rangle$ and $\langle\phi | \langle\psi |$ do not make sense.

Solution

(a) As will be explained later when we introduce the Hermitian adjoint of kets and bras, we want to mention that the bra $\langle\phi |$ can be obtained by simply taking the complex conjugate of the transpose of the ket $| \phi\rangle$:

$$\langle\phi | = (2 \quad i \quad 2+3i). \tag{2.39}$$

(b) The scalar product $\langle\phi \mid \psi\rangle$ can be calculated as follows:

$$\begin{aligned} \langle\phi \mid \psi\rangle &= (2 \quad i \quad 2+3i) \begin{pmatrix} -3i \\ 2+i \\ 4 \end{pmatrix} \\ &= 2(-3i) + i(2+i) + 4(2+3i) \\ &= 7+8i. \end{aligned} \tag{2.40}$$

(c) First, the product $| \psi\rangle | \phi\rangle$ cannot be performed because, from linear algebra, the product of two column matrices cannot be performed. Similarly, since two row matrices cannot be multiplied, the product $\langle\phi | \langle\psi |$ is meaningless.

Physical meaning of the scalar product
The scalar product can be interpreted in two ways. First, by analogy with the scalar product of ordinary vectors in the Euclidean space, where $\vec{A} \cdot \vec{B}$ represents the projection of $\vec{B}$ on $\vec{A}$, the product $\langle \phi \mid \psi \rangle$ also represents the projection of $\mid \psi \rangle$ onto $\mid \phi \rangle$. Second, in the case of normalized states and according to Born's probabilistic interpretation, the quantity $\langle \phi \mid \psi \rangle$ represents the probability amplitude that the system's state $\mid \psi \rangle$ will, after a measurement is performed on the system, be found to be in another state $\mid \phi \rangle$.

Example 2.4 (Bra-ket algebra)
Consider the states $\mid \psi \rangle = 3i \mid \phi_1 \rangle - 7i \mid \phi_2 \rangle$ and $\mid \chi \rangle = - \mid \phi_1 \rangle + 2i \mid \phi_2 \rangle$, where $\mid \phi_1 \rangle$ and $\mid \phi_2 \rangle$ are orthonormal.

(a) Calculate $\mid \psi + \chi \rangle$ and $\langle \psi + \chi \mid$.

(b) Calculate the scalar products $\langle \psi \mid \chi \rangle$ and $\langle \chi \mid \psi \rangle$. Are they equal?

(c) Show that the states $\mid \psi \rangle$ and $\mid \chi \rangle$ satisfy the Schwarz inequality.

(d) Show that the states $\mid \psi \rangle$ and $\mid \chi \rangle$ satisfy the triangle inequality.

Solution

(a) The calculation of $\mid \psi + \chi \rangle$ is straightforward:

$$\begin{aligned} \mid \psi + \chi \rangle &= \mid \psi \rangle + \mid \chi \rangle = (3i \mid \phi_1 \rangle - 7i \mid \phi_2 \rangle) + (- \mid \phi_1 \rangle + 2i \mid \phi_2 \rangle) \\ &= (-1 + 3i) \mid \phi_1 \rangle - 5i \mid \phi_2 \rangle. \end{aligned} \tag{2.41}$$

This leads at once to the expression of $\langle \psi + \chi \mid$:

$$\langle \psi + \chi \mid = (-1 + 3i)^* \langle \phi_1 \mid + (-5i)^* \langle \phi_2 \mid = (-1 - 3i) \langle \phi_1 \mid + 5i \langle \phi_2 \mid . \tag{2.42}$$

(b) Since $\langle \phi_1 \mid \phi_1 \rangle = \langle \phi_2 \mid \phi_2 \rangle = 1$, $\langle \phi_1 \mid \phi_2 \rangle = \langle \phi_2 \mid \phi_1 \rangle = 0$, and since the bras corresponding to the kets $\mid \psi \rangle = 3i \mid \phi_1 \rangle - 7i \mid \phi_2 \rangle$ and $\mid \chi \rangle = - \mid \phi_1 \rangle + 2i \mid \phi_2 \rangle$ are given by $\langle \psi \mid = -3i \langle \phi_1 \mid + 7i \langle \phi_2 \mid$ and $\langle \chi \mid = -\langle \phi_1 \mid - 2i \langle \phi_2 \mid$, the scalar products are

$$\begin{aligned} \langle \psi \mid \chi \rangle &= (-3i \langle \phi_1 \mid + 7i \langle \phi_2 \mid)(- \mid \phi_1 \rangle + 2i \mid \phi_2 \rangle) \\ &= (-3i)(-1) \langle \phi_1 \mid \phi_1 \rangle + (7i)(2i) \langle \phi_2 \mid \phi_2 \rangle \\ &= -14 + 3i, \end{aligned} \tag{2.43}$$

$$\begin{aligned} \langle \chi \mid \psi \rangle &= (-\langle \phi_1 \mid - 2i \langle \phi_2 \mid)(3i \mid \phi_1 \rangle - 7i \mid \phi_2 \rangle) \\ &= (-1)(3i) \langle \phi_1 \mid \phi_1 \rangle + (-2i)(-7i) \langle \phi_2 \mid \phi_2 \rangle \\ &= -14 - 3i. \end{aligned} \tag{2.44}$$

We see that $\langle \psi \mid \chi \rangle$ is equal to the complex conjugate of $\langle \chi \mid \psi \rangle$.

(c) Let us first calculate $\langle \psi \mid \psi \rangle$ and $\langle \chi \mid \chi \rangle$:

$$\langle \psi \mid \psi \rangle = (-3i \langle \phi_1 \mid + 7i \langle \phi_2 \mid)(3i \mid \phi_1 \rangle - 7i \mid \phi_2 \rangle) = (-3i)(3i) + (7i)(-7i) = 58, \tag{2.45}$$

$$\langle \chi \mid \chi \rangle = (-\langle \phi_1 \mid - 2i \langle \phi_2 \mid)(- \mid \phi_1 \rangle + 2i \mid \phi_2 \rangle) = (-1)(-1) + (-2i)(2i) = 5. \tag{2.46}$$

Since $\langle \psi \mid \chi \rangle = -14 + 3i$ we have $\mid \langle \psi \mid \chi \rangle \mid^2 = 14^2 + 3^2 = 205$. Combining the values of $\mid \langle \psi \mid \chi \rangle \mid^2$, $\langle \psi \mid \psi \rangle$, and $\langle \chi \mid \chi \rangle$, we see that the Schwarz inequality (2.34) is satisfied:

$$205 < (58)(5) \Longrightarrow \mid \langle \psi \mid \chi \rangle \mid^2 < \langle \psi \mid \psi \rangle \langle \chi \mid \chi \rangle. \tag{2.47}$$

(d) First, let us use (2.41) and (2.42) to calculate $\langle\psi+\chi \mid \psi+\chi\rangle$:

$$\begin{aligned}\langle\psi+\chi \mid \psi+\chi\rangle &= [(-1-3i)\langle\phi_1 \mid +5i\langle\phi_2 \mid][(-1+3i) \mid \phi_1\rangle - 5i \mid \phi_2\rangle] \\ &= (-1-3i)(-1+3i)+(5i)(-5i) \\ &= 35. \end{aligned} \tag{2.48}$$

Since $\langle\psi \mid \psi\rangle = 58$ and $\langle\chi \mid \chi\rangle = 5$, we infer that the triangle inequality (2.36) is satisfied:

$$\sqrt{35} < \sqrt{58}+\sqrt{5} \Longrightarrow \sqrt{\langle\psi+\chi \mid \psi+\chi\rangle} < \sqrt{\langle\psi \mid \psi\rangle}+\sqrt{\langle\chi \mid \chi\rangle}. \tag{2.49}$$

Example 2.5
Consider two states $|\psi_1\rangle = 2i|\phi_1\rangle+|\phi_2\rangle-a|\phi_3\rangle+4|\phi_4\rangle$ and $|\psi_2\rangle = 3|\phi_1\rangle-i|\phi_2\rangle+5|\phi_3\rangle-|\phi_4\rangle$, where $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, and $|\phi_4\rangle$ are orthonormal kets, and where a is a constant. Find the value of a so that $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal.

Solution
For the states $|\psi_1\rangle$ and $|\psi_2\rangle$ to be orthogonal, the scalar product $\langle\psi_2 \mid \psi_1\rangle$ must be zero. Using the relation $\langle\psi_2 | = 3\langle\phi_1| + i\langle\phi_2| + 5\langle\phi_3| - \langle\phi_4|$, we can easily find the scalar product

$$\begin{aligned}\langle\psi_2 \mid \psi_1\rangle &= (3\langle\phi_1|+i\langle\phi_2|+5\langle\phi_3|-\langle\phi_4|)\,(2i|\phi_1\rangle+|\phi_2\rangle-a|\phi_3\rangle+4|\phi_4\rangle) \\ &= 7i-5a-4. \end{aligned} \tag{2.50}$$

Since $\langle\psi_2 \mid \psi_1\rangle = 7i-5a-4=0$, the value of a is $a=(7i-4)/5$.

2.4 Operators

2.4.1 General Definitions

Definition of an operator: An operator[1] $\hat{A}$ is a *mathematical rule* that when applied to a ket $\mid \psi\rangle$ transforms it into another ket $\mid \psi'\rangle$ of the same space and when it acts on a bra $\langle\phi \mid$ transforms it into another bra $\langle\phi' \mid$:

$$\hat{A} \mid \psi\rangle = \mid \psi'\rangle, \qquad \langle\phi \mid \hat{A} = \langle\phi' \mid. \tag{2.51}$$

A similar definition applies to wave functions:

$$\hat{A}\psi(\vec{r}) = \psi'(\vec{r}), \qquad \phi(\vec{r})\hat{A} = \phi'(\vec{r}). \tag{2.52}$$

Examples of operators
Here are some of the operators that we will use in this text:

- Unity operator: it leaves any ket unchanged, $\hat{I} \mid \psi\rangle = \mid \psi\rangle$.
- The gradient operator: $\vec{\nabla}\psi(\vec{r}) = (\partial\psi(\vec{r})/\partial x)\vec{i} + (\partial\psi(\vec{r})/\partial y)\vec{j} + (\partial\psi(\vec{r})/\partial z)\vec{k}$.

[1] The hat on $\hat{A}$ will be used throughout this text to distinguish an operator $\hat{A}$ from a complex number or a matrix A.

- The linear momentum operator: $\vec{P}\psi(\vec{r}) = -i\hbar\vec{\nabla}\psi(\vec{r})$.
- The Laplacian operator: $\nabla^2\psi(\vec{r}) = \partial^2\psi(\vec{r})/\partial x^2 + \partial^2\psi(\vec{r})/\partial y^2 + \partial^2\psi(\vec{r})/\partial z^2$.
- The parity operator: $\hat{\mathcal{P}}\psi(\vec{r}) = \psi(-\vec{r})$.

Products of operators
The product of two operators is generally not commutative:

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}. \tag{2.53}$$

The product of operators is, however, associative:

$$\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}. \tag{2.54}$$

We may also write $\hat{A}^n\hat{A}^m = \hat{A}^{n+m}$. When the product $\hat{A}\hat{B}$ operates on a ket $|\,\psi\rangle$ (the order of application is important), the operator $\hat{B}$ acts first on $|\,\psi\rangle$ and then $\hat{A}$ acts on the new ket $(B\,|\,\psi\rangle)$:

$$\hat{A}\hat{B}\,|\,\psi\rangle \;=\; \hat{A}(\hat{B}\,|\,\psi\rangle). \tag{2.55}$$

Similarly, when $\hat{A}\hat{B}\hat{C}\hat{D}$ operates on a ket $|\,\psi\rangle$, $\hat{D}$ acts first, then $\hat{C}$, then $\hat{B}$, and then $\hat{A}$.

When an operator $\hat{A}$ is sandwiched between a bra $\langle\phi\,|$ and a ket $|\,\psi\rangle$, it yields in general a complex number: $\langle\phi\,|\,\hat{A}\,|\,\psi\rangle$ = complex number. The quantity $\langle\phi\,|\,\hat{A}\,|\,\psi\rangle$ can also be a purely real or a purely imaginary number. **Note:** In evaluating $\langle\phi\,|\,\hat{A}\,|\,\psi\rangle$ it does not matter if one first applies $\hat{A}$ to the ket and then takes the bra-ket or one first applies $\hat{A}$ to the bra and then takes the bra-ket; that is $(\langle\phi\,|\,\hat{A})\,|\,\psi\rangle = \langle\phi\,|\,(\hat{A}\,|\,\psi\rangle)$.

Linear operators
An operator $\hat{A}$ is said to be *linear* if it obeys the distributive law and, like all operators, it commutes with constants. That is, an operator $\hat{A}$ is linear if, for any vectors $|\,\psi_1\rangle$ and $|\,\psi_2\rangle$ and any complex numbers a_1 and a_2, we have

$$\hat{A}\,(a_1\,|\,\psi_1\rangle \,+\, a_2\,|\,\psi_2\rangle) = a_1\hat{A}\,|\,\psi_1\rangle \,+\, a_2\hat{A}\,|\,\psi_2\rangle, \tag{2.56}$$

and

$$(\langle\psi_1\,|\,a_1 \,+\, \langle\psi_2\,|\,a_2)\hat{A} = a_1\langle\psi_1\,|\,\hat{A} \,+\, a_2\langle\psi_2\,|\,\hat{A}. \tag{2.57}$$

Remarks

- The *expectation* or *mean* value $\langle\hat{A}\rangle$ of an operator $\hat{A}$ with respect to a state $|\,\psi\rangle$ is defined by

$$\langle\hat{A}\rangle = \frac{\langle\psi\,|\,\hat{A}\,|\,\psi\rangle}{\langle\psi\,|\,\psi\rangle}. \tag{2.58}$$

- The quantity $|\,\phi\rangle\langle\psi\,|$ (i.e., the product of a ket with a bra) is a linear operator in Dirac's notation. To see this, when $|\,\phi\rangle\langle\psi\,|$ is applied to a ket $|\,\psi'\rangle$, we obtain another ket:

$$|\,\phi\rangle\langle\psi\,|\,\psi'\rangle = \langle\psi\,|\,\psi'\rangle\,|\,\phi\rangle, \tag{2.59}$$

since $\langle\psi\,|\,\psi'\rangle$ is a complex number.

- Products of the type $|\,\psi\rangle\hat{A}$ and $\hat{A}\langle\psi\,|$ (i.e., when an operator stands on the right of a ket or on the left of a bra) are forbidden. They are not operators, or kets, or bras; they have no mathematical or physical meanings (see equation (2.219) for an illustration).

2.4.2 Hermitian Adjoint

The Hermitian adjoint or conjugate[2], $\alpha^\dagger$, of a complex number α is the complex conjugate of this number: $\alpha^\dagger = \alpha^*$. The Hermitian adjoint, or simply the adjoint, $\hat{A}^\dagger$, of an operator $\hat{A}$ is defined by this relation:

$$\langle \psi \mid \hat{A}^\dagger \mid \phi \rangle = \langle \phi \mid \hat{A} \mid \psi \rangle^*. \tag{2.60}$$

Properties of the Hermitian conjugate rule
To obtain the Hermitian adjoint of any expression, we must cyclically reverse the order of the factors and make three replacements:

- Replace constants by their complex conjugates: $\alpha^\dagger = \alpha^*$.
- Replace kets (bras) by the corresponding bras (kets): $(\mid \psi \rangle)^\dagger = \langle \psi \mid$ and $(\langle \psi \mid)^\dagger = \mid \psi \rangle$.
- Replace operators by their adjoints.

Following these rules, we can write

$$(\hat{A}^\dagger)^\dagger = \hat{A}, \tag{2.61}$$
$$(a\hat{A})^\dagger = a^*\hat{A}^\dagger, \tag{2.62}$$
$$(\hat{A}^n)^\dagger = (\hat{A}^\dagger)^n, \tag{2.63}$$
$$(\hat{A} + \hat{B} + \hat{C} + \hat{D})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger + \hat{C}^\dagger + \hat{D}^\dagger, \tag{2.64}$$
$$(\hat{A}\hat{B}\hat{C}\hat{D})^\dagger = \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger, \tag{2.65}$$
$$(\hat{A}\hat{B}\hat{C}\hat{D} \mid \psi\rangle)^\dagger = \langle \psi \mid D^\dagger C^\dagger B^\dagger A^\dagger. \tag{2.66}$$

The Hermitian adjoint of the operator $\mid \psi\rangle\langle\phi \mid$ is given by

$$(\mid \psi\rangle\langle\phi \mid)^\dagger = \mid \phi\rangle\langle\psi \mid. \tag{2.67}$$

Operators act inside kets and bras, respectively, as follows:

$$\mid \alpha\hat{A}\psi\rangle = \alpha\hat{A} \mid \psi\rangle, \qquad \langle\alpha\hat{A}\psi \mid = \alpha^*\langle\psi \mid \hat{A}^\dagger. \tag{2.68}$$

Note also that $\langle\alpha\hat{A}^\dagger\psi \mid = \alpha^*\langle\psi \mid (\hat{A}^\dagger)^\dagger = \alpha^*\langle\psi \mid \hat{A}$. Hence, we can also write:

$$\langle\psi \mid \hat{A} \mid \phi\rangle = \langle\hat{A}^\dagger\psi \mid \phi\rangle = \langle\psi \mid \hat{A}\phi\rangle. \tag{2.69}$$

Hermitian and skew-Hermitian operators
An operator $\hat{A}$ is said to be *Hermitian* if it is equal to its adjoint $\hat{A}^\dagger$:

$$\boxed{\hat{A} = \hat{A}^\dagger \quad \text{or} \quad \langle\psi \mid \hat{A} \mid \phi\rangle = \langle\phi \mid \hat{A} \mid \psi\rangle^*.} \tag{2.70}$$

[2] The terms “adjoint” and “conjugate” are used indiscriminately.

On the other hand, an operator $\hat{B}$ is said to be *skew-Hermitian* or *anti-Hermitian* if

$$\boxed{\hat{B}^\dagger = -\hat{B} \qquad \text{or} \quad \langle \psi \mid \hat{B} \mid \phi \rangle = -\langle \phi \mid \hat{B} \mid \psi \rangle^*.} \tag{2.71}$$

Remark

The Hermitian adjoint of an operator is not, in general, equal to its complex conjugate: $\hat{A}^\dagger \neq \hat{A}^*$.

Example 2.6

(a) Discuss the hermiticity of the operators $(\hat{A} + \hat{A}^\dagger)$, $i(\hat{A} + \hat{A}^\dagger)$, and $i(\hat{A} - \hat{A}^\dagger)$.

(b) Find the Hermitian adjoint of $f(\hat{A}) = (1 + i\hat{A} + 3\hat{A}^2)(1 - 2i\hat{A} - 9\hat{A}^2)/(5 + 7\hat{A})$.

(c) Show that the expectation value of a Hermitian operator is real and that of an anti-Hermitian operator is imaginary.

Solution

(a) The operator $\hat{B} = \hat{A} + \hat{A}^\dagger$ is Hermitian regardless of whether or not $\hat{A}$ is Hermitian, since

$$\hat{B}^\dagger = (\hat{A} + \hat{A}^\dagger)^\dagger = \hat{A}^\dagger + \hat{A} = \hat{B}. \tag{2.72}$$

Similarly, the operator $i(\hat{A} - \hat{A}^\dagger)$ is also Hermitian; but $i(\hat{A} + \hat{A}^\dagger)$ is anti-Hermitian, since $[i(\hat{A} + \hat{A}^\dagger)]^\dagger = -i(\hat{A} + \hat{A}^\dagger)$.

(b) Since the Hermitian adjoint of an operator function $f(\hat{A})$ is given by $f^\dagger(\hat{A}) = f^*(\hat{A}^\dagger)$, we can write

$$\left(\frac{(1 + i\hat{A} + 3\hat{A}^2)(1 - 2i\hat{A} - 9\hat{A}^2)}{5 + 7\hat{A}} \right)^\dagger = \frac{(1 + 2i\hat{A}^\dagger - 9\hat{A}^{\dagger 2})(1 - i\hat{A}^\dagger + 3\hat{A}^{\dagger 2})}{5 + 7\hat{A}^\dagger}. \tag{2.73}$$

(c) From (2.70) we immediately infer that the expectation value of a Hermitian operator is real, for it satisfies the following property:

$$\langle \psi \mid \hat{A} \mid \psi \rangle = \langle \psi \mid \hat{A} \mid \psi \rangle^*; \tag{2.74}$$

that is, if $\hat{A}^\dagger = \hat{A}$ then $\langle \psi \mid \hat{A} \mid \psi \rangle$ is real. Similarly, for an anti-Hermitian operator, $\hat{B}^\dagger = -\hat{B}$, we have

$$\langle \psi \mid \hat{B} \mid \psi \rangle = -\langle \psi \mid \hat{B} \mid \psi \rangle^*, \tag{2.75}$$

which means that $\langle \psi \mid \hat{B} \mid \psi \rangle$ is a purely imaginary number.

2.4.3 Projection Operators

An operator $\hat{P}$ is said to be a *projection operator* if it is Hermitian and equal to its own square:

$$\hat{P}^\dagger = \hat{P}, \qquad \hat{P}^2 = \hat{P}. \tag{2.76}$$

The unit operator $\hat{I}$ is a simple example of a projection operator, since $\hat{I}^\dagger = \hat{I}$, $\quad \hat{I}^2 = \hat{I}$.

Properties of projection operators

- The product of two commuting projection operators, $\hat{P}_1$ and $\hat{P}_2$, is also a projection operator, since

$$(\hat{P}_1\hat{P}_2)^\dagger = \hat{P}_2^\dagger\hat{P}_1^\dagger = \hat{P}_2\hat{P}_1 = \hat{P}_1\hat{P}_2 \text{ and } (\hat{P}_1\hat{P}_2)^2 = \hat{P}_1\hat{P}_2\hat{P}_1\hat{P}_2 = \hat{P}_1^2\hat{P}_2^2 = \hat{P}_1\hat{P}_2. \tag{2.77}$$

- The sum of two projection operators is generally not a projection operator.
- Two projection operators are said to be orthogonal if their product is zero.
- For a sum of projection operators $\hat{P}_1 + \hat{P}_2 + \hat{P}_3 + \cdots$ to be a projection operator, it is necessary and sufficient that these projection operators be mutually orthogonal (i.e., the cross-product terms must vanish).

Example 2.7
Show that the operator $|\,\psi\rangle\langle\psi\,|$ is a projection operator only when $|\,\psi\rangle$ is normalized.

Solution
It is easy to ascertain that the operator $|\,\psi\rangle\langle\psi\,|$ is Hermitian, since $(|\,\psi\rangle\langle\psi\,|)^\dagger = |\,\psi\rangle\langle\psi\,|$. As for the square of this operator, it is given by

$$(|\,\psi\rangle\langle\psi\,|)^2 = (|\,\psi\rangle\langle\psi\,|)(|\,\psi\rangle\langle\psi\,|) = |\,\psi\rangle\langle\psi\,|\,\psi\rangle\langle\psi\,|\,. \tag{2.78}$$

Thus, if $|\,\psi\rangle$ is normalized, we have $(|\,\psi\rangle\langle\psi\,|)^2 = |\,\psi\rangle\langle\psi\,|$. In sum, if the state $|\,\psi\rangle$ is normalized, the product of the ket $|\,\psi\rangle$ with the bra $\langle\psi\,|$ is a projection operator.

2.4.4 Commutator Algebra

The *commutator* of two operators $\hat{A}$ and $\hat{B}$, denoted by $[\hat{A},\ \hat{B}]$, is defined by

$$\boxed{[\hat{A},\ \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A},} \tag{2.79}$$

and the *anticommutator* $\{\hat{A},\ \hat{B}\}$ is defined by

$$\boxed{\{\hat{A},\ \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}.} \tag{2.80}$$

Two operators are said to commute if their commutator is equal to zero and hence $\hat{A}\hat{B} = \hat{B}\hat{A}$. Any operator commutes with itself:

$$[\hat{A},\ \hat{A}] = 0. \tag{2.81}$$

Note that if two operators are Hermitian and their product is also Hermitian, these operators commute:

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A}, \tag{2.82}$$

and since $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$ we have $\hat{A}\hat{B} = \hat{B}\hat{A}$.

As an example, we may mention the commutators involving the x-position operator, $\hat{X}$, and the x-component of the momentum operator, $\hat{P}_x = -i\hbar\partial/\partial x$, as well as the y and the z components

$$\boxed{[\hat{X},\ \hat{P}_x] = i\hbar\hat{I}, \qquad [\hat{Y},\ \hat{P}_y] = i\hbar\hat{I}, \qquad [\hat{Z},\ \hat{P}_z] = i\hbar\hat{I},} \tag{2.83}$$

where $\hat{I}$ is the unit operator.

Properties of commutators
Using the commutator relation (2.79), we can establish the following properties:

- Antisymmetry:
$$[\hat{A},\ \hat{B}] = -[\hat{B},\ \hat{A}] \tag{2.84}$$

- Linearity:
$$[\hat{A},\ \hat{B} + \hat{C} + \hat{D} + \cdots] = [\hat{A},\ \hat{B}] + [\hat{A},\ \hat{C}] + [\hat{A},\ \hat{D}] + \cdots \tag{2.85}$$

- Hermitian conjugate of a commutator:
$$[\hat{A},\ \hat{B}]^\dagger = [\hat{B}^\dagger,\ \hat{A}^\dagger] \tag{2.86}$$

- Distributivity:
$$[\hat{A},\ \hat{B}\hat{C}] = [\hat{A},\ \hat{B}]\hat{C} + \hat{B}[\hat{A},\ \hat{C}] \tag{2.87}$$
$$[\hat{A}\hat{B},\ \hat{C}] = \hat{A}[\hat{B},\ \hat{C}] + [\hat{A},\ \hat{C}]\hat{B} \tag{2.88}$$

- Jacobi identity:
$$[\hat{A}, [\hat{B},\ \hat{C}]] + [\hat{B},\ [\hat{C},\ \hat{A}]] + [\hat{C},\ [\hat{A},\ \hat{B}]] = 0 \tag{2.89}$$

- By repeated applications of (2.87), we can show that
$$[\hat{A},\ \hat{B}^n] = \sum_{j=0}^{n-1} \hat{B}^j[\hat{A},\ \hat{B}]\hat{B}^{n-j-1} \tag{2.90}$$
$$[\hat{A}^n,\ \hat{B}] = \sum_{j=0}^{n-1} \hat{A}^{n-j-1}[\hat{A},\ \hat{B}]\hat{A}^j \tag{2.91}$$

- Operators commute with scalars: an operator $\hat{A}$ commutes with any scalar b:
$$[\hat{A},\ b] = 0 \tag{2.92}$$

Example 2.8
(a) Show that the commutator of two Hermitian operators is anti-Hermitian.
(b) Evaluate the commutator $[\hat{A},\ [\hat{B},\ \hat{C}]\hat{D}]$.

Solution

(a) If $\hat{A}$ and $\hat{B}$ are Hermitian, we can write

$$[\hat{A},\ \hat{B}]^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A},\ \hat{B}]; \tag{2.93}$$

that is, the commutator of $\hat{A}$ and $\hat{B}$ is anti-Hermitian: $[\hat{A},\ \hat{B}]^\dagger = -[\hat{A},\ \hat{B}]$.

(b) Using the distributivity relation (2.87), we have

$$\begin{aligned}[\hat{A},\ [\hat{B},\ \hat{C}]\hat{D}] &= [\hat{B},\ \hat{C}][\hat{A},\ \hat{D}] + [\hat{A},\ [\hat{B},\ \hat{C}]]\hat{D} \\ &= (\hat{B}\hat{C} - \hat{C}\hat{B})(\hat{A}\hat{D} - \hat{D}\hat{A}) + \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B})\hat{D} - (\hat{B}\hat{C} - \hat{C}\hat{B})\hat{A}\hat{D} \\ &= \hat{C}\hat{B}\hat{D}\hat{A} - \hat{B}\hat{C}\hat{D}\hat{A} + \hat{A}\hat{B}\hat{C}\hat{D} - \hat{A}\hat{C}\hat{B}\hat{D}. \end{aligned} \tag{2.94}$$

2.4.5 Uncertainty Relation between Two Operators

An interesting application of the commutator algebra is to derive a general relation giving the uncertainties product of two operators, $\hat{A}$ and $\hat{B}$. In particular, we want to give a formal derivation of Heisenberg's uncertainty relations.

Let $\langle\hat{A}\rangle$ and $\langle\hat{B}\rangle$ denote the expectation values of two Hermitian operators $\hat{A}$ and $\hat{B}$ with respect to a normalized state vector $\mid\psi\rangle$: $\langle\hat{A}\rangle = \langle\psi\mid\hat{A}\mid\psi\rangle$ and $\langle\hat{B}\rangle = \langle\psi\mid\hat{B}\mid\psi\rangle$. Introducing the operators $\Delta\hat{A}$ and $\Delta\hat{B}$,

$$\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle, \qquad \Delta\hat{B} = \hat{B} - \langle\hat{B}\rangle, \tag{2.95}$$

we have $(\Delta\hat{A})^2 = \hat{A}^2 - 2\hat{A}\langle\hat{A}\rangle + \langle\hat{A}\rangle^2$ and $(\Delta\hat{B})^2 = \hat{B}^2 - 2\hat{B}\langle\hat{B}\rangle + \langle\hat{B}\rangle^2$, and hence

$$\langle\psi\mid(\Delta\hat{A})^2\mid\psi\rangle = \langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2, \qquad \langle(\Delta\hat{B})^2\rangle = \langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2, \tag{2.96}$$

where $\langle\hat{A}^2\rangle = \langle\psi\mid\hat{A}^2\mid\psi\rangle$ and $\langle\hat{B}^2\rangle = \langle\psi\mid\hat{B}^2\mid\psi\rangle$. The *uncertainties* ΔA and ΔB are defined by

$$\boxed{\Delta A = \sqrt{\langle(\Delta\hat{A})^2\rangle} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}, \qquad \Delta B = \sqrt{\langle(\Delta\hat{B})^2\rangle} = \sqrt{\langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2}.} \tag{2.97}$$

Let us write the action of the operators (2.95) on any state $\mid\psi\rangle$ as follows:

$$\mid\chi\rangle = \Delta\hat{A}\mid\psi\rangle = \left(\hat{A} - \langle\hat{A}\rangle\right)\mid\psi\rangle, \qquad \mid\phi\rangle = \Delta\hat{B}\mid\psi\rangle = \left(\hat{B} - \langle\hat{B}\rangle\right)\mid\psi\rangle. \tag{2.98}$$

The Schwarz inequality for the states $\mid\chi\rangle$ and $\mid\phi\rangle$ is given by

$$\langle\chi\mid\chi\rangle\langle\phi\mid\phi\rangle \geq |\langle\chi\mid\phi\rangle|^2. \tag{2.99}$$

Since $\hat{A}$ and $\hat{B}$ are Hermitian, $\Delta\hat{A}$ and $\Delta\hat{B}$ must also be Hermitian: $\Delta\hat{A}^\dagger = \hat{A}^\dagger - \langle\hat{A}\rangle = \hat{A} - \langle\hat{A}\rangle = \Delta\hat{A}$ and $\Delta\hat{B}^\dagger = \hat{B} - \langle\hat{B}\rangle = \Delta\hat{B}$. Thus, we can show the following three relations:

$$\langle\chi\mid\chi\rangle = \langle\psi\mid(\Delta\hat{A})^2\mid\psi\rangle, \quad \langle\phi\mid\phi\rangle = \langle\psi\mid(\Delta\hat{B})^2\mid\psi\rangle, \quad \langle\chi\mid\phi\rangle = \langle\psi\mid\Delta\hat{A}\Delta\hat{B}\mid\psi\rangle. \tag{2.100}$$

For instance, since $\Delta\hat{A}^\dagger = \Delta\hat{A}$ we have $\langle\chi \mid \chi\rangle = \langle\psi \mid \Delta\hat{A}^\dagger\Delta\hat{A} \mid \psi\rangle = \langle\psi \mid (\Delta\hat{A})^2 \mid \psi\rangle = \langle(\Delta\hat{A})^2\rangle$. Hence, the Schwarz inequality (2.99) becomes

$$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \;\geq\; \left|\langle\Delta\hat{A}\Delta\hat{B}\rangle\right|^2. \tag{2.101}$$

Notice that the last term $\Delta\hat{A}\Delta\hat{B}$ of this equation can be written as

$$\Delta\hat{A}\Delta\hat{B} = \frac{1}{2}[\Delta\hat{A},\ \Delta\hat{B}] + \frac{1}{2}\{\Delta\hat{A},\ \Delta\hat{B}\} = \frac{1}{2}[\hat{A},\ \hat{B}] + \frac{1}{2}\{\Delta\hat{A},\ \Delta\hat{B}\}, \tag{2.102}$$

where we have used the fact that $[\Delta\hat{A},\ \Delta\hat{B}] = [\hat{A},\ \hat{B}]$. Since $[\hat{A},\ \hat{B}]$ is anti-Hermitian and $\{\Delta\hat{A},\ \Delta\hat{B}\}$ is Hermitian and since the expectation value of a Hermitian operator is real and that the expectation value of an anti-Hermitian operator is imaginary (see Example 2.6), the expectation value $\langle\Delta\hat{A}\Delta\hat{B}\rangle$ of (2.102) becomes equal to the sum of a real part $\langle\{\Delta\hat{A},\ \Delta\hat{B}\}\rangle/2$ and an imaginary part $\langle[\hat{A},\ \hat{B}]\rangle/2$; hence

$$\left|\langle\Delta\hat{A}\Delta\hat{B}\rangle\right|^2 = \frac{1}{4}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|^2 + \frac{1}{4}\left|\langle\{\Delta\hat{A},\ \Delta\hat{B}\}\rangle\right|^2. \tag{2.103}$$

Since the last term is a positive real number, we can infer the following relation:

$$\left|\langle\Delta\hat{A}\Delta\hat{B}\rangle\right|^2 \;\geq\; \frac{1}{4}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|^2. \tag{2.104}$$

Comparing equations (2.101) and (2.104), we conclude that

$$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \;\geq\; \frac{1}{4}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|^2, \tag{2.105}$$

which (by taking its square root) can be reduced to

$$\boxed{\Delta A \Delta B \geq \frac{1}{2}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|.} \tag{2.106}$$

This uncertainty relation plays an important role in the formalism of quantum mechanics. Its application to position and momentum operators leads to the Heisenberg uncertainty relations, which represent one of the cornerstones of quantum mechanics; see the next example.

Example 2.9 (Heisenberg uncertainty relations)

Find the uncertainty relations between the components of the position and the momentum operators.

Solution

By applying (2.106) to the x-components of the position operator $\hat{X}$, and the momentum operator $\hat{P}_x$, we obtain $\Delta x\Delta p_x \;\geq\; \frac{1}{2} \mid \langle[\hat{X},\ \hat{P}_x]\rangle \mid$. But since $[\hat{X},\ \hat{P}_x] = i\hbar\hat{I}$, we have $\Delta x\Delta p_x \geq \hbar/2$; the uncertainty relations for the $y-$ and $z-$ components follow immediately:

$$\boxed{\Delta x\Delta p_x \geq \frac{\hbar}{2}, \qquad \Delta y\Delta p_y \geq \frac{\hbar}{2}, \qquad \Delta z\Delta p_z \geq \frac{\hbar}{2}.} \tag{2.107}$$

These are the Heisenberg uncertainty relations.

2.4.6 Functions of Operators

Let $F(\hat{A})$ be a function of an operator $\hat{A}$. If $\hat{A}$ is a linear operator, we can Taylor expand $F(\hat{A})$ in a power series of $\hat{A}$:

$$F(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n, \tag{2.108}$$

where a_n is just an expansion coefficient. As an illustration of an operator function, consider $e^{a\hat{A}}$, where a is a scalar which can be complex or real. We can expand it as follows:

$$e^{a\hat{A}} = \sum_{n=0}^{\infty} \frac{a^n}{n!} \hat{A}^n = \hat{I} + a\hat{A} + \frac{a^2}{2!}\hat{A}^2 + \frac{a^3}{3!}\hat{A}^3 + \cdots. \tag{2.109}$$

Commutators involving function operators

If $\hat{A}$ commutes with another operator $\hat{B}$, then $\hat{B}$ commutes with any operator function that depends on $\hat{A}$:

$$[\hat{A},\ \hat{B}] = 0 \quad \Longrightarrow \quad [\hat{B},\ F(\hat{A})] = 0; \tag{2.110}$$

in particular, $F(\hat{A})$ commutes with $\hat{A}$ and with any other function, $G(\hat{A})$, of $\hat{A}$:

$$[\hat{A},\ F(\hat{A})] = 0, \qquad [\hat{A}^n,\ F(\hat{A})] = 0, \qquad [F(\hat{A}),\ G(\hat{A})] = 0. \tag{2.111}$$

Hermitian adjoint of function operators

The adjoint of $F(\hat{A})$ is given by

$$[F(\hat{A})]^\dagger = F^*(\hat{A}^\dagger). \tag{2.112}$$

Note that if $\hat{A}$ is Hermitian, $F(\hat{A})$ is not necessarily Hermitian; $F(\hat{A})$ will be Hermitian only if F is a real function and $\hat{A}$ is Hermitian. An example is

$$(e^{\hat{A}})^\dagger = e^{\hat{A}^\dagger}, \qquad (e^{i\hat{A}})^\dagger = e^{-i\hat{A}^\dagger}, \qquad (e^{i\alpha\hat{A}})^\dagger = e^{-i\alpha^*\hat{A}^\dagger}, \tag{2.113}$$

where α is a complex number. So if $\hat{A}$ is Hermitian, an operator function which can be expanded as $F(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n$ will be Hermitian only if the expansion coefficients a_n are real numbers. But in general, $F(\hat{A})$ is not Hermitian even if $\hat{A}$ is Hermitian, since

$$F^*(\hat{A}^\dagger) = \sum_{n=0}^{\infty} a_n^* (\hat{A}^\dagger)^n. \tag{2.114}$$

Relations involving function operators

Note that

$$[\hat{A},\ \hat{B}] \neq 0 \quad \Longrightarrow \quad [\hat{B},\ F(\hat{A})] \neq 0; \tag{2.115}$$

in particular, $e^{\hat{A}}e^{\hat{B}} \neq e^{\hat{A}+\hat{B}}$. Using (2.109) we can ascertain that

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{[\hat{A},\ \hat{B}]/2}, \tag{2.116}$$

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\ \hat{B}] + \frac{1}{2!}[\hat{A},\ [\hat{A},\ \hat{B}]] + \frac{1}{3!}[\hat{A},\ [\hat{A},\ [\hat{A},\ \hat{B}]]] + \cdots. \tag{2.117}$$

2.4.7 Inverse and Unitary Operators

Inverse of an operator: Assuming it exists[3] the *inverse* $\hat{A}^{-1}$ of a linear operator $\hat{A}$ is defined by the relation

$$\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I}, \tag{2.118}$$

where $\hat{I}$ is the unit operator, the operator that leaves any state $| \psi\rangle$ unchanged.

Quotient of two operators: Dividing an operator $\hat{A}$ by another operator $\hat{B}$ (provided that the inverse $\hat{B}^{-1}$ exists) is equivalent to multiplying $\hat{A}$ by $\hat{B}^{-1}$:

$$\frac{\hat{A}}{\hat{B}} = \hat{A}\hat{B}^{-1}. \tag{2.119}$$

The side on which the quotient is taken matters:

$$\frac{\hat{A}}{\hat{B}} = \hat{A}\frac{\hat{I}}{\hat{B}} = \hat{A}\hat{B}^{-1} \quad \text{and} \quad \frac{\hat{I}}{\hat{B}}\hat{A} = \hat{B}^{-1}\hat{A}. \tag{2.120}$$

In general, we have $\hat{A}\hat{B}^{-1} \neq \hat{B}^{-1}\hat{A}$. For an illustration of these ideas, see Problem 2.12. We may mention here the following properties about the inverse of operators:

$$\left(\hat{A}\hat{B}\hat{C}\hat{D}\right)^{-1} = \hat{D}^{-1}\hat{C}^{-1}\hat{B}^{-1}\hat{A}^{-1}, \qquad \left(\hat{A}^{n}\right)^{-1} = \left(\hat{A}^{-1}\right)^{n}. \tag{2.121}$$

Unitary operators: A linear operator $\hat{U}$ is said to be *unitary* if its inverse $\hat{U}^{-1}$ is equal to its adjoint $\hat{U}^{\dagger}$:

$$\hat{U}^{\dagger} = \hat{U}^{-1} \qquad \text{or} \qquad \hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \hat{I}. \tag{2.122}$$

The product of two unitary operators is also unitary, since

$$(\hat{U}\hat{V})(\hat{U}\hat{V})^{\dagger} = (\hat{U}\hat{V})(\hat{V}^{\dagger}\hat{U}^{\dagger}) = \hat{U}(\hat{V}\hat{V}^{\dagger})\hat{U}^{\dagger} = \hat{U}\hat{U}^{\dagger} = \hat{I}, \tag{2.123}$$

or $(\hat{U}\hat{V})^{\dagger} = (\hat{U}\hat{V})^{-1}$. This result can be generalized to any number of operators; the product of a number of unitary operators is also unitary, since

$$\begin{aligned}(\hat{A}\hat{B}\hat{C}\hat{D}\cdots)(\hat{A}\hat{B}\hat{C}\hat{D}\cdots)^{\dagger} &= \hat{A}\hat{B}\hat{C}\hat{D}(\cdots)\hat{D}^{\dagger}\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{A}\hat{B}\hat{C}(\hat{D}\hat{D}^{\dagger})\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} \\ &= \hat{A}\hat{B}(\hat{C}\hat{C}^{\dagger})\hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{A}(\hat{B}\hat{B}^{\dagger})\hat{A}^{\dagger} \\ &= \hat{A}\hat{A}^{\dagger} = \hat{I}, \end{aligned} \tag{2.124}$$

or $(\hat{A}\hat{B}\hat{C}\hat{D}\cdots)^{\dagger} = (\hat{A}\hat{B}\hat{C}\hat{D}\cdots)^{-1}$.

Example 2.10 (Unitary operator)

What conditions must the parameter ε and the operator $\hat{G}$ satisfy so that the operator $\hat{U} = e^{i\varepsilon\hat{G}}$ is unitary?

[3]Not every operator has an inverse, just as in the case of matrices. The inverse of a matrix exists only when its determinant is nonzero.

Solution
Clearly, if ε is real and $\hat{G}$ is Hermitian, the operator $e^{i\varepsilon\hat{G}}$ would be unitary. Using the property $[F(\hat{A})]^\dagger = F^*(\hat{A}^\dagger)$, we see that

$$(e^{i\varepsilon\hat{G}})^\dagger = e^{-i\varepsilon\hat{G}} = (e^{i\varepsilon\hat{G}})^{-1}, \tag{2.125}$$

that is, $\hat{U}^\dagger = \hat{U}^{-1}$.

2.4.8 Eigenvalues and Eigenvectors of an Operator

Having studied the properties of operators and states, we are now ready to discuss how to find the eigenvalues and eigenvectors of an operator.

A state vector $|\,\psi\rangle$ is said to be an *eigenvector* (also called an eigenket or eigenstate) of an operator $\hat{A}$ if the application of $\hat{A}$ to $|\,\psi\rangle$ gives

$$\hat{A}\,|\,\psi\rangle = a\,|\,\psi\rangle, \tag{2.126}$$

where a is a complex number, called an *eigenvalue* of $\hat{A}$. This equation is known as the *eigenvalue equation*, or *eigenvalue problem*, of the operator $\hat{A}$. Its solutions yield the eigenvalues and eigenvectors of $\hat{A}$. In Section 2.5.3 we will see how to solve the eigenvalue problem in a discrete basis.

A simple example is the eigenvalue problem for the unity operator $\hat{I}$:

$$\hat{I}\,|\,\psi\rangle = |\,\psi\rangle. \tag{2.127}$$

This means that all vectors are eigenvectors of $\hat{I}$ with one eigenvalue, 1. Note that

$$\hat{A}\,|\,\psi\rangle = a\,|\,\psi\rangle \implies \hat{A}^n\,|\,\psi\rangle = a^n\,|\,\psi\rangle \quad \text{and} \quad F(\hat{A})\,|\,\psi\rangle = F(a)\,|\,\psi\rangle. \tag{2.128}$$

For instance, we have

$$\hat{A}\,|\,\psi\rangle = a\,|\,\psi\rangle \quad \Longrightarrow \quad e^{i\hat{A}}\,|\,\psi\rangle = e^{ia}\,|\,\psi\rangle. \tag{2.129}$$

Example 2.11 (Eigenvalues of the inverse of an operator)
Show that if $\hat{A}^{-1}$ exists, the eigenvalues of $\hat{A}^{-1}$ are just the inverses of those of $\hat{A}$.

Solution
Since $\hat{A}^{-1}\hat{A} = \hat{I}$ we have on the one hand

$$\hat{A}^{-1}\hat{A}\,|\,\psi\rangle = |\,\psi\rangle, \tag{2.130}$$

and on the other hand

$$\hat{A}^{-1}\hat{A}\,|\,\psi\rangle = \hat{A}^{-1}(\hat{A}\,|\,\psi\rangle) = a\hat{A}^{-1}\,|\,\psi\rangle. \tag{2.131}$$

Combining the previous two equations, we obtain

$$a\hat{A}^{-1}\,|\,\psi\rangle = |\,\psi\rangle, \tag{2.132}$$

hence

$$\hat{A}^{-1} \mid \psi\rangle = \frac{1}{a} \mid \psi\rangle. \tag{2.133}$$

This means that $\mid \psi\rangle$ is also an eigenvector of $\hat{A}^{-1}$ with eigenvalue $1/a$. That is, if $\hat{A}^{-1}$ exists, then

$$\boxed{\hat{A} \mid \psi\rangle = a \mid \psi\rangle \quad \Longrightarrow \quad \hat{A}^{-1} \mid \psi\rangle = \frac{1}{a} \mid \psi\rangle.} \tag{2.134}$$

Some useful theorems pertaining to the eigenvalue problem

Theorem 2.1 *For a Hermitian operator, all of its eigenvalues are real and the eigenvectors corresponding to different eigenvalues are orthogonal.*

$$\text{If } \hat{A}^{\dagger} = \hat{A}, \quad \hat{A} \mid \phi_n\rangle = a_n \mid \phi_n\rangle \quad \Longrightarrow \quad a_n = \text{real number, and } \langle\phi_m \mid \phi_n\rangle = \delta_{mn}. \tag{2.135}$$

Proof of Theorem 2.1
Note that

$$\hat{A} \mid \phi_n\rangle = a_n \mid \phi_n\rangle \quad \Longrightarrow \quad \langle\phi_m \mid \hat{A} \mid \phi_n\rangle = a_n\langle\phi_m \mid \phi_n\rangle, \tag{2.136}$$

and

$$\langle\phi_m \mid \hat{A}^{\dagger} = a_m^*\langle\phi_m \mid \quad \Longrightarrow \quad \langle\phi_m \mid \hat{A}^{\dagger} \mid \phi_n\rangle = a_m^*\langle\phi_m \mid \phi_n\rangle. \tag{2.137}$$

Subtracting (2.137) from (2.136) and using the fact that $\hat{A}$ is Hermitian, $\hat{A} = \hat{A}^{\dagger}$, we have

$$(a_n - a_m^*)\langle\phi_m \mid \phi_n\rangle = 0. \tag{2.138}$$

Two cases must be considered separately:

- Case $m = n$: since $\langle\phi_n \mid \phi_n\rangle > 0$, we must have $a_n = a_n^*$; hence the eigenvalues a_n must be real.
- Case $m \neq n$: since in general $a_n \neq a_m^*$, we must have $\langle\phi_m \mid \phi_n\rangle = 0$; that is, $\mid \phi_m\rangle$ and $\mid \phi_n\rangle$ must be orthogonal.

Theorem 2.2 *The eigenstates of a Hermitian operator define a complete set of mutually orthonormal basis states. The operator is diagonal in this eigenbasis with its diagonal elements equal to the eigenvalues. This basis set is unique if the operator has no degenerate eigenvalues and not unique (in fact it is infinite) if there is any degeneracy.*

Theorem 2.3 *If two Hermitian operators, $\hat{A}$ and $\hat{B}$, commute and if $\hat{A}$ has no degenerate eigenvalue, then each eigenvector of $\hat{A}$ is also an eigenvector of $\hat{B}$. In addition, we can construct a common orthonormal basis that is made of the joint eigenvectors of $\hat{A}$ and $\hat{B}$.*

Proof of Theorem 2.3
Since $\hat{A}$ is Hermitian with no degenerate eigenvalue, to each eigenvalue of $\hat{A}$ there corresponds only one eigenvector. Consider the equation

$$\hat{A} \mid \phi_n\rangle = a_n \mid \phi_n\rangle. \tag{2.139}$$

Since $\hat{A}$ commutes with $\hat{B}$ we can write

$$\hat{B}\hat{A} \mid \phi_n\rangle = \hat{A}\hat{B} \mid \phi_n\rangle \quad \text{or} \quad \hat{A}(\hat{B} \mid \phi_n\rangle) = a_n(\hat{B} \mid \phi_n\rangle); \tag{2.140}$$

that is, $(\hat{B} \mid \phi_n\rangle)$ is an eigenvector of $\hat{A}$ with eigenvalue a_n. But since this eigenvector is unique (apart from an arbitrary phase constant), the ket $\mid \phi_n\rangle$ must also be an eigenvector of $\hat{B}$:

$$\hat{B} \mid \phi_n\rangle = b_n \mid \phi_n\rangle. \tag{2.141}$$

Since each eigenvector of $\hat{A}$ is also an eigenvector of $\hat{B}$ (and vice versa), both of these operators must have a common basis. This basis is unique; it is made of the joint eigenvectors of $\hat{A}$ and $\hat{B}$. This theorem also holds for any number of mutually commuting Hermitian operators.

Now, if a_n is a degenerate eigenvalue, we can only say that $\hat{B} \mid \phi_n\rangle$ is an eigenvector of $\hat{A}$ with eigenvalue a_n; $\mid \phi_n\rangle$ is not necessarily an eigenvector of $\hat{B}$. If one of the operators is degenerate, there exist an infinite number of orthonormal basis sets that are common to these two operators; that is, the joint basis does exist and it is not unique.

Theorem 2.4 *The eigenvalues of an anti-Hermitian operator are either purely imaginary or equal to zero.*

Theorem 2.5 *The eigenvalues of a unitary operator are complex numbers of moduli equal to one; the eigenvectors of a unitary operator that has no degenerate eigenvalues are mutually orthogonal.*

Proof of Theorem 2.5

Let $\mid \phi_n\rangle$ and $\mid \phi_m\rangle$ be eigenvectors to the unitary operator $\hat{U}$ with eigenvalues a_n and a_m, respectively. We can write

$$(\langle\phi_m \mid \hat{U}^\dagger)(\hat{U} \mid \phi_n\rangle) = a_m^* a_n \langle\phi_m \mid \phi_n\rangle. \tag{2.142}$$

Since $\hat{U}^\dagger\hat{U} = \hat{I}$ this equation can be rewritten as

$$(a_m^* a_n - 1)\langle\phi_m \mid \phi_n\rangle = 0, \tag{2.143}$$

which in turn leads to the following two cases:

- Case $n = m$: since $\langle\phi_n \mid \phi_n\rangle > 0$ then $a_n^* a_n = \mid a_n \mid^2 = 1$, and hence $\mid a_n \mid = 1$.
- Case $n \neq m$: the only possibility for this case is that $\mid \phi_m\rangle$ and $\mid \phi_n\rangle$ are orthogonal, $\langle\phi_m \mid \phi_n\rangle = 0$.

2.4.9 Infinitesimal and Finite Unitary Transformations

We want to study here how quantities such as kets, bras, operators, and scalars transform under unitary transformations. A unitary transformation is the application of a unitary operator $\hat{U}$ to one of these quantities.

2.4.9.1 Unitary Transformations

Kets $|\,\psi\rangle$ and bras $\langle\psi\,|$ transform as follows:

$$|\,\psi'\rangle = \hat{U}\,|\,\psi\rangle, \qquad \langle\psi'\,| = \langle\psi\,|\,\hat{U}^\dagger. \tag{2.144}$$

Let us now find out how operators transform under unitary transformations. Since the transform of $\hat{A}\,|\,\psi\rangle = |\,\phi\rangle$ is $\hat{A}'\,|\,\psi'\rangle = |\,\phi'\rangle$, we can rewrite $\hat{A}'\,|\,\psi'\rangle = |\,\phi'\rangle$ as $\hat{A}'\hat{U}\,|\,\psi\rangle = \hat{U}\,|\,\phi\rangle = \hat{U}\hat{A}\,|\,\psi\rangle$ which, in turn, leads to $\hat{A}'\hat{U} = \hat{U}\hat{A}$. Multiplying both sides of $\hat{A}'\hat{U} = \hat{U}\hat{A}$ by $\hat{U}^\dagger$ and since $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$, we have

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger, \qquad \hat{A} = \hat{U}^\dagger\hat{A}'\hat{U}. \tag{2.145}$$

The results reached in (2.144) and (2.145) may be summarized as follows:

$$\boxed{|\,\psi'\rangle = \hat{U}\,|\,\psi\rangle, \qquad \langle\psi'\,| = \langle\psi\,|\,\hat{U}^\dagger, \qquad \hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger,} \tag{2.146}$$

$$\boxed{|\,\psi\rangle = \hat{U}^\dagger\,|\,\psi'\rangle, \qquad \langle\psi\,| = \langle\psi'\,|\,\hat{U}, \qquad \hat{A} = \hat{U}^\dagger\hat{A}'\hat{U}.} \tag{2.147}$$

Properties of unitary transformations

- If an operator $\hat{A}$ is Hermitian, its transformed $\hat{A}'$ is also Hermitian, since

$$\hat{A}'^{\,\dagger} = (\hat{U}\hat{A}\hat{U}^\dagger)^\dagger = \hat{U}\hat{A}^\dagger\hat{U}^\dagger = \hat{U}\hat{A}\hat{U}^\dagger = \hat{A}'. \tag{2.148}$$

- The eigenvalues of $\hat{A}$ and those of its transformed $\hat{A}'$ are the same:

$$\hat{A}\,|\,\psi_n\rangle = a_n\,|\,\psi_n\rangle \quad\Longrightarrow\quad \hat{A}'\,|\,\psi'_n\rangle = a_n\,|\,\psi'_n\rangle, \tag{2.149}$$

  since

$$\begin{aligned} \hat{A}'\,|\,\psi'_n\rangle &= (\hat{U}\hat{A}\hat{U}^\dagger)(\hat{U}\,|\,\psi_n\rangle) = \hat{U}\hat{A}(\hat{U}^\dagger\hat{U})\,|\,\psi_n\rangle \\ &= \hat{U}\hat{A}\,|\,\psi_n\rangle = a_n(\hat{U}\,|\,\psi_n\rangle) = a_n\,|\,\psi'_n\rangle. \end{aligned} \tag{2.150}$$

- Commutators that are equal to (complex) numbers remain unchanged under unitary transformations, since the transformation of $[\hat{A}, \hat{B}] = a$, where a is a complex number, is given by

$$\begin{aligned} [\hat{A}', \hat{B}'] &= [\hat{U}\hat{A}\hat{U}^\dagger, \hat{U}\hat{B}\hat{U}^\dagger] = (\hat{U}\hat{A}\hat{U}^\dagger)(\hat{U}\hat{B}\hat{U}^\dagger) - (\hat{U}\hat{B}\hat{U}^\dagger)(\hat{U}\hat{A}\hat{U}^\dagger) \\ &= \hat{U}[\hat{A}, \hat{B}]\hat{U}^\dagger = \hat{U}a\hat{U}^\dagger = a\hat{U}\hat{U}^\dagger = a \\ &= [\hat{A}, \hat{B}]. \end{aligned} \tag{2.151}$$

- We can also verify the following general relations:

$$\hat{A} = \beta\hat{B} + \gamma\hat{C} \quad\Longrightarrow\quad \hat{A}' = \beta\hat{B}' + \gamma\hat{C}', \tag{2.152}$$

$$\hat{A} = \alpha\hat{B}\hat{C}\hat{D} \quad\Longrightarrow\quad \hat{A}' = \alpha\hat{B}'\hat{C}'\hat{D}', \tag{2.153}$$

  where $\hat{A}'$, $\hat{B}'$, $\hat{C}'$, and $\hat{D}'$ are the transforms of $\hat{A}$, $\hat{B}$, $\hat{C}$, and $\hat{D}$, respectively.

- Since the result (2.151) is valid for any complex number, we can state that complex numbers, such as $\langle \psi \mid \hat{A} \mid \chi \rangle$, remain unchanged under unitary transformations, since

$$\langle \psi' \mid \hat{A}' \mid \chi' \rangle = (\langle \psi \mid \hat{U}^\dagger)(\hat{U}\hat{A}\hat{U}^\dagger)(\hat{U} \mid \chi \rangle) = \langle \psi \mid (\hat{U}^\dagger \hat{U})\hat{A}(\hat{U}^\dagger U) \mid \chi \rangle = \langle \psi \mid \hat{A} \mid \chi \rangle. \tag{2.154}$$

  Taking $\hat{A} = \hat{I}$ we see that scalar products of the type

$$\langle \psi' \mid \chi' \rangle = \langle \psi \mid \chi \rangle \tag{2.155}$$

  are invariant under unitary transformations; notably, the norm of a state vector is conserved:

$$\langle \psi' \mid \psi' \rangle = \langle \psi \mid \psi \rangle. \tag{2.156}$$

- We can also verify that $\left(\hat{U}\hat{A}\hat{U}^\dagger\right)^n = \hat{U}\hat{A}^n\hat{U}^\dagger$ since

$$\begin{aligned} \left(\hat{U}\hat{A}\hat{U}^\dagger\right)^n &= \left(\hat{U}\hat{A}\hat{U}^\dagger\right)\left(\hat{U}\hat{A}\hat{U}^\dagger\right)\cdots\left(\hat{U}\hat{A}\hat{U}^\dagger\right) = \hat{U}\hat{A}(\hat{U}^\dagger\hat{U})\hat{A}(\hat{U}^\dagger\hat{U})\cdots(\hat{U}^\dagger\hat{U})\hat{A}\hat{U}^\dagger \\ &= \hat{U}\hat{A}^n\hat{U}^\dagger. \end{aligned} \tag{2.157}$$

- We can generalize the previous result to obtain the transformation of any operator function $f(\hat{A})$:

$$\hat{U} f(\hat{A})\hat{U}^\dagger = f(\hat{U}\hat{A}\hat{U}^\dagger) = f(\hat{A}'), \tag{2.158}$$

  or more generally

$$\hat{U} f(\hat{A}, \hat{B}, \hat{C}, \cdots)\hat{U}^\dagger = f(\hat{U}\hat{A}\hat{U}^\dagger, \hat{U}\hat{B}\hat{U}^\dagger, \hat{U}\hat{C}\hat{U}^\dagger, \cdots) = f(\hat{A}', \hat{B}', \hat{C}', \cdots). \tag{2.159}$$

A unitary transformation does not change the physics of a system; it merely transforms one description of the system to another physically equivalent description.

In what follows we want to consider two types of unitary transformations: infinitesimal transformations and finite transformations.

2.4.9.2 Infinitesimal Unitary Transformations

Consider an operator $\hat{U}$ which depends on an infinitesimally small real parameter ε and which varies only slightly from the unity operator $\hat{I}$:

$$\hat{U}_\varepsilon(\hat{G}) = \hat{I} + i\varepsilon\hat{G}, \tag{2.160}$$

where $\hat{G}$ is called the *generator* of the infinitesimal transformation. Clearly, $\hat{U}_\varepsilon$ is a unitary transformation only when the parameter ε is real and $\hat{G}$ is Hermitian, since

$$\hat{U}_\varepsilon\hat{U}_\varepsilon^\dagger = (\hat{I} + i\varepsilon\hat{G})(\hat{I} - i\varepsilon\hat{G}^\dagger) \simeq \hat{I} + i\varepsilon(\hat{G} - \hat{G}^\dagger) = \hat{I}, \tag{2.161}$$

where we have neglected the quadratic terms in ε.

The transformation of a state vector $\mid \psi \rangle$ is

$$\mid \psi' \rangle = (\hat{I} + i\varepsilon\hat{G}) \mid \psi \rangle = \mid \psi \rangle + \delta \mid \psi \rangle, \tag{2.162}$$

where

$$\delta \mid \psi\rangle = i\varepsilon\hat{G} \mid \psi\rangle. \tag{2.163}$$

The transformation of an operator $\hat{A}$ is given by

$$\boxed{\hat{A}' = (\hat{I} + i\varepsilon\hat{G})\hat{A}(\hat{I} - i\varepsilon\hat{G}) \simeq \hat{A} + i\varepsilon[\hat{G}, \hat{A}].} \tag{2.164}$$

If $\hat{G}$ commutes with $\hat{A}$, the unitary transformation will leave $\hat{A}$ unchanged, $\hat{A}' = \hat{A}$:

$$[\hat{G}, \hat{A}] = 0 \quad \Longrightarrow \quad \hat{A}' = (\hat{I} + i\varepsilon\hat{G})\hat{A}(\hat{I} - i\varepsilon\hat{G}) = \hat{A}. \tag{2.165}$$

2.4.9.3 Finite Unitary Transformations

We can construct a *finite* unitary transformation from (2.160) by performing a succession of infinitesimal transformations in steps of ε; the application of a series of successive unitary transformations is equivalent to the application of a single unitary transformation. Denoting $\varepsilon = \alpha/N$, where N is an integer and α is a finite parameter, we can apply the same unitary transformation N times; in the limit $N \to +\infty$ we obtain

$$\hat{U}_\alpha(\hat{G}) = \lim_{N\to\infty} \prod_{k=1}^{N} \left(1 + i\frac{\alpha}{N}\hat{G}\right) = \lim_{N\to+\infty} \left(1 + i\frac{\alpha}{N}\hat{G}\right)^N = e^{i\alpha\hat{G}}, \tag{2.166}$$

where $\hat{G}$ is now the generator of the finite transformation and α is its parameter.

As shown in (2.125), $\hat{U}$ is unitary only when the parameter α is real and $\hat{G}$ is Hermitian, since

$$(e^{i\alpha\hat{G}})^\dagger = e^{-i\alpha\hat{G}} = (e^{i\alpha\hat{G}})^{-1}. \tag{2.167}$$

Using the commutation relation (2.117), we can write the transformation $\hat{A}'$ of an operator $\hat{A}$ as follows:

$$\boxed{e^{i\alpha\hat{G}}\hat{A}e^{-i\alpha\hat{G}} = \hat{A} + i\alpha[\hat{G}, \hat{A}] + \frac{(i\alpha)^2}{2!}\left[\hat{G}, [\hat{G}, \hat{A}]\right] + \frac{(i\alpha)^3}{3!}\left[\hat{G}, [\hat{G}, [\hat{G}, \hat{A}]]\right] + \cdots.} \tag{2.168}$$

If $\hat{G}$ commutes with $\hat{A}$, the unitary transformation will leave $\hat{A}$ unchanged, $\hat{A}' = \hat{A}$:

$$[\hat{G}, \hat{A}] = 0 \Longrightarrow \hat{A}' = e^{i\alpha\hat{G}}\hat{A}e^{-i\alpha\hat{G}} = \hat{A}. \tag{2.169}$$

In Chapter 3, we will consider some important applications of infinitesimal unitary transformations to study time translations, space translations, space rotations, and conservation laws.

2.5 Representation in Discrete Bases

By analogy with the expansion of Euclidean space vectors in terms of the basis vectors, we need to express any ket $\mid \psi\rangle$ of the Hilbert space in terms of a complete set of mutually orthonormal base kets. State vectors are then represented by their components in this basis.

2.5.1 Matrix Representation of Kets, Bras, and Operators

Consider a discrete, complete, and orthonormal basis which is made of an infinite[4] set of kets $| \phi_1\rangle, | \phi_2\rangle, | \phi_3\rangle, \ldots, | \phi_n\rangle$ and denote it by $\{| \phi_n\rangle\}$. Note that the basis $\{| \phi_n\rangle\}$ is discrete, yet it has an infinite number of unit vectors. In the limit $n \to \infty$, the ordering index n of the unit vectors $| \phi_n\rangle$ is *discrete* or *countable*; that is, the sequence $| \phi_1\rangle, | \phi_2\rangle, | \phi_3\rangle, \ldots$ is countably infinite. As an illustration, consider the special functions, such as the Hermite, Legendre, or Laguerre polynomials, $H_n(x)$, $P_n(x)$, and $L_n(x)$. These polynomials are identified by a discrete index n and by a continuous variable x; although n varies discretely, it can be infinite.

In Section 2.6, we will consider bases that have a continuous and infinite number of base vectors; in these bases the index n increases continuously. Thus, each basis has a continuum of base vectors.

In this section the notation $\{| \phi_n\rangle\}$ will be used to abbreviate an infinitely countable set of vectors (i.e., $| \phi_1\rangle, | \phi_2\rangle, | \phi_3\rangle, \ldots$) of the Hilbert space $\mathcal{H}$. The orthonormality condition of the base kets is expressed by

$$\langle\phi_n \mid \phi_m\rangle = \delta_{nm}, \tag{2.170}$$

where δ_{nm} is the *Kronecker delta* symbol defined by

$$\delta_{nm} = \begin{cases} 1, & n = m, \\ 0, & n \neq m. \end{cases} . \tag{2.171}$$

The completeness, or closure, relation for this basis is given by

$$\sum_{n=1}^{\infty} | \phi_n\rangle\langle\phi_n | = \hat{I}, \tag{2.172}$$

where $\hat{I}$ is the unit operator; when the unit operator acts on any ket, it leaves the ket unchanged.

2.5.1.1 Matrix Representation of Kets and Bras

Let us now examine how to represent the vector $| \psi\rangle$ within the context of the basis $\{| \phi_n\rangle\}$. The completeness property of this basis enables us to expand any state vector $| \psi\rangle$ in terms of the base kets $| \phi_n\rangle$:

$$| \psi\rangle = \hat{I} | \psi\rangle = \left(\sum_{n=1}^{\infty} | \phi_n\rangle\langle\phi_n |\right) | \psi\rangle = \sum_{n=1}^{\infty} a_n | \phi_n\rangle, \tag{2.173}$$

where the coefficient a_n, which is equal to $\langle\phi_n \mid \psi\rangle$, represents the projection of $| \psi\rangle$ onto $| \phi_n\rangle$; a_n is the component of $| \psi\rangle$ along the vector $| \phi_n\rangle$. Recall that the coefficients a_n are complex numbers. So, within the basis $\{| \phi_n\rangle\}$, the ket $| \psi\rangle$ is represented by the set of its components, $a_1, a_2, a_3, \ldots$ along $| \phi_1\rangle, | \phi_2\rangle, | \phi_3\rangle, \ldots$, respectively. Hence $| \psi\rangle$ can be represented by a *column* vector which has a countably infinite number of components:

$$| \psi\rangle \longrightarrow \begin{pmatrix} \langle\phi_1 \mid \psi\rangle \\ \langle\phi_2 \mid \psi\rangle \\ \vdots \\ \langle\phi_n \mid \psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}. \tag{2.174}$$

[4] Kets are elements of the Hilbert space, and the dimension of a Hilbert space is infinite.

The bra $\langle\psi\mid$ can be represented by a *row* vector:

$$\begin{aligned}\langle\psi\mid\longrightarrow & \; (\langle\psi\mid\phi_1\rangle \;\; \langle\psi\mid\phi_2\rangle \;\; \cdots \;\; \langle\psi\mid\phi_n\rangle \;\; \cdots) \\ &= \; (\langle\phi_1\mid\psi\rangle^* \;\; \langle\phi_2\mid\psi\rangle^* \;\; \cdots \;\; \langle\phi_n\mid\psi\rangle^* \;\; \cdots) \\ &= \; (a_1^* \;\; a_2^* \;\; \cdots \;\; a_n^* \;\; \cdots).\end{aligned} \tag{2.175}$$

Using this representation, we see that a bra-ket $\langle\psi\mid\phi\rangle$ is a complex number equal to the matrix product of the row matrix corresponding to the bra $\langle\psi\mid$ with the column matrix corresponding to the ket $\mid\phi\rangle$:

$$\langle\psi\mid\phi\rangle = (a_1^* \;\; a_2^* \;\; \cdots \;\; a_n^* \;\; \cdots)\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \\ \vdots \end{pmatrix} = \sum_n a_n^* b_n, \tag{2.176}$$

where $b_n = \langle\phi_n\mid\phi\rangle$. We see that, within this representation, the matrices representing $\mid\psi\rangle$ and $\langle\psi\mid$ are Hermitian adjoints of each other.

Remark

A ket $|\psi\rangle$ is normalized if $\langle\psi\mid\psi\rangle = \sum_n |a_n|^2 = 1$. If $|\psi\rangle$ is not normalized and we want to normalized it, we need simply to multiply it by a constant α so that $\langle\alpha\psi\mid\alpha\psi\rangle = |\alpha|^2\langle\psi\mid\psi\rangle = 1$, and hence $\alpha = 1/\sqrt{\langle\psi\mid\psi\rangle}$.

Example 2.12

Consider the following two kets:

$$\mid\psi\rangle = \begin{pmatrix} 5i \\ 2 \\ -i \end{pmatrix}, \qquad \mid\phi\rangle = \begin{pmatrix} 3 \\ 8i \\ -9i \end{pmatrix}.$$

(a) Find $\mid\psi\rangle^*$ and $\langle\psi\mid$.
(b) Is $\mid\psi\rangle$ normalized? If not, normalize it.
(c) Are $\mid\psi\rangle$ and $\mid\phi\rangle$ orthogonal?

Solution

(a) The expressions of $\mid\psi\rangle^*$ and $\langle\psi\mid$ are given by

$$\mid\psi\rangle^* = \begin{pmatrix} -5i \\ 2 \\ i \end{pmatrix}, \qquad \langle\psi\mid \; = \; (-5i \quad 2 \quad i), \tag{2.177}$$

where we have used the fact that $\langle\psi\mid$ is equal to the complex conjugate of the transpose of the ket $\mid\psi\rangle$. Hence, we should reiterate the important fact that $\mid\psi\rangle^* \neq \langle\psi\mid$.

(b) The norm of $\mid\psi\rangle$ is given by

$$\langle\psi\mid\psi\rangle = (-5i \quad 2 \quad i)\begin{pmatrix} 5i \\ 2 \\ -i \end{pmatrix} = (-5i)(5i) + (2)(2) + (i)(-i) = 30. \tag{2.178}$$

Thus, $\mid \psi\rangle$ is not normalized. By multiplying it with $1/\sqrt{30}$, it becomes normalized:

$$\mid \chi\rangle = \frac{1}{\sqrt{30}} \mid \psi\rangle = \frac{1}{\sqrt{30}} \begin{pmatrix} 5i \\ 2 \\ -i \end{pmatrix} \qquad \Longrightarrow \qquad \langle \chi \mid \chi\rangle = 1. \tag{2.179}$$

(c) The kets $\mid \psi\rangle$ and $\mid \phi\rangle$ are not orthogonal since their scalar product is not zero:

$$\langle \psi \mid \phi\rangle = (-5i \quad 2 \quad i) \begin{pmatrix} 3 \\ 8i \\ -9i \end{pmatrix} = (-5i)(3) + (2)(8i) + (i)(-9i) = 9 + i. \tag{2.180}$$

2.5.1.2 Matrix Representation of Operators

For each linear operator $\hat{A}$, we can write

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum_{n=1}^{\infty} \mid \phi_n\rangle\langle\phi_n \mid\right)\hat{A}\left(\sum_{m=1}^{\infty} \mid \phi_m\rangle\langle\phi_m \mid\right) = \sum_{nm} A_{nm} \mid \phi_n\rangle\langle\phi_m \mid, \tag{2.181}$$

where A_{nm} is the nm matrix element of the operator $\hat{A}$:

$$A_{nm} = \langle\phi_n \mid \hat{A} \mid \phi_m\rangle. \tag{2.182}$$

We see that the operator $\hat{A}$ is represented, within the basis $\{\mid \phi_n\rangle\}$, by a *square* matrix A (A without a hat designates a matrix), which has a countably infinite number of columns and a countably infinite number of rows:

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{2.183}$$

For instance, the *unit* operator $\hat{I}$ is represented by the unit matrix; when the unit matrix is multiplied with another matrix, it leaves that unchanged:

$$I = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2.184}$$

In summary, *kets are represented by column vectors, bras by row vectors, and operators by square matrices*.

2.5.1.3 Matrix Representation of Some Other Operators

(a) Hermitian adjoint operation

Let us now look at the matrix representation of the Hermitian adjoint operation of an operator. First, recall that the *transpose* of a matrix A, denoted by A^T, is obtained by interchanging the rows with the columns:

$$(A^T)_{nm} = A_{mn} \quad \text{or} \quad \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}^T = \begin{pmatrix} A_{11} & A_{21} & A_{31} & \cdots \\ A_{12} & A_{22} & A_{32} & \cdots \\ A_{13} & A_{23} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2.185}$$

Similarly, the transpose of a column matrix is a row matrix, and the transpose of a row matrix is a column matrix:

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}^T = \begin{pmatrix} a_1 & a_2 & \cdots & a_n & \cdots \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a_1 & a_2 & \cdots & a_n & \cdots \end{pmatrix}^T = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}. \tag{2.186}$$

So a square matrix A is symmetric if it is equal to its transpose, $A^T = A$. A skew-symmetric matrix is a square matrix whose transpose equals the negative of the matrix, $A^T = -A$.

The *complex conjugate* of a matrix is obtained by simply taking the complex conjugate of all its elements: $(A^*)_{nm} = (A_{nm})^*$.

The matrix which represents the operator $\hat{A}^\dagger$ is obtained by taking the complex conjugate of the matrix transpose of A:

$$A^\dagger = (A^T)^* \quad \text{or} \quad (\hat{A}^\dagger)_{nm} = \langle \phi_n \mid \hat{A}^\dagger \mid \phi_m \rangle = \langle \phi_m \mid \hat{A} \mid \phi_n \rangle^* = A^*_{mn}; \tag{2.187}$$

that is,

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}^\dagger = \begin{pmatrix} A^*_{11} & A^*_{21} & A^*_{31} & \cdots \\ A^*_{12} & A^*_{22} & A^*_{32} & \cdots \\ A^*_{13} & A^*_{23} & A^*_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2.188}$$

If an operator $\hat{A}$ is Hermitian, its matrix satisfies this condition:

$$(A^T)^* = A \quad \text{or} \quad A^*_{mn} = A_{nm}. \tag{2.189}$$

The diagonal elements of a Hermitian matrix therefore must be real numbers. Note that *a Hermitian matrix must be square*.

(b) Inverse and unitary operators

A matrix has an inverse only if it is square and its determinant is nonzero; a matrix that has an inverse is called a nonsingular matrix and a matrix that has no inverse is called a singular matrix. The elements A^{-1}_{nm} of the inverse matrix A^{-1}, representing an operator $\hat{A}^{-1}$, are given by the relation

$$A^{-1}_{nm} = \frac{\text{cofactor of } A_{mn}}{\text{determinant of } A} \quad \text{or} \quad A^{-1} = \frac{B^T}{\text{determinant of } A}, \tag{2.190}$$

where B is the matrix of *cofactors* (also called the minor); the cofactor of element A_{mn} is equal to $(-1)^{m+n}$ times the determinant of the submatrix obtained from A by removing the mth row and the nth column. Note that when the matrix, representing an operator, has a determinant equal to zero, this operator does not possess an inverse. Note that $A^{-1}A = AA^{-1} = I$ where I is the unit matrix.

The inverse of a product of matrices is obtained as follows:

$$(ABC \cdots PQ)^{-1} = Q^{-1}P^{-1} \cdots C^{-1}B^{-1}A^{-1}. \tag{2.191}$$

The inverse of the inverse of a matrix is equal to the matrix itself, $\left(A^{-1}\right)^{-1} = A$.

A *unitary* operator $\hat{U}$ is represented by a unitary matrix. A matrix U is said to be unitary if its inverse is equal to its adjoint:

$$U^{-1} = U^{\dagger} \quad \text{or} \quad U^{\dagger}U = I, \tag{2.192}$$

where I is the unit matrix.

Example 2.13 (Inverse of a matrix)

Calculate the inverse of the matrix $A = \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix}$. Is this matrix unitary?

Solution

Since the determinant of A is $\det(A) = -4 + 16i$, we have $A^{-1} = B^T/(-4 + 16i)$, where the elements of the cofactor matrix B are given by $B_{nm} = (-1)^{n+m}$ times the determinant of the submatrix obtained from A by removing the nth row and the mth column. In this way, we have

$$B_{11} = (-1)^{1+1} \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} = (-1)^2 \begin{vmatrix} 1 & 5 \\ -i & -2 \end{vmatrix} = -2 + 5i, \tag{2.193}$$

$$B_{12} = (-1)^{1+2} \begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} = (-1)^3 \begin{vmatrix} 3 & 5 \\ 0 & -2 \end{vmatrix} = 6, \tag{2.194}$$

$$B_{13} = (-1)^{1+3} \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix} = (-1)^4 \begin{vmatrix} 3 & 1 \\ 0 & -i \end{vmatrix} = -3i, \tag{2.195}$$

$$B_{21} = (-1)^3 \begin{vmatrix} i & 0 \\ -i & -2 \end{vmatrix} = 2i, \qquad B_{22} = (-1)^4 \begin{vmatrix} 2 & 0 \\ 0 & -2 \end{vmatrix} = -4, \tag{2.196}$$

$$B_{23} = (-1)^5 \begin{vmatrix} 2 & i \\ 0 & -i \end{vmatrix} = 2i, \qquad B_{31} = (-1)^4 \begin{vmatrix} i & 0 \\ 1 & 5 \end{vmatrix} = 5i, \tag{2.197}$$

$$B_{32} = (-1)^5 \begin{vmatrix} 2 & 0 \\ 3 & 5 \end{vmatrix} = -10, \qquad B_{33} = (-1)^6 \begin{vmatrix} 2 & i \\ 3 & 1 \end{vmatrix} = 2 - 3i, \tag{2.198}$$

and hence

$$B = \begin{pmatrix} -2+5i & 6 & -3i \\ 2i & -4 & 2i \\ 5i & -10 & 2-3i \end{pmatrix}. \tag{2.199}$$

Taking the transpose of B, we obtain

$$\begin{aligned} A^{-1} &= \frac{1}{-4+16i} B^T = \frac{-1-4i}{68} \begin{pmatrix} -2+5i & 2i & 5i \\ 6 & -4 & -10 \\ -3i & 2i & 2-3i \end{pmatrix} \\ &= \frac{1}{68} \begin{pmatrix} 22+3i & 8-2i & 20-5i \\ -6-24i & 4+16i & 10+40i \\ -12+3i & 8-2i & -14-5i \end{pmatrix}. \end{aligned} \tag{2.200}$$

Clearly, this matrix is not unitary since its inverse is not equal to its Hermitian adjoint: $A^{-1} \neq A^{\dagger}$.

(c) Matrix representation of $\mid \psi\rangle\langle\psi \mid$

It is now easy to see that the product $\mid \psi\rangle\langle\psi \mid$ is indeed an operator, since its representation within $\{\mid \phi_n\rangle\}$ is a square matrix:

$$\mid \psi\rangle\langle\psi \mid = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} (a_1^* \quad a_2^* \quad a_3^* \quad \cdots) = \begin{pmatrix} a_1a_1^* & a_1a_2^* & a_1a_3^* & \cdots \\ a_2a_1^* & a_2a_2^* & a_2a_3^* & \cdots \\ a_3a_1^* & a_3a_2^* & a_3a_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2.201}$$

(d) Trace of an operator

The trace $\text{Tr}(\hat{A})$ of an operator $\hat{A}$ is given, within an orthonormal basis $\{\mid \phi_n\rangle\}$, by the expression

$$\text{Tr}(\hat{A}) = \sum_n \langle\phi_n \mid \hat{A} \mid \phi_n\rangle = \sum_n A_{nn}; \tag{2.202}$$

we will see later that the trace of an operator does not depend on the basis. The trace of a matrix is equal to the sum of its diagonal elements:

$$\text{Tr} \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = A_{11} + A_{22} + A_{33} + \cdots. \tag{2.203}$$

Properties of the trace

We can ascertain that

$$\text{Tr}(\hat{A}^{\dagger}) = (\text{Tr}(\hat{A}))^*, \tag{2.204}$$

$$\text{Tr}(\alpha\hat{A} + \beta\hat{B} + \gamma\hat{C} + \cdots) = \alpha\text{Tr}(\hat{A}) + \beta\text{Tr}(\hat{B}) + \gamma\text{Tr}(\hat{C}) + \cdots, \tag{2.205}$$

and the trace of a product of operators is invariant under the cyclic permutations of these operators:

$$\text{Tr}(\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}) = \text{Tr}(\hat{E}\hat{A}\hat{B}\hat{C}\hat{D}) = \text{Tr}(\hat{D}\hat{E}\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{D}\hat{E}\hat{A}\hat{B}) = \cdots. \tag{2.206}$$

Example 2.14

(a) Show that $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.

(b) Show that the trace of a commutator is always zero.

(c) Illustrate the results shown in (a) and (b) on the following matrices:

$$A = \begin{pmatrix} 8-2i & 4i & 0 \\ 1 & 0 & 1-i \\ -8 & i & 6i \end{pmatrix}, \qquad B = \begin{pmatrix} -i & 2 & 1-i \\ 6 & 1+i & 3i \\ 1 & 5+7i & 0 \end{pmatrix}.$$

Solution

(a) Using the definition of the trace,

$$\mathrm{Tr}(\hat{A}\hat{B}) = \sum_n \langle \phi_n \mid \hat{A}\hat{B} \mid \phi_n \rangle, \tag{2.207}$$

and inserting the unit operator between $\hat{A}$ and $\hat{B}$ we have

$$\begin{aligned} \mathrm{Tr}(\hat{A}\hat{B}) &= \sum_n \langle \phi_n \mid \hat{A}\left(\sum_m \mid \phi_m\rangle\langle\phi_m \mid\right)\hat{B} \mid \phi_n\rangle = \sum_{nm} \langle \phi_n \mid \hat{A} \mid \phi_m\rangle\langle\phi_m \mid \hat{B} \mid \phi_n\rangle \\ &= \sum_{nm} A_{nm} B_{mn}. \end{aligned} \tag{2.208}$$

On the other hand, since $\mathrm{Tr}(\hat{A}\hat{B}) = \sum_n \langle \phi_n \mid \hat{A}\hat{B} \mid \phi_n\rangle$, we have

$$\begin{aligned} \mathrm{Tr}(\hat{B}\hat{A}) &= \sum_m \langle \phi_m \mid \hat{B}\left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right)\hat{A} \mid \phi_m\rangle = \sum_{m} \langle \phi_m \mid \hat{B} \mid \phi_n\rangle\langle\phi_n \mid \hat{A} \mid \phi_m\rangle \\ &= \sum_{nm} B_{mn} A_{nm}. \end{aligned} \tag{2.209}$$

Comparing (2.208) and (2.209), we see that $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.

(b) Since $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$ we can infer at once that the trace of any commutator is always zero:

$$\mathrm{Tr}([\hat{A},\ \hat{B}]) = \mathrm{Tr}(\hat{A}\hat{B}) - \mathrm{Tr}(\hat{B}\hat{A}) = 0. \tag{2.210}$$

(c) Let us verify that the traces of the products AB and BA are equal. Since

$$AB = \begin{pmatrix} -2+16i & 12 & -6-10i \\ 1-2i & 14+2i & 1-i \\ 20i & -59+31i & -11+8i \end{pmatrix}, \quad BA = \begin{pmatrix} -8 & 5+i & 8+4i \\ 49-35i & -3+24i & -16 \\ 13+5i & 4i & 12+2i \end{pmatrix}, \tag{2.211}$$

we have

$$\mathrm{Tr}(AB) = \mathrm{Tr}\begin{pmatrix} -2+16i & 12 & -6-10i \\ 1-2i & 14+2i & 1-i \\ 20i & -59+31i & -11+8i \end{pmatrix} = 1+26i, \tag{2.212}$$

$$\mathrm{Tr}(BA) = \mathrm{Tr}\begin{pmatrix} -8 & 5+i & 8+4i \\ 49-35i & -3+24i & -16 \\ 13+5i & 4i & 12+2i \end{pmatrix} = 1+26i = \mathrm{Tr}(AB). \tag{2.213}$$

This leads to $\mathrm{Tr}(AB) - \mathrm{Tr}(BA) = (1+26i) - (1+26i) = 0$ or $\mathrm{Tr}([A,\ B]) = 0$.

2.5.1.4 Matrix Representation of Several Other Quantities

(a) Matrix representation of $|\,\phi\rangle = \hat{A}\,|\,\psi\rangle$
The relation $|\,\phi\rangle = \hat{A}\,|\,\psi\rangle$ can be cast into the algebraic form $\hat{I}\,|\,\phi\rangle = \hat{I}\hat{A}\hat{I}\,|\,\psi\rangle$ or

$$\left(\sum_n |\,\phi_n\rangle\langle\phi_n\,|\right)|\,\phi\rangle = \left(\sum_n |\,\phi_n\rangle\langle\phi_n\,|\right)\hat{A}\left(\sum_m |\,\phi_m\rangle\langle\phi_m\,|\right)|\,\psi\rangle, \tag{2.214}$$

which in turn can be written as

$$\sum_n b_n\,|\,\phi_n\rangle = \sum_{nm} a_m\,|\,\phi_n\rangle\langle\phi_n\,|\,\hat{A}\,|\,\phi_m\rangle = \sum_{nm} a_m A_{nm}\,|\,\phi_n\rangle, \tag{2.215}$$

where $b_n = \langle\phi_n\,|\,\phi\rangle$, $A_{nm} = \langle\phi_n\,|\,\hat{A}\,|\,\phi_m\rangle$, and $a_m = \langle\phi_m\,|\,\psi\rangle$. It is easy to see that (2.215) yields $b_n = \sum_m A_{nm}a_m$; hence the matrix representation of $|\,\phi\rangle = \hat{A}\,|\,\psi\rangle$ is given by

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}. \tag{2.216}$$

(b) Matrix representation of $\langle\phi\,|\,\hat{A}\,|\,\psi\rangle$
As for $\langle\phi\,|\,\hat{A}\,|\,\psi\rangle$ we have

$$\begin{aligned}\langle\phi\,|\,\hat{A}\,|\,\psi\rangle &= \langle\phi\,|\,\hat{I}\hat{A}\hat{I}\,|\,\psi\rangle = \langle\phi\,|\left(\sum_{n=1}^{\infty} |\,\phi_n\rangle\langle\phi_n\,|\right)\hat{A}\left(\sum_{m=1}^{\infty} |\,\phi_m\rangle\langle\phi_m\,|\right)|\,\psi\rangle \\ &= \sum_{nm}\langle\phi\,|\,\phi_n\rangle\langle\phi_n\,|\,\hat{A}\,|\,\phi_m\rangle\langle\phi_m\,|\,\psi\rangle \\ &= \sum_{nm} b_n^* A_{nm} a_m. \end{aligned} \tag{2.217}$$

This is a complex number; its matrix representation goes as follows:

$$\langle\phi\,|\,\hat{A}\,|\,\psi\rangle \longrightarrow (b_1^* \quad b_2^* \quad b_3^* \quad \cdots)\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}. \tag{2.218}$$

Remark
It is now easy to see explicitly why products of the type $|\,\psi\rangle\,|\,\phi\rangle$, $\langle\psi\,|\,\langle\phi\,|$, $\hat{A}\langle\psi\,|$, or $|\,\psi\rangle\hat{A}$ are forbidden. They cannot have matrix representations; they are nonsensical. For instance, $|\,\psi\rangle\,|\,\phi\rangle$ is represented by the product of two column matrices:

$$|\,\psi\rangle\,|\,\phi\rangle \longrightarrow \begin{pmatrix} \langle\phi_1\,|\,\psi\rangle \\ \langle\phi_2\,|\,\psi\rangle \\ \vdots \end{pmatrix}\begin{pmatrix} \langle\phi_1\,|\,\phi\rangle \\ \langle\phi_2\,|\,\phi\rangle \\ \vdots \end{pmatrix}. \tag{2.219}$$

This product is clearly not possible to perform, for the product of two matrices is possible only when the number of columns of the first is equal to the number of rows of the second; in (2.219) the first matrix has one single column and the second an infinite number of rows.

2.5.1.5 Properties of a Matrix A

- Real if $A = A^*$ or $A_{mn} = A^*_{mn}$
- Imaginary if $A = -A^*$ or $A_{mn} = -A^*_{mn}$
- Symmetric if $A = A^T$ or $A_{mn} = A_{nm}$
- Antisymmetric if $A = -A^T$ or $A_{mn} = -A_{nm}$ with $A_{mm} = 0$
- Hermitian if $A = A^\dagger$ or $A_{mn} = A^*_{nm}$
- Anti-Hermitian if $A = -A^\dagger$ or $A_{mn} = -A^*_{nm}$
- Orthogonal if $A^T = A^{-1}$ or $AA^T = I$ or $(AA^T)_{mn} = \delta_{mn}$
- Unitary if $A^\dagger = A^{-1}$ or $AA^\dagger = I$ or $(AA^\dagger)_{mn} = \delta_{mn}$

Example 2.15
Consider a matrix A (which represents an operator $\hat{A}$), a ket $\mid \psi\rangle$, and a bra $\langle \phi \mid$:

$$A = \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix}, \quad \mid \psi\rangle = \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix}, \quad \langle\phi\mid = \begin{pmatrix} 6 & -i & 5 \end{pmatrix}.$$

(a) Calculate the quantities $A \mid \psi\rangle$, $\langle\phi \mid A$, $\langle\phi \mid A \mid \psi\rangle$, and $\mid \psi\rangle\langle\phi \mid$.

(b) Find the complex conjugate, the transpose, and the Hermitian conjugate of A, $\mid \psi\rangle$, and $\langle\phi \mid$.

(c) Calculate $\langle\phi \mid \psi\rangle$ and $\langle\psi \mid \phi\rangle$; are they equal? Comment on the differences between the complex conjugate, Hermitian conjugate, and transpose of kets and bras.

Solution

(a) The calculations are straightforward:

$$A \mid \psi\rangle = \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix} \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = \begin{pmatrix} -5+17i \\ 17+34i \\ 11+14i \end{pmatrix}, \tag{2.220}$$

$$\langle\phi \mid A = \begin{pmatrix} 6 & -i & 5 \end{pmatrix} \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix} = \begin{pmatrix} 34-5i & 26+12i & 20+10i \end{pmatrix}, \tag{2.221}$$

$$\langle\phi \mid A \mid \psi\rangle = \begin{pmatrix} 6 & -i & 5 \end{pmatrix} \begin{pmatrix} 5 & 3+2i & 3i \\ -i & 3i & 8 \\ 1-i & 1 & 4 \end{pmatrix} \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = 59+155i, \tag{2.222}$$

$$\mid \psi\rangle\langle\phi \mid = \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} \begin{pmatrix} 6 & -i & 5 \end{pmatrix} = \begin{pmatrix} -6+6i & 1+i & -5+5i \\ 18 & -3i & 15 \\ 12+18i & 3-2i & 10+15i \end{pmatrix}. \tag{2.223}$$

(b) To obtain the complex conjugate of A, $\mid \psi\rangle$, and $\langle\phi \mid$, we need simply to take the complex conjugate of their elements:

$$A^* = \begin{pmatrix} 5 & 3-2i & -3i \\ i & -3i & 8 \\ 1+i & 1 & 4 \end{pmatrix}, \quad \mid \psi\rangle^* = \begin{pmatrix} -1-i \\ 3 \\ 2-3i \end{pmatrix}, \quad \langle\phi \mid^* = \begin{pmatrix} 6 & i & 5 \end{pmatrix}. \tag{2.224}$$

For the transpose of A, $\mid \psi\rangle$, and $\langle\phi \mid$, we simply interchange columns with rows:

$$A^T = \begin{pmatrix} 5 & -i & 1-i \\ 3+2i & 3i & 1 \\ 3i & 8 & 4 \end{pmatrix}, \quad \mid \psi\rangle^T = \begin{pmatrix} -1+i & 3 & 2+3i \end{pmatrix}, \quad \langle\phi \mid^T = \begin{pmatrix} 6 \\ -i \\ 5 \end{pmatrix}. \tag{2.225}$$

The Hermitian conjugate can be obtained by taking the complex conjugates of the transpose expressions calculated above: $A^\dagger = (A^T)^*$, $\mid \psi\rangle^\dagger = \left(\mid \psi\rangle^T\right)^* = \langle\psi \mid$, $\langle\phi \mid^\dagger = \left(\langle\phi \mid^T\right)^* = \mid \phi\rangle$:

$$A^\dagger = \begin{pmatrix} 5 & i & 1+i \\ 3-2i & -3i & 1 \\ -3i & 8 & 4 \end{pmatrix}, \quad \langle\psi \mid = \begin{pmatrix} -1-i & 3 & 2-3i \end{pmatrix}, \quad \mid \phi\rangle = \begin{pmatrix} 6 \\ i \\ 5 \end{pmatrix}. \tag{2.226}$$

(c) Using the kets and bras above, we can easily calculate the needed scalar products:

$$\langle\phi \mid \psi\rangle = \begin{pmatrix} 6 & -i & 5 \end{pmatrix} \begin{pmatrix} -1+i \\ 3 \\ 2+3i \end{pmatrix} = 6(-1+i)+(-i)(3)+5(2+3i) = 4+18i, \tag{2.227}$$

$$\langle\psi \mid \phi\rangle = \begin{pmatrix} -1-i & 3 & 2-3i \end{pmatrix} \begin{pmatrix} 6 \\ i \\ 5 \end{pmatrix} = 6(-1-i)+(i)(3)+5(2-3i) = 4-18i. \tag{2.228}$$

We see that $\langle\phi \mid \psi\rangle$ and $\langle\psi \mid \phi\rangle$ are not equal; they are complex conjugates of each other:

$$\langle\psi \mid \phi\rangle = \langle\phi \mid \psi\rangle^* = 4-18i. \tag{2.229}$$

Remark

We should underscore the importance of the differences between $\mid \psi\rangle^*$, $\mid \psi\rangle^T$, and $\mid \psi\rangle^\dagger$. Most notably, we should note (from equations (2.224)–(2.226)) that $\mid \psi\rangle^*$ is a ket, while $\mid \psi\rangle^T$ and $\mid \psi\rangle^\dagger$ are bras. Additionally, we should note that $\langle\phi \mid^*$ is a bra, while $\langle\phi \mid^T$ and $\langle\phi \mid^\dagger$ are kets.

2.5.2 Change of Bases and Unitary Transformations

In a Euclidean space, a vector $\vec{A}$ may be represented by its components in different coordinate systems or in different bases. The transformation from one basis to the other is called a change of basis. The components of $\vec{A}$ in a given basis can be expressed in terms of the components of $\vec{A}$ in another basis by means of a *transformation* matrix.

Similarly, state vectors and operators of quantum mechanics may also be represented in different bases. In this section we are going to study how to transform from one basis to another. That is, knowing the components of kets, bras, and operators in a basis $\{\mid \phi_n\rangle\}$, how does one determine the corresponding components in a different basis $\{| \phi'_n\rangle\}$? Assuming that $\{| \phi_n\rangle\}$ and $\{| \phi'_n\rangle\}$ are two different bases, we can expand each ket $| \phi_n\rangle$ of the old basis in terms of the new basis $\{| \phi'_n\rangle\}$ as follows:

$$| \phi_n\rangle = \left(\sum_m | \phi'_m\rangle\langle\phi'_m |\right) | \phi_n\rangle = \sum_m U_{mn} | \phi'_m\rangle, \tag{2.230}$$

where

$$U_{mn} = \langle\phi'_m | \phi_n\rangle. \tag{2.231}$$

The matrix U, providing the transformation from the old basis $\{| \phi_n\rangle\}$ to the new basis $\{| \phi'_n\rangle\}$, is given by

$$U = \begin{pmatrix} \langle\phi'_1 | \phi_1\rangle & \langle\phi'_1 | \phi_2\rangle & \langle\phi'_1 | \phi_3\rangle \\ \langle\phi'_2 | \phi_1\rangle & \langle\phi'_2 | \phi_2\rangle & \langle\phi'_2 | \phi_3\rangle \\ \langle\phi'_3 | \phi_1\rangle & \langle\phi'_3 | \phi_2\rangle & \langle\phi'_3 | \phi_3\rangle \end{pmatrix}. \tag{2.232}$$

Example 2.16 (Unitarity of the transformation matrix)
Let U be a transformation matrix which connects two *complete* and *orthonormal* bases $\{| \phi_n\rangle\}$ and $\{| \phi'_n\rangle\}$. Show that U is *unitary*.

Solution
For this we need to prove that $\hat{U}\hat{U}^\dagger = \hat{I}$, which reduces to showing that $\langle\phi_m | \hat{U}\hat{U}^\dagger | \phi_n\rangle = \delta_{mn}$. This goes as follows:

$$\langle\phi_m | \hat{U}\hat{U}^\dagger | \phi_n\rangle = \langle\phi_m | \hat{U}\left(\sum_l | \phi_l\rangle\langle\phi_l |\right)\hat{U}^\dagger | \phi_n\rangle = \sum_l U_{ml}U^*_{nl}, \tag{2.233}$$

where $U_{ml} = \langle\phi_m | \hat{U} | \phi_l\rangle$ and $U^*_{nl} = \langle\phi_l | \hat{U}^\dagger | \phi_n\rangle = \langle\phi_n | \hat{U} | \phi_l\rangle^*$. According to (2.231), $U_{ml} = \langle\phi'_m | \phi_l\rangle$ and $U^*_{nl} = \langle\phi_l | \phi'_n\rangle$; we can thus rewrite (2.233) as

$$\sum_l U_{ml}U^*_{nl} = \sum_l \langle\phi'_m | \phi_l\rangle\langle\phi_l | \phi'_n\rangle = \langle\phi'_m | \phi'_n\rangle = \delta_{mn}. \tag{2.234}$$

Combining (2.233) and (2.234), we infer $\langle\phi_m | \hat{U}\hat{U}^\dagger | \phi_n\rangle = \delta_{mn}$, or $\hat{U}\hat{U}^\dagger = \hat{I}$.

2.5.2.1 Transformations of Kets, Bras, and Operators

The components $\langle\phi'_n | \psi\rangle$ of a state vector $| \psi\rangle$ in a new basis $\{| \phi'_n\rangle\}$ can be expressed in terms of the components $\langle\phi_n | \psi\rangle$ of $| \psi\rangle$ in an old basis $\{| \phi_n\rangle\}$ as follows:

$$\langle\phi'_m | \psi\rangle = \langle\phi'_m | \hat{I} | \psi\rangle = \langle\phi'_m | \left(\sum_n | \phi_n\rangle\langle\phi_n |\right) | \psi\rangle = \sum_n U_{mn}\langle\phi_n | \psi\rangle. \tag{2.235}$$

This relation, along with its complex conjugate, can be generalized into

$$| \psi_{new}\rangle = \hat{U} | \psi_{old}\rangle, \qquad \langle\psi_{new} | = \langle\psi_{old} | \hat{U}^\dagger. \tag{2.236}$$

Let us now examine how operators transform when we change from one basis to another. The matrix elements $A'_{mn} = \langle \phi'_m \mid \hat{A} \mid \phi'_n \rangle$ of an operator $\hat{A}$ in the new basis can be expressed in terms of the old matrix elements, $A_{jl} = \langle \phi_j \mid \hat{A} \mid \phi_l \rangle$, as follows:

$$A'_{mn} = \langle \phi'_m \mid \left(\sum_j \mid \phi_j \rangle \langle \phi_j \mid \right) \hat{A} \left(\sum_l \mid \phi_l \rangle \langle \phi_l \mid \right) \mid \phi'_n \rangle = \sum_{jl} U_{mj} A_{jl} U^*_{nl}; \qquad (2.237)$$

that is,

$$\hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^\dagger \qquad \text{or} \qquad \hat{A}_{old} = \hat{U}^\dagger \hat{A}_{new} \hat{U}. \qquad (2.238)$$

We may summarize the results of the change of basis in the following relations:

$$\boxed{\mid \psi_{new} \rangle = \hat{U} \mid \psi_{old} \rangle, \qquad \langle \psi_{new} \mid = \langle \psi_{old} \mid \hat{U}^\dagger, \qquad \hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^\dagger,} \qquad (2.239)$$

or

$$\boxed{\mid \psi_{old} \rangle = \hat{U}^\dagger \mid \psi_{new} \rangle, \qquad \langle \psi_{old} \mid = \langle \psi_{new} \mid \hat{U}, \qquad \hat{A}_{old} = \hat{U}^\dagger \hat{A}_{new} \hat{U}.} \qquad (2.240)$$

These relations are similar to the ones we derived when we studied unitary transformations; see (2.146) and (2.147).

Example 2.17
Show that the operator $\hat{U} = \sum_n \mid \phi'_n \rangle \langle \phi_n \mid$ satisfies all the properties discussed above.

Solution
First, note that $\hat{U}$ is unitary:

$$\hat{U}\hat{U}^\dagger = \sum_{nl} \mid \phi'_n \rangle \langle \phi_n \mid \phi_l \rangle \langle \phi'_l \mid = \sum_{nl} \mid \phi'_n \rangle \langle \phi'_l \mid \delta_{nl} = \sum_n \mid \phi'_n \rangle \langle \phi'_n \mid = \hat{I}. \qquad (2.241)$$

Second, the action of $\hat{U}$ on a ket of the old basis gives the corresponding ket from the new basis:

$$\hat{U} \mid \phi_m \rangle = \sum_n \mid \phi'_n \rangle \langle \phi_n \mid \phi_m \rangle = \sum_n \mid \phi'_n \rangle \delta_{nm} = \mid \phi'_m \rangle. \qquad (2.242)$$

We can also verify that the action $\hat{U}^\dagger$ on a ket of the new basis gives the corresponding ket from the old basis:

$$\hat{U}^\dagger \mid \phi'_m \rangle = \sum_l \mid \phi_l \rangle \langle \phi'_l \mid \phi'_m \rangle = \sum_l \mid \phi_l \rangle \delta_{lm} = \mid \phi_m \rangle. \qquad (2.243)$$

How does a trace transform under unitary transformations? Using the cyclic property of the trace, $\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{C}\hat{A})$, we can ascertain that

$$\text{Tr}(\hat{A}') = \text{Tr}(\hat{U}\hat{A}\hat{U}^\dagger) = \text{Tr}(\hat{U}^\dagger\hat{U}\hat{A}) = \text{Tr}(\hat{A}), \qquad (2.244)$$

$$\begin{aligned}\mathrm{Tr}\left(\mid \phi_n\rangle\langle\phi_m \mid\right) &= \sum_l \langle\phi_l \mid \phi_n\rangle\langle\phi_m \mid \phi_l\rangle = \sum_l \langle\phi_m \mid \phi_l\rangle\langle\phi_l \mid \phi_n\rangle \\ &= \langle\phi_m \mid \left(\sum_l \mid \phi_l\rangle\langle\phi_l \mid\right) \mid \phi_n\rangle = \langle\phi_m \mid \phi_n\rangle = \delta_{mn}, \end{aligned} \tag{2.245}$$

$$\mathrm{Tr}\left(\mid \phi'_m\rangle\langle\phi_n \mid\right) = \langle\phi_n \mid \phi'_m\rangle. \tag{2.246}$$

Example 2.18 (The trace is base independent)
Show that the trace of an operator does not depend on the basis in which it is expressed.

Solution
Let us show that the trace of an operator $\hat{A}$ in a basis $\{\mid \phi_n\rangle\}$ is equal to its trace in another basis $\{\mid \phi'_n\rangle\}$. First, the trace of $\hat{A}$ in the basis $\{\mid \phi_n\rangle\}$ is given by

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle\phi_n \mid \hat{A} \mid \phi_n\rangle \tag{2.247}$$

and in $\{\mid \phi'_n\rangle\}$ by

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle\phi'_n \mid \hat{A} \mid \phi'_n\rangle. \tag{2.248}$$

Starting from (2.247) and using the completeness of the other basis, $\{\mid \phi'_n\rangle\}$, we have

$$\begin{aligned}\mathrm{Tr}(\hat{A}) &= \sum_n \langle\phi_n \mid \hat{A} \mid \phi_n\rangle = \sum_n \langle\phi_n \mid \left(\sum_m \mid \phi'_m\rangle\langle\phi'_m \mid\right) \hat{A} \mid \phi_n\rangle \\ &= \sum_{nm} \langle\phi_n \mid \phi'_m\rangle\langle\phi'_m \mid \hat{A} \mid \phi_n\rangle. \end{aligned} \tag{2.249}$$

All we need to do now is simply to interchange the positions of the numbers (scalars) $\langle\phi_n \mid \phi'_m\rangle$ and $\langle\phi'_m \mid \hat{A} \mid \phi_n\rangle$:

$$\mathrm{Tr}(\hat{A}) = \sum_m \langle\phi'_m \mid \hat{A} \left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right) \mid \phi'_m\rangle = \sum_m \langle\phi'_m \mid \hat{A} \mid \phi'_m\rangle. \tag{2.250}$$

From (2.249) and (2.250) we see that

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle\phi_n \mid \hat{A} \mid \phi_n\rangle = \sum_n \langle\phi'_n \mid \hat{A} \mid \phi'_n\rangle. \tag{2.251}$$

2.5.3 Matrix Representation of the Eigenvalue Problem

At issue here is to work out the matrix representation of the eigenvalue problem (2.126) and then solve it. That is, we want to find the eigenvalues a and the eigenvectors $\mid \psi\rangle$ of an operator $\hat{A}$ such that

$$\hat{A} \mid \psi\rangle = a \mid \psi\rangle, \tag{2.252}$$

where a is a complex number. Inserting the unit operator between $\hat{A}$ and $\mid \psi\rangle$ and multiplying by $\langle\phi_m \mid$, we can cast the eigenvalue equation in the form

$$\langle\phi_m \mid \hat{A}\left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right)\mid \psi\rangle \;=\; a\langle\phi_m \mid\left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right)\mid \psi\rangle, \tag{2.253}$$

or

$$\sum_n A_{mn}\langle\phi_n \mid \psi\rangle \;=\; a\sum_n\langle\phi_n \mid \psi\rangle\delta_{nm}, \tag{2.254}$$

which can be rewritten as

$$\sum_n \left[A_{mn} - a\delta_{nm}\right]\langle\phi_n \mid \psi\rangle = 0, \tag{2.255}$$

with $A_{mn} \;=\; \langle\phi_m \mid \hat{A} \mid \phi_n\rangle$.

This equation represents an infinite, homogeneous system of equations for the coefficients $\langle\phi_n \mid \psi\rangle$, since the basis $\{\mid \phi_n\rangle\}$ is made of an infinite number of base kets. This system of equations can have nonzero solutions only if its determinant vanishes:

$$\det\left(A_{mn} - a\delta_{nm}\right) = 0. \tag{2.256}$$

The problem that arises here is that this determinant corresponds to a matrix with an infinite number of columns and rows. To solve (2.256) we need to truncate the basis $\{\mid \phi_n\rangle\}$ and assume that it contains only N terms, where N must be large enough to guarantee convergence. In this case we can reduce (2.256) to the following Nth degree determinant:

$$\begin{vmatrix} A_{11}-a & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22}-a & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33}-a & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN}-a \end{vmatrix} = 0. \tag{2.257}$$

This is known as the *secular* or *characteristic equation*. The solutions of this equation yield the N *eigenvalues* $a_1, a_2, a_3, \ldots, a_N$, since it is an Nth order equation in a. The set of these N eigenvalues is called the spectrum of $\hat{A}$. Knowing the set of eigenvalues $a_1, a_2, a_3, \ldots, a_N$, we can easily determine the corresponding set of *eigenvectors* $\mid \phi_1\rangle, \mid \phi_2\rangle, \ldots, \mid \phi_N\rangle$. For each eigenvalue a_m of $\hat{A}$, we can obtain from the "secular" equation (2.257) the N components $\langle\phi_1 \mid \psi\rangle, \langle\phi_2 \mid \psi\rangle, \langle\phi_3 \mid \psi\rangle, \ldots, \langle\phi_N \mid \psi\rangle$ of the corresponding eigenvector $\mid \phi_m\rangle$.

If a number of different eigenvectors (two or more) have the same eigenvalue, this eigenvalue is said to be *degenerate*. The order of degeneracy is determined by the number of linearly independent eigenvectors that have the same eigenvalue. For instance, if an eigenvalue has five different eigenvectors, it is said to be fivefold degenerate.

In the case where the set of eigenvectors $\mid \phi_n\rangle$ of $\hat{A}$ is complete and orthonormal, this set can be used as a basis. In this basis the matrix representing the operator $\hat{A}$ is diagonal,

$$A = \begin{pmatrix} a_1 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & \cdots \\ 0 & 0 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{2.258}$$

the diagonal elements being the eigenvalues a_n of $\hat{A}$, since

$$\langle \phi_m \mid \hat{A} \mid \phi_n \rangle = a_n \langle \phi_m \mid \phi_n \rangle = a_n \delta_{mn}. \tag{2.259}$$

Note that the trace and determinant of a matrix are given, respectively, by the sum and product of the *eigenvalues*:

$$\mathrm{Tr}(A) = \sum_n a_n = a_1 + a_2 + a_3 + \cdots, \tag{2.260}$$

$$\det(A) = \prod_n a_n = a_1 a_2 a_3 \cdots. \tag{2.261}$$

Properties of determinants
Let us mention several useful properties that pertain to determinants. The determinant of a product of matrices is equal to the product of their determinants:

$$\det(ABCD\cdots) = \det(A)\cdot\det(B)\cdot\det(C)\cdot\det(D)\cdots, \tag{2.262}$$

$$\det(A^*) = (\det(A))^*, \qquad \det(A^\dagger) = (\det(A))^*, \tag{2.263}$$

$$\det(A^T) = \det(A), \qquad \det(A) = e^{\mathrm{Tr}(\ln A)}. \tag{2.264}$$

Some theorems pertaining to the eigenvalue problem
Here is a list of useful theorems (the proofs are left as exercises):

- The eigenvalues of a symmetric matrix are real; the eigenvectors form an orthonormal basis.
- The eigenvalues of an antisymmetric matrix are purely imaginary or zero.
- The eigenvalues of a Hermitian matrix are real; the eigenvectors form an orthonormal basis.
- The eigenvalues of a skew-Hermitian matrix are purely imaginary or zero.
- The eigenvalues of a unitary matrix have absolute value equal to one.
- If the eigenvalues of a square matrix are not degenerate (distinct), the corresponding eigenvectors form a basis (i.e., they form a linearly independent set).

Example 2.19 (Eigenvalues and eigenvectors of a matrix)
Find the eigenvalues and the normalized eigenvectors of the matrix

$$A = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}.$$

Solution

To find the eigenvalues of A, we simply need to solve the secular equation $\det(A - aI) = 0$:

$$0 = \begin{vmatrix} 7-a & 0 & 0 \\ 0 & 1-a & -i \\ 0 & i & -1-a \end{vmatrix} = (7-a)\left[-(1-a)(1+a)+i^2\right] = (7-a)(a^2-2). \tag{2.265}$$

The eigenvalues of A are thus given by

$$a_1 = 7, \quad a_2 = \sqrt{2}, \quad a_3 = -\sqrt{2}. \tag{2.266}$$

Let us now calculate the eigenvectors of A. To find the eigenvector corresponding to the first eigenvalue, $a_1 = 7$, we need to solve the matrix equation

$$\begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 7 \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Longrightarrow \begin{array}{rcl} 7x & = & 7x \\ y - iz & = & 7y \\ iy - z & = & 7z \end{array} ; \tag{2.267}$$

this yields $x = 1$ (because the eigenvector is normalized) and $y = z = 0$. So the eigenvector corresponding to $a_1 = 7$ is given by the column matrix

$$|\, a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{2.268}$$

This eigenvector is normalized since $\langle a_1 \mid a_1\rangle = 1$.

The eigenvector corresponding to the second eigenvalue, $a_2 = \sqrt{2}$, can be obtained from the matrix equation

$$\begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{2} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Longrightarrow \begin{array}{rcl} (7-\sqrt{2})x & = & 0 \\ (1-\sqrt{2})y - iz & = & 0 \\ iy - (1+\sqrt{2})z & = & 0 \end{array} ; \tag{2.269}$$

this yields $x = 0$ and $z = i(\sqrt{2}-1)y$. So the eigenvector corresponding to $a_2 = \sqrt{2}$ is given by the column matrix

$$|\, a_2\rangle = \begin{pmatrix} 0 \\ y \\ i(\sqrt{2}-1)y \end{pmatrix}. \tag{2.270}$$

The value of the variable y can be obtained from the normalization condition of $|\, a_2\rangle$:

$$1 = \langle a_2 \mid a_2\rangle = \begin{pmatrix} 0 & y^* & -i(\sqrt{2}-1)y^* \end{pmatrix} \begin{pmatrix} 0 \\ y \\ i(\sqrt{2}-1)y \end{pmatrix} = 2(2-\sqrt{2}) \mid y \mid^2 . \tag{2.271}$$

Taking only the positive value of y (a similar calculation can be performed easily if one is interested in the negative value of y), we have $y = 1/\sqrt{2(2-\sqrt{2})}$; hence the eigenvector (2.270) becomes

$$|\, a_2\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2(2-\sqrt{2})}} \\ \frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} \end{pmatrix}. \tag{2.272}$$

Following the same procedure that led to (2.272), we can show that the third eigenvector is given by

$$| a_3\rangle = \begin{pmatrix} 0 \\ y \\ -i(1+\sqrt{2})y \end{pmatrix}; \tag{2.273}$$

its normalization leads to $y = 1/\sqrt{2(2+\sqrt{2})}$ (we have considered only the positive value of y); hence

$$| a_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2(2+\sqrt{2})}} \\ -\frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix}. \tag{2.274}$$

2.6 Representation in Continuous Bases

In this section we are going to consider the representation of state vectors, bras, and operators in *continuous* bases. After presenting the general formalism, we will consider two important applications: representations in the *position* and *momentum* spaces.

In the previous section we saw that the representations of kets, bras, and operators in a discrete basis are given by discrete matrices. We will show here that these quantities are represented in a *continuous* basis by *continuous matrices*, that is, by noncountable infinite matrices.

2.6.1 General Treatment

The orthonormality condition of the base *kets* of the continuous basis $| \chi_k\rangle$ is expressed not by the usual discrete Kronecker delta as in (2.170) but by Dirac's *continuous delta* function:

$$\langle \chi_k \mid \chi_{k'}\rangle = \delta(k'-k), \tag{2.275}$$

where k and k' are continuous parameters and where $\delta(k'-k)$ is the Dirac delta function (see Appendix A), which is defined by

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}\,dk. \tag{2.276}$$

As for the completeness condition of this continuous basis, it is not given by a discrete sum as in (2.172), but by an integral over the continuous variable

$$\int_{-\infty}^{+\infty} dk \mid \chi_k\rangle\langle\chi_k \mid = \hat{I}, \tag{2.277}$$

where $\hat{I}$ is the unit operator.

Every state vector $| \psi\rangle$ can be expanded in terms of the complete set of basis *kets* $| \chi_k\rangle$:

$$| \psi\rangle = \hat{I} \mid \psi\rangle = \left(\int_{-\infty}^{+\infty} dk \mid \chi_k\rangle\langle\chi_k \mid\right) \mid \psi\rangle = \int_{-\infty}^{+\infty} dk\, b(k) \mid \chi_k\rangle, \tag{2.278}$$

where $b(_k)$, which is equal to $\langle \chi_k \mid \psi \rangle$, represents the projection of $\mid \psi \rangle$ on $\mid \chi_k \rangle$.

The norm of the discrete base *kets* is finite ($\langle \phi_n \mid \phi_n \rangle = 1$), but the norm of the continuous base *kets* is infinite; a combination of (2.275) and (2.276) leads to

$$\langle \chi_k \mid \chi_k \rangle = \delta(0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \quad \longrightarrow \quad \infty. \tag{2.279}$$

This implies that the kets $\mid \chi_k \rangle$ are not square integrable and hence are not elements of the Hilbert space; recall that the space spanned by square-integrable functions is a Hilbert space. Despite the divergence of the norm of $\mid \chi_k \rangle$, the set $\mid \chi_k \rangle$ does constitute a valid basis of vectors that span the Hilbert space, since for any state vector $\mid \psi \rangle$, the scalar product $\langle \chi_k \mid \psi \rangle$ is finite.

The Dirac delta function

Before dealing with the representation of kets, bras, and operators, let us make a short detour to list some of the most important properties of the Dirac delta function (for a more detailed presentation, see Appendix A):

$$\delta(x) = 0, \qquad \text{for} \qquad x \neq 0, \tag{2.280}$$

$$\int_a^b f(x)\delta(x - x_0)\, dx = \begin{cases} f(x_0) & \text{if} \quad a < x_0 < b, \\ 0 & \text{elsewhere,} \end{cases} \tag{2.281}$$

$$\int_{-\infty}^{\infty} f(x) \frac{d^n \delta(x-a)}{dx^n}\, dx = (-1)^n \left. \frac{d^n f(x)}{dx^n} \right|_{x=a}, \tag{2.282}$$

$$\delta(\vec{r} - \vec{r}\,') = \delta(x - x')\delta(y - y')\delta(z - z') = \frac{1}{r^2 \sin\theta}\delta(r - r')\delta(\theta - \theta')\delta(\varphi - \varphi'). \tag{2.283}$$

Representation of kets, bras, and operators

The representation of kets, bras, and operators can be easily inferred from the study that was carried out in the previous section, for the case of a discrete basis. For instance, the ket $\mid \psi \rangle$ is represented by a single column matrix which has a continuous (noncountable) and infinite number of components (rows) $b(k)$:

$$\mid \psi \rangle \longrightarrow \begin{pmatrix} \vdots \\ \langle \chi_k \mid \psi \rangle \\ \vdots \end{pmatrix}. \tag{2.284}$$

The bra $\langle \psi \mid$ is represented by a single row matrix which has a continuous (noncountable) and infinite number of components (columns):

$$\langle \psi \mid \longrightarrow (\cdots\cdots \quad \langle \psi \mid \chi_k \rangle \quad \cdots\cdots). \tag{2.285}$$

Operators are represented by square continuous matrices whose rows and columns have continuous and infinite numbers of components:

$$\hat{A} \longrightarrow \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & A(k, k') & \cdots \\ \ddots & \vdots & \ddots \end{pmatrix}. \tag{2.286}$$

As an application, we are going to consider the representations in the position and momentum bases.

2.6.2 Position Representation

In the position representation, the basis consists of an infinite set of vectors $\{| \vec{r}\rangle\}$ which are eigenkets to the position operator $\hat{\vec{R}}$:

$$\hat{\vec{R}} \mid \vec{r}\rangle = \vec{r} \mid \vec{r}\rangle, \tag{2.287}$$

where $\vec{r}$ (without a hat), the position vector, is the eigenvalue of the operator $\hat{\vec{R}}$. The orthonormality and completeness conditions are respectively given by

$$\langle\vec{r} \mid \vec{r}\,'\rangle = \delta(\vec{r} - \vec{r}\,') = \delta(x - x')\delta(y - y')\delta(z - z'), \tag{2.288}$$

$$\int d^3 r \mid \vec{r}\rangle\langle\vec{r} \mid = \hat{I}, \tag{2.289}$$

since, as discussed in Appendix A, the three-dimensional delta function is given by

$$\delta(\vec{r} - \vec{r}\,') = \frac{1}{(2\pi)^3} \int d^3 k\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}. \tag{2.290}$$

So every state vector $| \psi\rangle$ can be expanded as follows:

$$| \psi\rangle = \int d^3 r \mid \vec{r}\rangle\langle\vec{r} \mid \psi\rangle \equiv \int d^3 r\, \psi(\vec{r}) \mid \vec{r}\rangle, \tag{2.291}$$

where $\psi(\vec{r})$ denotes the components of $| \psi\rangle$ in the $\{| \vec{r}\rangle\}$ basis:

$$\langle\vec{r} \mid \psi\rangle = \psi(\vec{r}). \tag{2.292}$$

This is known as the *wave function* for the state vector $| \psi\rangle$. Recall that, according to the probabilistic interpretation of Born, the quantity $| \langle\vec{r} \mid \psi\rangle |^2\, d^3 r$ represents the probability of finding the system in the volume element $d^3 r$.

The scalar product between two state vectors, $| \psi\rangle$ and $| \phi\rangle$, can be expressed in this form:

$$\langle\phi \mid \psi\rangle = \langle\phi \mid \left(\int d^3 r \mid \vec{r}\rangle\langle\vec{r} \mid\right) \mid \psi\rangle = \int d^3 r\, \phi^*(\vec{r})\psi(\vec{r}). \tag{2.293}$$

Since $\hat{\vec{R}} \mid \vec{r}\rangle = \vec{r} \mid \vec{r}\rangle$ we have

$$\langle\vec{r}\,' \mid \hat{\vec{R}}^{\,n} \mid \vec{r}\rangle = \vec{r}^{\,n}\delta(\vec{r}\,' - \vec{r}). \tag{2.294}$$

Note that the operator $\hat{\vec{R}}$ is Hermitian, since

$$\begin{aligned} \langle\phi \mid \hat{\vec{R}} \mid \psi\rangle &= \int d^3 r\, \vec{r}\langle\phi \mid \vec{r}\rangle\langle\vec{r} \mid \psi\rangle = \left[\int d^3 r\, \vec{r}\langle\psi \mid \vec{r}\rangle\langle\vec{r} \mid \phi\rangle\right]^* \\ &= \langle\psi \mid \hat{\vec{R}} \mid \phi\rangle^*. \end{aligned} \tag{2.295}$$

2.6.3 Momentum Representation

The basis $\{| \vec{p}\rangle\}$ of the momentum representation is obtained from the eigenkets of the momentum operator $\hat{\vec{P}}$:

$$\hat{\vec{P}} \mid \vec{p}\rangle = \vec{p} \mid \vec{p}\rangle, \tag{2.296}$$

where $\vec{p}$ is the momentum vector. The algebra relevant to this representation can be easily inferred from the position representation. The orthonormality and completeness conditions of the momentum space basis $| \vec{p}\rangle$ are given by

$$\langle \vec{p} \mid \vec{p}\,'\rangle = \delta(\vec{p} - \vec{p}\,') \qquad \text{and} \qquad \int d^3p \; | \vec{p}\rangle\langle\vec{p} \,| = \hat{I}. \tag{2.297}$$

Expanding $| \psi\rangle$ in this basis, we obtain

$$| \psi\rangle = \int d^3p \; | \vec{p}\rangle\langle\vec{p} \mid \psi\rangle = \int d^3p \; \Psi(\vec{p}) \mid \vec{p}\rangle, \tag{2.298}$$

where the expansion coefficient $\Psi(\vec{p})$ represents the *momentum space wave function*. The quantity $| \Psi(\vec{p}) |^2 \; d^3p$ is the probability of finding the system's momentum in the volume element d^3p located between $\vec{p}$ and $\vec{p} + d\vec{p}$.

By analogy with (2.293) the scalar product between two states is given in the momentum space by

$$\langle \phi \mid \psi\rangle = \langle \phi \mid \left(\int d^3p \; | \vec{p}\rangle\langle\vec{p} \,|\right) | \psi\rangle = \int d^3p \; \Phi^*(\vec{p})\Psi(\vec{p}). \tag{2.299}$$

Since $\hat{\vec{P}} \mid \vec{p}\rangle = \vec{p} \mid \vec{p}\rangle$ we have

$$\langle \vec{p}\,' \mid \hat{\vec{P}}^{\,n} \mid \vec{p}\rangle = \vec{p}^{\,n}\delta(\vec{p}\,' - \vec{p}). \tag{2.300}$$

2.6.4 Connecting the Position and Momentum Representations

Let us now study how to establish a connection between the position and the momentum representations. By analogy with the foregoing study, when changing from the $\{| \vec{r}\rangle\}$ basis to the $\{| \vec{p}\rangle\}$ basis, we encounter the *transformation* function $\langle\vec{r} \mid \vec{p}\rangle$.

To find the expression for the transformation function $\langle\vec{r} \mid \vec{p}\rangle$, let us establish a connection between the position and momentum representations of the state vector $| \psi\rangle$:

$$\langle\vec{r} \mid \psi\rangle = \langle\vec{r} \mid \left(\int d^3p \; | \vec{p}\rangle\langle\vec{p} \,|\right) | \psi\rangle = \int d^3p \; \langle\vec{r} \mid \vec{p}\rangle\Psi(\vec{p}); \tag{2.301}$$

that is,

$$\psi(\vec{r}) = \int d^3p \, \langle\vec{r} \mid \vec{p}\rangle\Psi(\vec{p}). \tag{2.302}$$

Similarly, we can write

$$\Psi(\vec{p}) = \langle\vec{p} \mid \psi\rangle = \langle\vec{p} \mid \int d^3r \; | \vec{r}\rangle\langle\vec{r} \mid \psi\rangle = \int d^3r \langle\vec{p} \mid \vec{r}\rangle\psi(\vec{r}). \tag{2.303}$$

The last two relations imply that $\psi(\vec{r})$ and $\Psi(\vec{p})$ are to be viewed as Fourier transforms of each other. In quantum mechanics the Fourier transform of a function $f(\vec{r})$ is given by

$$f(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, e^{i\vec{p}\cdot\vec{r}/\hbar} g(\vec{p}); \tag{2.304}$$

notice the presence of Planck's constant. Hence the function $\langle \vec{r} \mid \vec{p} \rangle$ is given by

$$\boxed{\langle \vec{r} \mid \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}.} \tag{2.305}$$

This function transforms from the momentum to the position representation. The function corresponding to the inverse transformation, $\langle \vec{p} \mid \vec{r} \rangle$, is given by

$$\boxed{\langle \vec{p} \mid \vec{r} \rangle = \langle \vec{r} \mid \vec{p} \rangle^* = \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar}.} \tag{2.306}$$

The quantity $|\langle \vec{r} \mid \vec{p} \rangle|^2$ represents the probability density of finding the particle in a region around $\vec{r}$ where its momentum is equal to $\vec{p}$.

Remark
If the position wave function

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, e^{i\vec{p}\cdot\vec{r}/\hbar} \Psi(\vec{p}) \tag{2.307}$$

is normalized (i.e., $\int d^3r\ \psi(\vec{r})\psi^*(\vec{r}) = 1$), its Fourier transform

$$\Psi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r\ e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi(\vec{r}) \tag{2.308}$$

must also be normalized, since

$$\begin{aligned}
\int d^3p\, \Psi^*(\vec{p})\Psi(\vec{p}) &= \int d^3p \Psi^*(\vec{p}) \left[\frac{1}{(2\pi\hbar)^{3/2}} \int d^3r\ e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi(\vec{r}) \right] \\
&= \int d^3r\ \psi(\vec{r}) \left[\frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\ \Psi^*(\vec{p}) e^{-i\vec{p}\cdot\vec{r}/\hbar} \right] \\
&= \int d^3r\ \psi(\vec{r})\psi^*(\vec{r}) \\
&= 1.
\end{aligned} \tag{2.309}$$

This result is known as *Parseval's theorem*.

2.6.4.1 Momentum Operator in the Position Representation

To determine the form of the momentum operator $\hat{\vec{P}}$ in the position representation, let us calculate $\langle \vec{r} \mid \hat{\vec{P}} \mid \psi \rangle$:

$$\begin{aligned}
\langle \vec{r} \mid \hat{\vec{P}} \mid \psi \rangle &= \int \langle \vec{r} \mid \hat{\vec{P}} \mid \vec{p} \rangle \langle \vec{p} \mid \psi \rangle d^3p = \int \vec{p} \langle \vec{r} \mid \vec{p} \rangle \langle \vec{p} \mid \psi \rangle d^3p \\
&= \frac{1}{(2\pi\hbar)^{3/2}} \int \vec{p}\, e^{i\vec{p}\cdot\vec{r}/\hbar} \Psi(\vec{p}) d^3p,
\end{aligned} \tag{2.310}$$

where we have used the relation $\int \mid \vec{p}\rangle\langle\vec{p} \mid d^3p = \hat{I}$ along with Eq. (2.305). Now, since $\vec{p}\, e^{i\vec{p}\cdot\vec{r}/\hbar} = -i\hbar\vec{\nabla}e^{i\vec{p}\cdot\vec{r}/\hbar}$, and using Eq. (2.305) again, we can rewrite (2.310) as

$$\begin{aligned}\langle\vec{r} \mid \hat{\vec{P}} \mid \psi\rangle &= -i\hbar\vec{\nabla}\left(\frac{1}{(2\pi\hbar)^{3/2}}\int e^{i\vec{p}\cdot\vec{r}/\hbar}\Psi(\vec{p})d^3p\right)\\ &= -i\hbar\vec{\nabla}\left(\int\langle\vec{r} \mid \vec{p}\rangle\langle\vec{p} \mid \psi\rangle d^3p\right)\\ &= -i\hbar\vec{\nabla}\langle\vec{r} \mid \psi\rangle. \end{aligned} \tag{2.311}$$

Thus, $\hat{\vec{P}}$ is given in the position representation by

$$\boxed{\hat{\vec{P}} = -i\hbar\vec{\nabla}.} \tag{2.312}$$

Its Cartesian components are

$$\boxed{\hat{P}_x = -i\hbar\frac{\partial}{\partial x}, \qquad \hat{P}_y = -i\hbar\frac{\partial}{\partial y}, \qquad \hat{P}_z = -i\hbar\frac{\partial}{\partial z}.} \tag{2.313}$$

Note that the form of the momentum operator (2.312) can be derived by simply applying the gradient operator $\vec{\nabla}$ on a *plane* wave function $\psi(\vec{r}, t) = Ae^{i(\vec{p}\cdot\vec{r}-Et)/\hbar}$:

$$-i\hbar\vec{\nabla}\psi(\vec{r}, t) = \vec{p}\psi(\vec{r}, t) = \hat{\vec{P}}\psi(\vec{r}, t). \tag{2.314}$$

It is easy to verify that $\hat{\vec{P}}$ is Hermitian (see equation (2.378)).

Now, since $\hat{\vec{P}} = -i\hbar\vec{\nabla}$, we can write the Hamiltonian operator $\hat{H} = \hat{\vec{P}}^{\,2}/(2m) + \hat{V}$ in the position representation as follows:

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r}) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \hat{V}(\vec{r}),} \tag{2.315}$$

where ∇^2 is the Laplacian operator; it is given in Cartesian coordinates by $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$.

2.6.4.2 Position Operator in the Momentum Representation

The form of the position operator $\hat{\vec{R}}$ in the momentum representation can be easily inferred from the representation of $\hat{\vec{P}}$ in the position space. In momentum space the position operator can be written as follows:

$$\hat{R}_j = i\hbar\frac{\partial}{\partial p_j} \qquad (j = x, y, z) \tag{2.316}$$

or

$$\boxed{\hat{X} = i\hbar\frac{\partial}{\partial p_x}, \qquad \hat{Y} = i\hbar\frac{\partial}{\partial p_y}, \qquad \hat{Z} = i\hbar\frac{\partial}{\partial p_z}.} \tag{2.317}$$

2.6.4.3 Important Commutation Relations

Let us now calculate the commutator $[\hat{R}_j, \hat{P}_k]$ in the position representation. As the separate actions of $\hat{X}\hat{P}_x$ and $\hat{P}_x\hat{X}$ on the wave function $\psi(\vec{r})$ are given by

$$\hat{X}\hat{P}_x\psi(\vec{r}) = -i\hbar x\frac{\partial\psi(\vec{r})}{\partial x}, \tag{2.318}$$

$$\hat{P}_x\hat{X}\psi(\vec{r}) = -i\hbar\frac{\partial}{\partial x}(x\psi(\vec{r})) = -i\hbar\psi(\vec{r}) - i\hbar x\frac{\partial\psi(\vec{r})}{\partial x}, \tag{2.319}$$

we have

$$\begin{aligned}[\hat{X}, \hat{P}_x]\psi(\vec{r}) &= \hat{X}\hat{P}_x\psi(\vec{r}) - \hat{P}_x\hat{X}\psi(\vec{r}) = -i\hbar x\frac{\partial\psi(\vec{r})}{\partial x} + i\hbar\psi(\vec{r}) + i\hbar x\frac{\partial\psi(\vec{r})}{\partial x} \\ &= i\hbar\psi(\vec{r}) \end{aligned}\tag{2.320}$$

or

$$[\hat{X}, \hat{P}_x] = i\hbar. \tag{2.321}$$

Similar relations can be derived at once for the y and the z components:

$$\boxed{[\hat{X}, \hat{P}_x] = i\hbar, \qquad [\hat{Y}, \hat{P}_Y] = i\hbar, \qquad [\hat{Z}, \hat{P}_Z] = i\hbar.} \tag{2.322}$$

We can verify that

$$[\hat{X}, \hat{P}_y] = [\hat{X}, \hat{P}_z] = [\hat{Y}, \hat{P}_x] = [\hat{Y}, \hat{P}_z] = [\hat{Z}, \hat{P}_x] = [\hat{Z}, \hat{P}_y] = 0, \tag{2.323}$$

since the x, y, z degrees of freedom are independent; the previous two relations can be grouped into

$$\boxed{[\hat{R}_j, \hat{P}_k] = i\hbar\delta_{jk}, \qquad [\hat{R}_j, \hat{R}_k] = 0, \qquad [\hat{P}_j, \hat{P}_k] = 0 \qquad (j,\ k = x, y, z).} \tag{2.324}$$

These relations are often called the *canonical commutation relations*.

Now, from (2.321) we can show that (for the proof see Problem 2.8 on page 139)

$$\boxed{[\hat{X}^n, \hat{P}_x] = i\hbar n\hat{X}^{n-1}, \qquad [\hat{X}, \hat{P}_x^n] = i\hbar n\hat{P}_x^{n-1}.} \tag{2.325}$$

Following the same procedure that led to (2.320), we can obtain a more general commutation relation of $\hat{P}_x$ with an arbitrary function $f(\hat{X})$:

$$\boxed{[f(\hat{X}), \hat{P}_x] = i\hbar\frac{df(\hat{X})}{d\hat{X}} \quad\Longrightarrow\quad \left[\hat{\vec{P}},\ F(\hat{\vec{R}})\right] = -i\hbar\vec{\nabla}F(\hat{\vec{R}})),} \tag{2.326}$$

where F is a function of the operator $\hat{\vec{R}}$.

The explicit form of operators thus depends on the representation adopted. We have seen, however, that the *commutation relations for operators are representation independent*. In particular, the commutator $[\hat{R}_j, \hat{P}_k]$ is given by $i\hbar\delta_{jk}$ in the position and the momentum representations; see the next example.

Example 2.20 (Commutators are representation independent)
Calculate the commutator $[\hat{X}, \hat{P}]$ in the momentum representation and verify that it is equal to $i\hbar$.

Solution
As the operator $\hat{X}$ is given in the momentum representation by $\hat{X} = i\hbar\partial/\partial p$, we have

$$\begin{aligned}[\hat{X}, \hat{P}]\psi(p) &= \hat{X}\hat{P}\psi(p) - \hat{P}\hat{X}\psi(p) = i\hbar\frac{\partial}{\partial p}(p\psi(p)) - i\hbar p\frac{\partial\psi(p)}{\partial p} \\ &= i\hbar\psi(p) + i\hbar p\frac{\partial\psi(p)}{\partial p} - i\hbar p\frac{\partial\psi(p)}{\partial p} = i\hbar\psi(p). \end{aligned} \tag{2.327}$$

Thus, the commutator $[\hat{X}, \hat{P}]$ is given in the *momentum representation* by

$$[\hat{X}, \hat{P}] = \left[i\hbar\frac{\partial}{\partial p},\ \hat{P}\right] = i\hbar. \tag{2.328}$$

The commutator $[\hat{X}, \hat{P}]$ was also shown to be equal to $i\hbar$ in the *position representation* (see equation (2.321):

$$[\hat{X}, \hat{P}] = -\left[\hat{X},\ i\hbar\frac{\partial}{\partial p_x}\right] = i\hbar. \tag{2.329}$$

2.6.5 Parity Operator

The *space reflection* about the origin of the coordinate system is called an *inversion* or a *parity* operation. This transformation is *discrete*. The parity operator $\hat{\mathcal{P}}$ is defined by its action on the kets $|\vec{r}\rangle$ of the position space:

$$\hat{\mathcal{P}} \mid \vec{r}\rangle = \mid -\vec{r}\rangle, \qquad \langle\vec{r} \mid \hat{\mathcal{P}}^\dagger = \langle -\vec{r} \mid, \tag{2.330}$$

such that

$$\hat{\mathcal{P}}\psi(\vec{r}) = \psi(-\vec{r}). \tag{2.331}$$

The parity operator is Hermitian, $\hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}}$, since

$$\begin{aligned}\int d^3r\ \phi^*(\vec{r})\left[\hat{\mathcal{P}}\psi(\vec{r})\right] &= \int d^3r\phi^*(\vec{r})\psi(-\vec{r}) = \int d^3r\ \phi^*(-\vec{r})\psi(\vec{r}) \\ &= \int d^3r\ \left[\hat{\mathcal{P}}\phi(\vec{r})\right]^*\psi(\vec{r}). \end{aligned} \tag{2.332}$$

From the definition (2.331), we have

$$\hat{\mathcal{P}}^2\psi(\vec{r}) = \hat{\mathcal{P}}\psi(-\vec{r}) = \psi(\vec{r}); \tag{2.333}$$

hence $\hat{\mathcal{P}}^2$ is equal to the unity operator:

$$\hat{\mathcal{P}}^2 = \hat{I} \qquad \text{or} \qquad \hat{\mathcal{P}} = \hat{\mathcal{P}}^{-1}. \tag{2.334}$$

The parity operator is therefore *unitary*, since its Hermitian adjoint is equal to its inverse:

$$\hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}}^{-1}. \tag{2.335}$$

Now, since $\hat{\mathcal{P}}^2 = \hat{I}$, the eigenvalues of $\hat{\mathcal{P}}$ are $+1$ or -1 with the corresponding eigenstates

$$\hat{\mathcal{P}}\psi_+(\vec{r}) = \psi_+(-\vec{r}) = \psi_+(\vec{r}), \qquad \hat{\mathcal{P}}\psi_-(\vec{r}) = \psi_-(-\vec{r}) = -\psi_-(\vec{r}). \tag{2.336}$$

The eigenstate $\mid \psi_+\rangle$ is said to be *even* and $\mid \psi_-\rangle$ is *odd*. Therefore, the eigenfunctions of the parity operator have *definite parity*: they are either even or odd.

Since $\mid \psi_+\rangle$ and $\mid \psi_-\rangle$ are joint eigenstates of the same Hermitian operator $\hat{\mathcal{P}}$ but with different eigenvalues, these eigenstates must be orthogonal:

$$\langle\psi_+ \mid \psi_-\rangle = \int d^3r\ \psi_+^*(-\vec{r})\psi_-(-\vec{r}) \equiv -\int d^3r\ \psi_+^*(\vec{r})\psi_-(\vec{r}) = -\langle\psi_+ \mid \psi_-\rangle; \tag{2.337}$$

hence $\langle\psi_+ \mid \psi_-\rangle$ is zero. The states $\mid \psi_+\rangle$ and $\mid \psi_-\rangle$ form a complete set since any function can be written as $\psi(\vec{r}) = \psi_+(\vec{r}) + \psi_-(\vec{r})$, which leads to

$$\psi_+(\vec{r}) = \frac{1}{2}\left[\psi(\vec{r}) + \psi(-\vec{r})\right], \qquad \psi_-(\vec{r}) = \frac{1}{2}\left[\psi(\vec{r}) - \psi(-\vec{r})\right]. \tag{2.338}$$

Since $\hat{\mathcal{P}}^2 = I$ we have

$$\hat{\mathcal{P}}^n = \begin{cases} \hat{\mathcal{P}} & \text{when } n \text{ is odd,} \\ \hat{I} & \text{when } n \text{ is even.} \end{cases} \tag{2.339}$$

Even and odd operators

An operator $\hat{A}$ is said to be *even* if it obeys the condition

$$\hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}} = \hat{A} \tag{2.340}$$

and an operator $\hat{B}$ is *odd* if

$$\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}} = -\hat{B}. \tag{2.341}$$

We can easily verify that even operators commute with the parity operator $\hat{\mathcal{P}}$ and that odd operators anticommute with $\hat{\mathcal{P}}$:

$$\hat{A}\hat{\mathcal{P}} = (\hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}})\hat{\mathcal{P}} = \hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}}^2 = \hat{\mathcal{P}}\hat{A}, \tag{2.342}$$

$$\hat{B}\hat{\mathcal{P}} = -(\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}})\hat{\mathcal{P}} = -\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}}^2 = -\hat{\mathcal{P}}\hat{B}. \tag{2.343}$$

The fact that even operators commute with the parity operator has very useful consequences. Let us examine the following two important cases depending on whether an even operator has nondegenerate or degenerate eigenvalues:

- If an even operator is Hermitian and none of its eigenvalues is degenerate, then this operator has the same eigenvectors as those of the parity operator. And since the eigenvectors of the parity operator are either even or odd, the eigenvectors of an even, Hermitian, and nondegenerate operator must also be either even or odd; they are said to have a *definite parity*. This property will have useful applications when we solve the Schrödinger equation for even Hamiltonians.

- If the even operator has a degenerate spectrum, its eigenvectors do not necessarily have a definite parity.

What about the parity of the position and momentum operators, $\hat{\vec{R}}$ and $\hat{\vec{P}}$? We can easily show that both of them are odd, since they anticommute with the parity operator:

$$\hat{\mathcal{P}}\hat{\vec{R}} = -\hat{\vec{R}}\hat{\mathcal{P}}, \qquad \hat{\mathcal{P}}\hat{\vec{P}} = -\hat{\vec{P}}\hat{\mathcal{P}}; \tag{2.344}$$

hence

$$\hat{\mathcal{P}}\hat{\vec{R}}\hat{\mathcal{P}}^{\dagger} = -\hat{\vec{R}}, \qquad \hat{\mathcal{P}}\hat{\vec{P}}\hat{\mathcal{P}}^{\dagger} = -\hat{\vec{P}}, \tag{2.345}$$

since $\hat{\mathcal{P}}\hat{\mathcal{P}}^{\dagger} = 1$. For instance, to show that $\hat{\vec{R}}$ anticommutes with $\hat{\mathcal{P}}$, we need simply to look at the following relations:

$$\hat{\mathcal{P}}\hat{\vec{R}} \mid \vec{r}\rangle = \vec{r}\hat{\mathcal{P}} \mid \vec{r}\rangle = \vec{r} \mid -\vec{r}\rangle, \tag{2.346}$$

$$\hat{\vec{R}}\hat{\mathcal{P}} \mid \vec{r}\rangle = \hat{\vec{R}} \mid -\vec{r}\rangle = -\vec{r} \mid -\vec{r}\rangle. \tag{2.347}$$

If the operators $\hat{A}$ and $\hat{B}$ are even and odd, respectively, we can verify that

$$\hat{\mathcal{P}}\hat{A}^{n}\hat{\mathcal{P}} = \hat{A}^{n}, \qquad \hat{\mathcal{P}}\hat{B}^{n}\hat{\mathcal{P}} = (-1)^{n}\hat{B}^{n}. \tag{2.348}$$

These relations can be shown as follows:

$$\hat{\mathcal{P}}\hat{A}^{n}\hat{\mathcal{P}} = (\hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}})\,(\hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}})\cdots(\hat{\mathcal{P}}\hat{A}\hat{\mathcal{P}}) = \hat{A}^{n}, \tag{2.349}$$

$$\hat{\mathcal{P}}\hat{B}^{n}\hat{\mathcal{P}} = (\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}})\,(\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}})\cdots(\hat{\mathcal{P}}\hat{B}\hat{\mathcal{P}}) = (-1)^{n}\hat{B}^{n}. \tag{2.350}$$

2.7 Matrix and Wave Mechanics

In this chapter we have so far worked out the mathematics pertaining to quantum mechanics in two different representations: *discrete* basis systems and *continuous* basis systems. The theory of quantum mechanics deals in essence with solving the following eigenvalue problem:

$$\hat{H} \mid \psi\rangle = E \mid \psi\rangle, \tag{2.351}$$

where $\hat{H}$ is the Hamiltonian of the system. This equation is general and does not depend on any coordinate system or representation. But to solve it, we need to represent it in a given basis system. The complexity associated with solving this eigenvalue equation will then vary from one basis to another.

In what follows we are going to examine the representation of this eigenvalue equation in a *discrete* basis and then in a *continuous* basis.

2.7.1 Matrix Mechanics

The representation of quantum mechanics in a *discrete* basis yields a *matrix* eigenvalue problem. That is, the representation of (2.351) in a discrete basis $\{\mid \phi_n\rangle\}$ yields the following matrix eigenvalue equation (see (2.257)):

$$\begin{vmatrix} H_{11}-E & H_{12} & H_{13} & \cdots & H_{1N} \\ H_{21} & H_{22}-E & H_{23} & \cdots & H_{2N} \\ H_{31} & H_{32} & H_{33}-E & \cdots & H_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & H_{N3} & \cdots & H_{NN}-E \end{vmatrix} = 0. \tag{2.352}$$

This is an Nth order equation in E; its solutions yield the energy spectrum of the system: E_1, E_2, E_3, ..., E_N. Knowing the set of eigenvalues E_1, E_2, E_3, ..., E_N, we can easily determine the corresponding set of eigenvectors $\mid \phi_1\rangle$, $\mid \phi_2\rangle$, ..., $\mid \phi_N\rangle$.

The diagonalization of the Hamiltonian matrix (2.352) of a system yields the energy spectrum as well as the state vectors of the system. This procedure, which was worked out by Heisenberg, involves only matrix quantities and matrix eigenvalue equations. This formulation of quantum mechanics is known as *matrix mechanics*.

The starting point of Heisenberg, in his attempt to find a theoretical foundation to Bohr's ideas, was the atomic transition relation, $\nu_{mn} = (E_m - E_n)/h$, which gives the frequencies of the radiation associated with the electron's transition from orbit m to orbit n. The frequencies ν_{mn} can be arranged in a square matrix, where the mn element corresponds to the transition from the mth to the nth quantum state.

We can also construct matrices for other dynamical quantities related to the transition $m \to n$. In this way, every physical quantity is represented by a matrix. For instance, we represent the energy levels by an energy matrix, the position by a position matrix, the momentum by a momentum matrix, the angular momentum by an angular momentum matrix, and so on. In calculating the various physical magnitudes, one has thus to deal with the algebra of matrix quantities. So, within the context of matrix mechanics, one deals with noncommuting quantities, for the product of matrices does not commute. This is an essential feature that distinguishes matrix mechanics from classical mechanics, where all the quantities commute. Take, for instance, the position and momentum quantities. While commuting in classical mechanics, $px = xp$, they do not commute within the context of matrix mechanics; they are related by the commutation relation $[\hat{X},\ \hat{P}_x] = i\hbar$. The same thing applies for the components of angular momentum. We should note that the role played by the commutation relations within the context of matrix mechanics is similar to the role played by Bohr's quantization condition in atomic theory. Heisenberg's matrix mechanics therefore requires the introduction of some mathematical machinery—linear vector spaces, Hilbert space, commutator algebra, and matrix algebra—that is entirely different from the mathematical machinery of classical mechanics. Here lies the justification for having devoted a somewhat lengthy section, Section 2.5, to study the matrix representation of quantum mechanics.

2.7.2 Wave Mechanics

Representing the formalism of quantum mechanics in a *continuous* basis yields an eigenvalue problem not in the form of a matrix equation, as in Heisenberg's formulation, but in the form of a *differential equation*. The representation of the eigenvalue equation (2.351) in the *position* space yields

$$\langle \vec{r} \mid \hat{H} \mid \psi\rangle = E\langle \vec{r} \mid \psi\rangle. \tag{2.353}$$

As shown in (2.315), the Hamiltonian is given in the position representation by $-\hbar^2\nabla^2/(2m)+\hat{V}(\vec{r})$, so we can rewrite (2.353) in a more familiar form:

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+\hat{V}(\vec{r})\psi(\vec{r})=E\psi(\vec{r}),} \tag{2.354}$$

where $\langle\vec{r}\mid\psi\rangle = \psi(\vec{r})$ is the *wave function* of the system. This differential equation is known as the *Schrödinger equation* (its origin will be discussed in Chapter 3). Its solutions yield the energy spectrum of the system as well as its wave function. This formulation of quantum mechanics in *the position representation* is called *wave mechanics*.

Unlike Heisenberg, Schödinger took an entirely different starting point in his quest to find a theoretical justification for Bohr's ideas. He started from the de Broglie particle–wave hypothesis and extended it to the electrons orbiting around the nucleus. Schrödinger aimed at finding an equation that describes the motion of the electron within an atom. Here the focus is on the *wave* aspect of the electron. We can show, as we did in Chapter 1, that the Bohr quantization condition, $L = n\hbar$, is equivalent to the de Broglie relation, $\lambda = 2\pi\hbar/p$. To establish this connection, we need simply to make three assumptions: (a) the wavelength of the wave associated with the orbiting electron is connected to the electron's linear momentum p by $\lambda = 2\pi\hbar/p$, (b) the electron's orbit is circular, and (c) the circumference of the electron's orbit is an integer multiple of the electron's wavelength, i.e., $2\pi r = n\lambda$. This leads at once to $2\pi r = n \times (2\pi\hbar/p)$ or $n\hbar = rp \equiv L$. This means that, for every orbit, there is only one wavelength (or one wave) associated with the electron while revolving in that orbit. This wave can be described by means of a *wave function*. So Bohr's quantization condition implies, in essence, a uniqueness of the wave function for each orbit of the electron. In Chapter 3 we will show how Schrödinger obtained his differential equation (2.354) to describe the motion of an electron in an atom.

2.8 Concluding Remarks

Historically, the matrix formulation of quantum mechanics was worked out by Heisenberg shortly before Schrödinger introduced his wave theory. The equivalence between the matrix and wave formulations was proved a few years later by using the theory of unitary transformations. Different in form, yet identical in contents, wave mechanics and matrix mechanics achieve the same goal: finding the energy spectrum and the states of quantum systems.

The matrix formulation has the advantage of greater (formal) generality, yet it suffers from a number of disadvantages. On the conceptual side, it offers no visual idea about the structure of the atom; it is less intuitive than wave mechanics. On the technical side, it is difficult to use in some problems of relative ease such as finding the stationary states of atoms. Matrix mechanics, however, becomes powerful and practical in solving problems such as the harmonic oscillator or in treating the formalism of angular momentum.

But most of the efforts of quantum mechanics focus on solving the Schrödinger equation, not the Heisenberg matrix eigenvalue problem. So in the rest of this text we deal mostly with wave mechanics. Matrix mechanics is used only in a few problems, such as the harmonic oscillator, where it is more suitable than Schrödinger's wave mechanics.

In wave mechanics we need only to specify the potential in which the particle moves; the Schrödinger equation takes care of the rest. That is, knowing $\hat{V}(\vec{r})$, we can in principle solve equation (2.354) to obtain the various energy levels of the particle and their corresponding wave functions. The complexity we encounter in solving the differential equation depends entirely on the form of the potential; the simpler the potential the easier the solution. Exact solutions of the Schrödinger equation are possible only for a few idealized systems; we deal with such systems in Chapters 4 and 6. However, exact solutions are generally not possible, for real systems do not yield themselves to exact solutions. In such cases one has to resort to approximate solutions. We deal with such approximate treatments in Chapters 9 and 10; Chapter 9 deals with time-independent potentials and Chapter 10 with time-dependent potentials.

Before embarking on the applications of the Schrödinger equation, we need first to lay down the theoretical foundations of quantum mechanics. We take up this task in Chapter 3, where we deal with the postulates of the theory as well as their implications; the postulates are the bedrock on which the theory is built.

2.9 Solved Problems

Problem 2.1

Consider the states $\mid \psi\rangle = 9i \mid \phi_1\rangle + 2 \mid \phi_2\rangle$ and $\mid \chi\rangle = -\frac{i}{\sqrt{2}} \mid \phi_1\rangle + \frac{1}{\sqrt{2}} \mid \phi_2\rangle$, where the two vectors $\mid \phi_1\rangle$ and $\mid \phi_2\rangle$ form a complete and orthonormal basis.

(a) Calculate the operators $\mid \psi\rangle\langle\chi \mid$ and $\mid \chi\rangle\langle\psi \mid$. Are they equal?

(b) Find the Hermitian conjugates of $\mid \psi\rangle$, $\mid \chi\rangle$, $\mid \psi\rangle\langle\chi \mid$, and $\mid \chi\rangle\langle\psi \mid$.

(c) Calculate $\text{Tr}(\mid \psi\rangle\langle\chi \mid)$ and $\text{Tr}(\mid \chi\rangle\langle\psi \mid)$. Are they equal?

(d) Calculate $\mid \psi\rangle\langle\psi \mid$ and $\mid \chi\rangle\langle\chi \mid$ and the traces $\text{Tr}(\mid \psi\rangle\langle\psi \mid)$ and $\text{Tr}(\mid \chi\rangle\langle\chi \mid)$. Are they projection operators?

Solution

(a) The bras corresponding to $\mid \psi\rangle = 9i \mid \phi_1\rangle + 2 \mid \phi_2\rangle$ and $\mid \chi\rangle = -i \mid \phi_1\rangle/\sqrt{2} + \mid \phi_2\rangle/\sqrt{2}$ are given by $\langle\psi \mid = -9i\langle\phi_1 \mid +2\langle\phi_2 \mid$ and $\langle\chi \mid = \frac{i}{\sqrt{2}}\langle\phi_1 \mid + \frac{1}{\sqrt{2}}\langle\phi_2 \mid$, respectively. Hence we have

$$\begin{aligned} \mid \psi\rangle\langle\chi \mid &= \frac{1}{\sqrt{2}}\left(9i \mid \phi_1\rangle + 2 \mid \phi_2\rangle\right)\left(i\langle\phi_1 \mid + \langle\phi_2 \mid\right) \\ &= \frac{1}{\sqrt{2}}\left(-9 \mid \phi_1\rangle\langle\phi_1 \mid + 9i \mid \phi_1\rangle\langle\phi_2 \mid + 2i \mid \phi_2\rangle\langle\phi_1 \mid + 2 \mid \phi_2\rangle\langle\phi_2 \mid\right), \end{aligned} \tag{2.355}$$

$$\mid \chi\rangle\langle\psi \mid = \frac{1}{\sqrt{2}}\left(-9 \mid \phi_1\rangle\langle\phi_1 \mid - 2i \mid \phi_1\rangle\langle\phi_2 \mid - 9i \mid \phi_2\rangle\langle\phi_1 \mid + 2 \mid \phi_2\rangle\langle\phi_2 \mid\right). \tag{2.356}$$

As expected, $\mid \psi\rangle\langle\chi \mid$ and $\mid \chi\rangle\langle\psi \mid$ are not equal; they would be equal only if the states $\mid \psi\rangle$ and $\mid \chi\rangle$ were proportional and the proportionality constant real.

(b) To find the Hermitian conjugates of $\mid \psi\rangle$, $\mid \chi\rangle$, $\mid \psi\rangle\langle\chi \mid$, and $\mid \chi\rangle\langle\psi \mid$, we need simply to replace the factors with their respective complex conjugates, the bras with kets, and the kets with bras:

$$\mid \psi\rangle^\dagger = \langle\psi \mid = -9i\langle\phi_1 \mid + 2\langle\phi_2 \mid, \qquad \mid \chi\rangle^\dagger = \langle\chi \mid = \frac{1}{\sqrt{2}}\left(i\langle\phi_1 \mid + \langle\phi_2 \mid\right), \tag{2.357}$$

$$
\begin{aligned}
(|\psi\rangle\langle\chi|)^\dagger = |\chi\rangle\langle\psi| &= \frac{1}{\sqrt{2}}\,(-9\,|\phi_1\rangle\langle\phi_1| - 2i\,|\phi_1\rangle\langle\phi_2| \\
&\quad - 9i\,|\phi_2\rangle\langle\phi_1| + 2\,|\phi_2\rangle\langle\phi_2|)\,, \qquad (2.358)\\
(|\chi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\chi| &= \frac{1}{\sqrt{2}}\,(-9\,|\phi_1\rangle\langle\phi_1| + 9i\,|\phi_1\rangle\langle\phi_2| \\
&\quad + 2i\,|\phi_2\rangle\langle\phi_1| + 2\,|\phi_2\rangle\langle\phi_2|)\,. \qquad (2.359)
\end{aligned}
$$

(c) Using the property $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ and since $\langle\phi_1 \mid \phi_1\rangle = \langle\phi_2 \mid \phi_2\rangle = 1$ and $\langle\phi_1 \mid \phi_2\rangle = \langle\phi_2 \mid \phi_1\rangle = 0$, we obtain

$$
\begin{aligned}
\mathrm{Tr}(|\psi\rangle\langle\chi|) &= \mathrm{Tr}(\langle\chi \mid \psi\rangle) = \langle\chi \mid \psi\rangle \\
&= \left(\frac{i}{\sqrt{2}}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2|\right)(9i\,|\phi_1\rangle + 2\,|\phi_2\rangle) = -\frac{7}{\sqrt{2}}, \qquad (2.360)\\
\mathrm{Tr}(|\chi\rangle\langle\psi|) &= \mathrm{Tr}(\langle\psi \mid \chi\rangle) = \langle\psi \mid \chi\rangle \\
&= (-9i\langle\phi_1| + 2\langle\phi_2|)\left(-\frac{i}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle\right) = -\frac{7}{\sqrt{2}} \\
&= \mathrm{Tr}(|\psi\rangle\langle\chi|). \qquad (2.361)
\end{aligned}
$$

The traces $\mathrm{Tr}(|\psi\rangle\langle\chi|)$ and $\mathrm{Tr}(|\chi\rangle\langle\psi|)$ are equal only because the scalar product of $|\psi\rangle$ and $|\chi\rangle$ is a real number. Were this product a complex number, the traces would be different; in fact, they would be the complex conjugate of one another.

(d) The expressions $|\psi\rangle\langle\psi|$ and $|\chi\rangle\langle\chi|$ are

$$
\begin{aligned}
|\psi\rangle\langle\psi| &= (9i\,|\phi_1\rangle + 2\,|\phi_2\rangle)\,(-9i\langle\phi_1| + 2\langle\phi_2|) \\
&= 81\,|\phi_1\rangle\langle\phi_1| + 18i\,|\phi_1\rangle\langle\phi_2| - 18i\,|\phi_2\rangle\langle\phi_1| + 4\,|\phi_2\rangle\langle\phi_2|, \qquad (2.362)
\end{aligned}
$$

$$
\begin{aligned}
|\chi\rangle\langle\chi|) &= \frac{1}{2}\,(|\phi_1\rangle\langle\phi_1| - i\,|\phi_1\rangle\langle\phi_2| + i\,|\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|) \\
&= \frac{1}{2}\,(1 - i\,|\phi_1\rangle\langle\phi_2| + i\,|\phi_2\rangle\langle\phi_1|)\,. \qquad (2.363)
\end{aligned}
$$

In deriving (2.363) we have used the fact that the basis is complete, $|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| = 1$. The traces $\mathrm{Tr}(|\psi\rangle\langle\psi|)$ and $\mathrm{Tr}(|\chi\rangle\langle\chi|)$ can then be calculated immediately:

$$
\begin{aligned}
\mathrm{Tr}(|\psi\rangle\langle\psi|) &= \langle\psi \mid \psi\rangle = (-9i\langle\phi_1| + 2\langle\phi_2|)\,(9i\,|\phi_1\rangle + 2\,|\phi_2\rangle) = 85, \qquad (2.364)\\
\mathrm{Tr}(|\chi\rangle\langle\chi|) &= \langle\chi \mid \chi\rangle = \frac{1}{2}\,(i\langle\phi_1| + \langle\phi_2|)\,(-i\,|\phi_1\rangle + |\phi_2\rangle) = 1. \qquad (2.365)
\end{aligned}
$$

So $|\chi\rangle$ is normalized but $|\psi\rangle$ is not. Since $|\chi\rangle$ is normalized, we can easily ascertain that $|\chi\rangle\langle\chi|$ is a projection operator, because it is Hermitian, $(|\chi\rangle\langle\chi|)^\dagger = |\chi\rangle\langle\chi|$, and equal to its own square:

$$
(|\chi\rangle\langle\chi|)^2 = |\chi\rangle\langle\chi \mid \chi\rangle\langle\chi| = (\langle\chi \mid \chi\rangle)\,|\chi\rangle\langle\chi| = |\chi\rangle\langle\chi|\,. \qquad (2.366)
$$

As for $|\psi\rangle\langle\psi|$, although it is Hermitian, it cannot be a projection operator since $|\psi\rangle$ is not normalized. That is, $|\psi\rangle\langle\psi|$ is not equal to its own square:

$$
(|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi \mid \psi\rangle\langle\psi| = (\langle\psi \mid \psi\rangle)\,|\psi\rangle\langle\psi| = 85\,|\psi\rangle\langle\psi|\,. \qquad (2.367)
$$

Problem 2.2

(a) Find a complete and orthonormal basis for a space of the trigonometric functions of the form $\psi(\theta) = \sum_{n=0}^{N} a_n \cos(n\theta)$.

(b) Illustrate the results derived in (a) for the case $N = 5$; find the basis vectors.

Solution

(a) Since $\cos(n\theta) = \frac{1}{2}\left(e^{in\theta} + e^{-in\theta}\right)$, we can write $\sum_{n=0}^{N} a_n \cos(n\theta)$ as

$$\frac{1}{2}\sum_{n=0}^{N} a_n \left(e^{in\theta} + e^{-in\theta}\right) = \frac{1}{2}\left[\sum_{n=0}^{N} a_n e^{in\theta} + \sum_{n=-N}^{0} a_{-n} e^{in\theta}\right] = \sum_{n=-N}^{N} C_n e^{in\theta}, \tag{2.368}$$

where $C_n = a_n/2$ for $n > 0$, $C_n = a_{-n}/2$ for $n < 0$, and $C_0 = a_0$. Since any trigonometric function of the form $\psi(x) = \sum_{n=0}^{N} a_n \cos(n\theta)$ can be expressed in terms of the functions $\phi_n(\theta) = e^{in\theta}/\sqrt{2\pi}$, we can try to take the set $\phi_n(\theta)$ as a basis. As this set is complete, let us see if it is orthonormal. The various functions $\phi_n(\theta)$ are indeed orthonormal, since their scalar products are given by

$$\langle \phi_m \mid \phi_n \rangle = \int_{-\pi}^{\pi} \phi_m^*(\theta)\phi_n(\theta) d\theta = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(n-m)\theta}\, d\theta = \delta_{nm}. \tag{2.369}$$

In deriving this result, we have considered two cases: $n = m$ and $n \neq m$. First, the case $n = m$ is obvious, since $\langle \phi_n \mid \phi_n \rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta = 1$. On the other hand, when $n \neq m$ we have

$$\langle \phi_m \mid \phi_n \rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(n-m)\theta} d\theta = \frac{1}{2\pi}\frac{e^{i(n-m)\pi} - e^{-i(n-m)\pi}}{i(n-m)} = \frac{2i\,\sin((n-m)\pi)}{2i\pi(n-m)} = 0, \tag{2.370}$$

since $\sin((n-m)\pi) = 0$. So the functions $\phi_n(\theta) = e^{in\theta}/\sqrt{2\pi}$ form a complete and orthonormal basis. From (2.368) we see that the basis has $2N+1$ functions $\phi_n(\theta)$; hence the dimension of this space of functions is equal to $2N + 1$.

(b) In the case where $N = 5$, the dimension of the space is equal to 11, for the basis has 11 vectors: $\phi_{-5}(\theta) = e^{-5i\theta}/\sqrt{2\pi}$, $\phi_{-4}(\theta) = e^{-4i\theta}/\sqrt{2\pi}$, ..., $\phi_0(\theta) = 1/\sqrt{2\pi}$, ..., $\phi_4(\theta) = e^{4i\theta}/\sqrt{2\pi}$, $\phi_5(\theta) = e^{5i\theta}/\sqrt{2\pi}$.

Problem 2.3

(a) Show that the sum of two projection operators cannot be a projection operator unless their product is zero.

(b) Show that the product of two projection operators cannot be a projection operator unless they commute.

Solution

Recall that an operator $\hat{P}$ is a projection operator if it satisfies $\hat{P}^\dagger = \hat{P}$ and $\hat{P}^2 = \hat{P}$.

(a) If two operators $\hat{A}$ and $\hat{B}$ are projection operators and if $\hat{A}\hat{B} = \hat{B}\hat{A}$, we want to show that $(\hat{A} + \hat{B})^\dagger = \hat{A} + \hat{B}$ and that $(\hat{A} + \hat{B})^2 = \hat{A} + \hat{B}$. First, the hermiticity is easy to ascertain since $\hat{A}$ and $\hat{B}$ are both Hermitian: $(\hat{A} + \hat{B})^\dagger = \hat{A} + \hat{B}$. Let us now look at the square of $(\hat{A} + \hat{B})$; since $\hat{A}^2 = \hat{A}$ and $\hat{B}^2 = \hat{B}$, we can write

$$(\hat{A} + \hat{B})^2 = \hat{A}^2 + \hat{B}^2 + (\hat{A}\hat{B} + \hat{B}\hat{A}) = \hat{A} + \hat{B} + (\hat{A}\hat{B} + \hat{B}\hat{A}). \tag{2.371}$$

Clearly, only when the product of $\hat{A}$ and $\hat{B}$ is zero will their sum be a projection operator.

(b) At issue here is to show that if two operators $\hat{A}$ and $\hat{B}$ are projection operators and if they commute, $[\hat{A},\ \hat{B}] = 0$, their product is a projection operator. That is, we need to show that $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$ and $(\hat{A}\hat{B})^2 = \hat{A}\hat{B}$. Again, since $\hat{A}$ and $\hat{B}$ are Hermitian and since they commute, we see that $(\hat{A}\hat{B})^\dagger = \hat{B}\hat{A} = \hat{A}\hat{B}$. As for the square of $\hat{A}\hat{B}$, we have

$$(\hat{A}\hat{B})^2 = (\hat{A}\hat{B})(\hat{A}\hat{B}) = \hat{A}(\hat{B}\hat{A})\hat{B} = \hat{A}(\hat{A}\hat{B})\hat{B} = \hat{A}^2\hat{B}^2 = \hat{A}\hat{B}, \tag{2.372}$$

hence the product $\hat{A}\hat{B}$ is a projection operator.

Problem 2.4

Consider a state $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle$ which is given in terms of three orthonormal eigenstates $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$ of an operator $\hat{B}$ such that $\hat{B}|\phi_n\rangle = n^2|\phi_n\rangle$. Find the expectation value of $\hat{B}$ for the state $|\psi\rangle$.

Solution

Using Eq (2.58), we can write the expectation value of $\hat{B}$ for the state $|\psi\rangle$ as $\langle\hat{B}\rangle = \langle\psi \mid \hat{B} \mid \psi\rangle/\langle\psi \mid \psi\rangle$ where

$$\begin{aligned} \langle\psi \mid \psi\rangle &= \left(\frac{1}{\sqrt{2}}\langle\phi_1 \mid + \frac{1}{\sqrt{5}}\langle\phi_2 \mid + \frac{1}{\sqrt{10}}\langle\phi_3 \mid\right)\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right) \\ &= \frac{8}{10} \end{aligned} \tag{2.373}$$

and

$$\begin{aligned} \langle\psi \mid \hat{B} \mid \psi\rangle &= \left(\frac{1}{\sqrt{2}}\langle\phi_1 \mid + \frac{1}{\sqrt{5}}\langle\phi_2 \mid + \frac{1}{\sqrt{10}}\langle\phi_3 \mid\right)\hat{B}\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right) \\ &= \frac{1}{2} + \frac{2^2}{5} + \frac{3^2}{10} \\ &= \frac{22}{10}. \end{aligned} \tag{2.374}$$

Hence, the expectation value of $\hat{B}$ is given by

$$\langle\hat{B}\rangle = \frac{\langle\psi \mid \hat{B} \mid \psi\rangle}{\langle\psi \mid \psi\rangle} = \frac{22/10}{8/10} = \frac{11}{4}. \tag{2.375}$$

Problem 2.5

(a) Study the hermiticity of these operators: $\hat{X}$, d/dx, and id/dx. What about the complex conjugate of these operators? Are the Hermitian conjugates of the position and momentum operators equal to their complex conjugates?

(b) Use the results of (a) to discuss the hermiticity of the operators $e^{\hat{X}}$, $e^{d/dx}$, and $e^{id/dx}$.

(c) Find the Hermitian conjugate of the operator $\hat{X}d/dx$.

(d) Use the results of (a) to discuss the hermiticity of the components of the angular momentum operator (Chapter 5): $\hat{L}_x = -i\hbar\left(\hat{Y}\partial/\partial z - \hat{Z}\partial/\partial y\right)$, $\hat{L}_y = -i\hbar\left(\hat{Z}\partial/\partial x - \hat{X}\partial/\partial z\right)$, $\hat{L}_z = -i\hbar\left(\hat{X}\partial/\partial y - \hat{Y}\partial/\partial x\right)$.

Solution

(a) Using (2.69) and (2.70), and using the fact that the eigenvalues of $\hat{X}$ are real (i.e., $\hat{X}^* = \hat{X}$ or $x^* = x$), we can verify that $\hat{X}$ is Hermitian (i.e., $\hat{X}^\dagger = \hat{X}$) since

$$\begin{aligned}\langle\psi \mid \hat{X}\psi\rangle &= \int_{-\infty}^{+\infty} \psi^*(x)\,(x\,\psi(x))\,dx = \int_{-\infty}^{+\infty} \left(x\,\psi(x)^*\right)\psi(x)\,dx \\ &= \int_{-\infty}^{+\infty} (x\,\psi(x))^*\,\psi(x)\,dx = \langle\hat{X}\psi \mid \psi\rangle. \end{aligned} \tag{2.376}$$

Now, since $\psi(x)$ vanishes as $x \to \pm\infty$, an integration by parts leads to

$$\begin{aligned}\langle\psi \mid \frac{d}{dx}\psi\rangle &= \int_{-\infty}^{+\infty}\psi^*(x)\left(\frac{d\psi(x)}{dx}\right)dx = \psi^*(x)\psi(x)\Big|_{x=-\infty}^{x=+\infty} - \int_{-\infty}^{+\infty}\left(\frac{d\psi^*(x)}{dx}\right)\psi(x)\,dx \\ &= -\int_{-\infty}^{+\infty}\left(\frac{d\psi(x)}{dx}\right)^*\psi(x)\,dx = -\langle\frac{d}{dx}\psi \mid \psi\rangle. \end{aligned} \tag{2.377}$$

So, d/dx is anti-Hermitian: $(d/dx)^\dagger = -d/dx$. Since d/dx is anti-Hermitian, id/dx must be Hermitian, since $(id/dx)^\dagger = -i\,(-d/dx) = id/dx$. The results derived above are

$$\boxed{\hat{X}^\dagger = \hat{X}, \qquad \left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}, \qquad \left(i\frac{d}{dx}\right)^\dagger = i\frac{d}{dx}.} \tag{2.378}$$

From this relation we see that the momentum operator $\hat{P} = -i\hbar d/dx$ is Hermitian: $\hat{P}^\dagger = \hat{P}$. We can also infer that, although the momentum operator is Hermitian, its complex conjugate is not equal to $\hat{P}$, since $\hat{P}^* = (-i\hbar d/dx)^* = i\hbar d/dx = -\hat{P}$. We may group these results into the following relation:

$$\boxed{\hat{X}^\dagger = \hat{X}, \quad \hat{X}^* = \hat{X}, \qquad \hat{P}^\dagger = \hat{P}, \quad \hat{P}^* = -\hat{P}.} \tag{2.379}$$

(b) Using the relations $(e^{\hat{A}})^\dagger = e^{\hat{A}^\dagger}$ and $(e^{i\hat{A}})^\dagger = e^{-i\hat{A}^\dagger}$ derived in (2.113), we infer

$$\boxed{(e^{\hat{X}})^\dagger = e^{\hat{X}}, \qquad (e^{d/dx})^\dagger = e^{-d/dx}, \qquad (e^{id/dx})^\dagger = e^{id/dx}.} \tag{2.380}$$

(c) Since $\hat{X}$ is Hermitian and d/dx is anti-Hermitian, we have

$$\left(\hat{X}\frac{d}{dx}\right)^\dagger = \left(\frac{d}{dx}\right)^\dagger(\hat{X})^\dagger = -\frac{d}{dx}\hat{X}, \tag{2.381}$$

where $d\hat{X}/dx$ is given by

$$\frac{d}{dx}\left(\hat{X}\psi(x)\right) = \left(1 + x\frac{d}{dx}\right)\psi(x); \tag{2.382}$$

hence

$$\left(\hat{X}\frac{d}{dx}\right)^\dagger = -\hat{X}\frac{d}{dx} - 1. \tag{2.383}$$

(d) From the results derived in (a), we infer that the operators $\hat{Y}$, $\hat{Z}$, $i\partial/\partial x$, and $i\partial/\partial y$ are Hermitian. We can verify that $\hat{L}_x$ is also Hermitian:

$$\hat{L}_x^\dagger = -i\hbar\left(\frac{\partial}{\partial z}\hat{Y} - \frac{\partial}{\partial y}\hat{Z}\right) = -i\hbar\left(\hat{Y}\frac{\partial}{\partial z} - \hat{Z}\frac{\partial}{\partial y}\right) = \hat{L}_x; \tag{2.384}$$

in deriving this relation, we used the fact that the y and z degrees of freedom commute (i.e., $\partial\hat{Y}/\partial z = \hat{Y}\partial/\partial z$ and $\partial\hat{Z}/\partial y = \hat{Z}\partial/\partial y$), for they are independent. Similarly, the hermiticity of $\hat{L}_y = -i\hbar\left(\hat{Z}\partial/\partial x - \hat{X}\partial/\partial z\right)$ and $\hat{L}_z = -i\hbar\left(\hat{X}\partial/\partial y - \hat{Y}\partial/\partial x\right)$ is obvious.

Problem 2.6

(a) Show that the operator $\hat{A} = i(\hat{X}^2 + 1)d/dx + i\hat{X}$ is Hermitian.

(b) Find the state $\psi(x)$ for which $\hat{A}\psi(x) = 0$ and normalize it.

(c) Calculate the probability of finding the particle (represented by $\psi(x)$) in the region: $-1 \leq x \leq 1$.

Solution

(a) From the previous problem we know that $\hat{X}^\dagger = \hat{X}$ and $(d/dx)^\dagger = -d/dx$. We can thus infer the Hermitian conjugate of $\hat{A}$:

$$\begin{aligned} \hat{A}^\dagger &= -i\left(\frac{d}{dx}\right)^\dagger(\hat{X}^2)^\dagger - i\left(\frac{d}{dx}\right)^\dagger - i\hat{X}^\dagger = i\left(\frac{d}{dx}\right)(\hat{X}^2) + i\left(\frac{d}{dx}\right) - i\hat{X} \\ &= i\hat{X}^2\frac{d}{dx} + i\left[\frac{d}{dx},\ \hat{X}^2\right] + i\frac{d}{dx} - i\hat{X}. \end{aligned} \tag{2.385}$$

Using the relation $[\hat{B},\ \hat{C}^2] = \hat{C}[\hat{B},\ \hat{C}] + [\hat{B},\ \hat{C}]\hat{C}$ along with $[d/dx,\ \hat{X}] = 1$, we can easily evaluate the commutator $[d/dx,\ \hat{X}^2]$:

$$\left[\frac{d}{dx},\ \hat{X}^2\right] = \hat{X}\left[\frac{d}{dx},\ \hat{X}\right] + \left[\frac{d}{dx},\ \hat{X}\right]\hat{X} = 2\hat{X}. \tag{2.386}$$

A combination of (2.385) and (2.386) shows that $\hat{A}$ is Hermitian:

$$\hat{A}^\dagger = i(\hat{X}^2 + 1)\frac{d}{dx} + i\hat{X} = \hat{A}. \tag{2.387}$$

(b) The state $\psi(x)$ for which $\hat{A}\psi(x) = 0$, i.e.,

$$i(\hat{X}^2 + 1)\frac{d\psi(x)}{dx} + i\hat{X}\psi(x) = 0, \tag{2.388}$$

corresponds to

$$\frac{d\psi(x)}{dx} = -\frac{x}{x^2 + 1}\psi(x). \tag{2.389}$$

The solution to this equation is given by

$$\psi(x) = \frac{B}{\sqrt{x^2 + 1}}. \tag{2.390}$$

Since $\int_{-\infty}^{+\infty} dx/(x^2+1) = \pi$ we have

$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = B^2 \int_{-\infty}^{+\infty} \frac{dx}{x^2+1} = B^2\pi, \tag{2.391}$$

which leads to $B = 1/\sqrt{\pi}$ and hence $\psi(x) = \frac{1}{\sqrt{\pi(x^2+1)}}$.

(c) Using the integral $\int_{-1}^{+1} dx/(x^2+1) = \pi/2$, we can obtain the probability immediately:

$$P = \int_{-1}^{+1} |\psi(x)|^2\, dx = \frac{1}{\pi}\int_{-1}^{+1} \frac{dx}{x^2+1} = \frac{1}{2}. \tag{2.392}$$

Problem 2.7
Discuss the conditions for these operators to be unitary: (a) $(1+i\hat{A})/(1-i\hat{A})$, (b) $(\hat{A}+i\hat{B})/\sqrt{\hat{A}^2+\hat{B}^2}$.

Solution
An operator $\hat{U}$ is unitary if $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$ (see (2.122)).

(a) Since

$$\left(\frac{1+i\hat{A}}{1-i\hat{A}}\right)^\dagger = \frac{1-i\hat{A}^\dagger}{1+i\hat{A}^\dagger}, \tag{2.393}$$

we see that if $\hat{A}$ is Hermitian, the expression $(1+i\hat{A})/(1-i\hat{A})$ is unitary:

$$\left(\frac{1+i\hat{A}}{1-i\hat{A}}\right)^\dagger \frac{1+i\hat{A}}{1-i\hat{A}} = \frac{1-i\hat{A}}{1+i\hat{A}}\frac{1+i\hat{A}}{1-i\hat{A}} = \hat{I}. \tag{2.394}$$

(b) Similarly, if $\hat{A}$ and $\hat{B}$ are Hermitian and commute, the expression $(\hat{A}+i\hat{B})/\sqrt{\hat{A}^2+\hat{B}^2}$ is unitary:

$$\begin{aligned}\left(\frac{\hat{A}+i\hat{B}}{\sqrt{\hat{A}^2+\hat{B}^2}}\right)^\dagger \frac{\hat{A}+i\hat{B}}{\sqrt{\hat{A}^2+\hat{B}^2}} &= \frac{\hat{A}-i\hat{B}}{\sqrt{\hat{A}^2+\hat{B}^2}}\frac{\hat{A}+i\hat{B}}{\sqrt{\hat{A}^2+\hat{B}^2}} = \frac{\hat{A}^2+\hat{B}^2+i(\hat{A}\hat{B}-\hat{B}\hat{A})}{\hat{A}^2+\hat{B}^2} \\ &= \frac{\hat{A}^2+\hat{B}^2}{\hat{A}^2+\hat{B}^2} = \hat{I}. \end{aligned} \tag{2.395}$$

Problem 2.8
(a) Using the commutator $[\hat{X},\ \hat{p}] = i\hbar$, show that $[\hat{X}^m,\ \hat{P}] = im\hbar\hat{X}^{m-1}$, with $m > 1$. Can you think of a direct way to get to the same result?

(b) Use the result of (a) to show the general relation $[F(\hat{X}),\ \hat{P}] = i\hbar dF(\hat{X})/d\hat{X}$, where $F(\hat{X})$ is a differentiable operator function of $\hat{X}$.

Solution

(a) Let us attempt a proof by induction. Assuming that $[\hat{X}^m,\ \hat{P}] = im\hbar\hat{X}^{m-1}$ is valid for $m = k$ (note that it holds for $n = 1$; i.e., $[\hat{X},\ \hat{P}] = i\hbar$),

$$[\hat{X}^k,\ \hat{P}] = ik\hbar\hat{X}^{k-1}, \tag{2.396}$$

let us show that it holds for $m = k + 1$:

$$[\hat{X}^{k+1},\ \hat{P}] = [\hat{X}^k\hat{X},\ \hat{P}] = \hat{X}^k[\hat{X},\ \hat{P}] + [\hat{X}^k,\ \hat{P}]\hat{X}, \tag{2.397}$$

where we have used the relation $[\hat{A}\hat{B},\ \hat{C}] = \hat{A}[\hat{B},\ \hat{C}] + [\hat{A},\ \hat{C}]\hat{B}$. Now, since $[\hat{X},\ \hat{P}] = i\hbar$ and $[\hat{X}^k,\ \hat{P}] = ik\hbar\hat{X}^{k-1}$, we rewrite (2.397) as

$$[\hat{X}^{k+1},\ \hat{P}] = i\hbar\hat{X}^k + (ik\hbar\hat{X}^{k-1})\hat{X} = i\hbar(k+1)\hat{X}^k. \tag{2.398}$$

So this relation is valid for any value of k, notably for $k = m - 1$:

$$\boxed{[\hat{X}^m,\ \hat{P}] = im\hbar\hat{X}^{m-1}.} \tag{2.399}$$

In fact, it is easy to arrive at this result *directly* through brute force as follows. Using the relation $[\hat{A}^n, \hat{B}] = \hat{A}^{n-1}[\hat{A}, \hat{B}] + [\hat{A}^{n-1}, \hat{B}]\hat{A}$ along with $[\hat{X}, \hat{P}_x] = i\hbar$, we can obtain

$$[\hat{X}^2, \hat{P}_x] = \hat{X}[\hat{X}, \hat{P}_x] + [\hat{X}, \hat{P}_x]\hat{X} = 2i\hbar\hat{X}, \tag{2.400}$$

which leads to

$$[\hat{X}^3, \hat{P}_x] = \hat{X}^2[\hat{X}, \hat{P}_x] + [\hat{X}^2, \hat{P}_x]\hat{X} = 3i\hat{X}^2\hbar; \tag{2.401}$$

this in turn leads to

$$[\hat{X}^4, \hat{P}_x] = \hat{X}^3[\hat{X}, \hat{P}_x] + [\hat{X}^3, \hat{P}_x]\hat{X} = 4i\hat{X}^3\hbar. \tag{2.402}$$

Continuing in this way, we can get to any power of $\hat{X}$: $[\hat{X}^m,\ \hat{P}] = im\hbar\hat{X}^{m-1}$.

A more direct and simpler method is to apply the commutator $[\hat{X}^m,\ \hat{P}]$ on some wave function $\psi(x)$:

$$\begin{aligned}
[\hat{X}^m, \hat{P}_x]\psi(x) &= \left(\hat{X}^m\hat{P}_x - \hat{P}_x\hat{X}^m\right)\psi(x) \\
&= x^m\left(-i\hbar\frac{d\psi(x)}{dx}\right) + i\hbar\frac{d}{dx}\left(x^m\psi(x)\right) \\
&= x^m\left(-i\hbar\frac{d\psi(x)}{dx}\right) + im\hbar x^{m-1}\psi(x) - x^m\left(-i\hbar\frac{d\psi(x)}{dx}\right) \\
&= im\hbar x^{m-1}\psi(x).
\end{aligned} \tag{2.403}$$

Since $[\hat{X}^m, \hat{P}_x]\psi(x) = im\hbar x^{m-1}\psi(x)$ we see that $[\hat{X}^m,\ \hat{P}] = im\hbar\hat{X}^{m-1}$.

(b) Let us Taylor expand $F(\hat{X})$ in powers of $\hat{X}$, $F(\hat{X}) = \sum_k a_k\hat{X}^k$, and insert this expression into $[F(\hat{X}),\ \hat{P}]$:

$$\left[F(\hat{X}),\ \hat{P}\right] = \left[\sum_k a_k\hat{X}^k,\ \hat{P}\right] = \sum_k a_k[\hat{X}^k,\ \hat{P}], \tag{2.404}$$

where the commutator $[\hat{X}^k,\ \hat{P}]$ is given by (2.396). Thus, we have

$$\left[F(\hat{X}),\ \hat{P}\right] = i\hbar \sum_k k a_k \hat{X}^{k-1} = i\hbar \frac{d(\sum_k a_k \hat{X}^k)}{d\hat{X}} = i\hbar \frac{dF(\hat{X})}{d\hat{X}}. \tag{2.405}$$

A much simpler method again consists in applying the commutator $\left[F(\hat{X}),\ \hat{P}\right]$ on some wave function $\psi(x)$. Since $F(\hat{X})\psi(x) = F(x)\psi(x)$, we have

$$\begin{aligned}\left[F(\hat{X}),\ \hat{P}\right]\psi(x) &= F(\hat{X})\hat{P}\psi(x) + i\hbar\frac{d}{dx}\left(F(x)\psi(x)\right)\\ &= F(\hat{X})\hat{P}\psi(x) - \left(-i\hbar\frac{d\psi(x)}{dx}\right)F(x) + i\hbar\frac{dF(x)}{dx}\psi(x)\\ &= F(\hat{X})\hat{P}\psi(x) - F(\hat{X})\hat{P}\psi(x) + i\hbar\frac{dF(x)}{dx}\psi(x)\\ &= i\hbar\frac{dF(x)}{dx}\psi(x).\end{aligned} \tag{2.406}$$

Since $\left[F(\hat{X}),\ \hat{P}\right]\psi(x) = i\hbar\frac{dF(x)}{dx}\psi(x)$ we see that $\left[F(\hat{X}),\ \hat{P}\right] = i\hbar\frac{dF(\hat{X})}{d\hat{X}}$.

Problem 2.9

Consider the matrices $A = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 & 3 \\ 0 & 2i & 0 \\ i & 0 & -5i \end{pmatrix}$.

(a) Are A and B Hermitian? Calculate AB and BA and verify that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$; then calculate $[A,\ B]$ and verify that $\mathrm{Tr}([A,\ B]) = 0$.

(b) Find the eigenvalues and the normalized eigenvectors of A. Verify that the sum of the eigenvalues of A is equal to the value of $\mathrm{Tr}(A)$ calculated in (a) and that the three eigenvectors form a basis.

(c) Verify that $U^\dagger AU$ is diagonal and that $U^{-1} = U^\dagger$, where U is the matrix formed by the normalized eigenvectors of A.

(d) Calculate the inverse of $A' = U^\dagger AU$ and verify that A'^{-1} is a diagonal matrix whose eigenvalues are the inverse of those of A'.

Solution

(a) Taking the Hermitian adjoints of the matrices A and B (see (2.188))

$$A^\dagger = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}, \qquad B^\dagger = \begin{pmatrix} 1 & 0 & -i \\ 0 & -2i & 0 \\ 3 & 0 & 5i \end{pmatrix}, \tag{2.407}$$

we see that A is Hermitian and B is not. Using the products

$$AB = \begin{pmatrix} 7 & 0 & 21 \\ 1 & 2i & -5 \\ -i & -2 & 5i \end{pmatrix}, \quad BA = \begin{pmatrix} 7 & 3i & -3 \\ 0 & 2i & 2 \\ 7i & 5 & 5i \end{pmatrix}, \tag{2.408}$$

we can obtain the commutator

$$[A, B] = \begin{pmatrix} 0 & -3i & 24 \\ 1 & 0 & -7 \\ -8i & -7 & 0 \end{pmatrix}. \tag{2.409}$$

From (2.408) we see that

$$\text{Tr}(AB) = 7 + 2i + 5i = 7 + 7i = \text{Tr}(BA). \tag{2.410}$$

That is, the cyclic permutation of matrices leaves the trace unchanged; see (2.206). On the other hand, (2.409) shows that the trace of the commutator $[A, B]$ is zero: $\text{Tr}([A, B]) = 0+0+0 = 0$.

(b) The eigenvalues and eigenvectors of A were calculated in Example 2.19 (see (2.266), (2.268), (2.272), (2.274)). We have $a_1 = 7$, $a_2 = \sqrt{2}$, and $a_3 = -\sqrt{2}$:

$$| a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad | a_2\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2(2-\sqrt{2})}} \\ \frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} \end{pmatrix}, \quad | a_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2(2+\sqrt{2})}} \\ -\frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix}. \tag{2.411}$$

One can easily verify that the eigenvectors $| a_1\rangle$, $| a_2\rangle$, and $| a_3\rangle$ are mutually orthogonal: $\langle a_i \mid a_j\rangle = \delta_{ij}$ where $i, j = 1, 2, 3$. Since the set of $| a_1\rangle$, $| a_2\rangle$, and $| a_3\rangle$ satisfy the completeness condition

$$\sum_{j=1}^{3} | a_j\rangle\langle a_j | = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.412}$$

and since they are orthonormal, they form a complete and orthonormal basis.

(c) The columns of the matrix U are given by the eigenvectors (2.411):

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2(2-\sqrt{2})}} & \frac{1}{\sqrt{2(2+\sqrt{2})}} \\ 0 & \frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} & -\frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix}. \tag{2.413}$$

We can show that the product $U^\dagger AU$ is diagonal where the diagonal elements are the eigenvalues of the matrix A; $U^\dagger AU$ is given by

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2(2-\sqrt{2})}} & -\frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} \\ 0 & \frac{1}{\sqrt{2(2+\sqrt{2})}} & \frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix} \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2(2-\sqrt{2})}} & \frac{1}{\sqrt{2(2+\sqrt{2})}} \\ 0 & \frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} & -\frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix}$$

$$= \begin{pmatrix} 7 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & -\sqrt{2} \end{pmatrix}. \tag{2.414}$$

We can also show that $U^\dagger U = 1$:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2(2-\sqrt{2})}} & -\frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} \\ 0 & \frac{1}{\sqrt{2(2+\sqrt{2})}} & \frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2(2-\sqrt{2})}} & \frac{1}{\sqrt{2(2+\sqrt{2})}} \\ 0 & \frac{i(\sqrt{2}-1)}{\sqrt{2(2-\sqrt{2})}} & -\frac{i(1+\sqrt{2})}{\sqrt{2(2+\sqrt{2})}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.415}$$

This implies that the matrix U is unitary: $U^\dagger = U^{-1}$. Note that, from (2.413), we have $|\det(U)| = |-i| = 1$.

(d) Using (2.414) we can verify that the inverse of $A' = U^\dagger A U$ is a diagonal matrix whose elements are given by the inverse of the diagonal elements of A':

$$A' = \begin{pmatrix} 7 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & -\sqrt{2} \end{pmatrix} \implies A'^{-1} = \begin{pmatrix} \frac{1}{7} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}. \tag{2.416}$$

Problem 2.10

Consider a particle whose Hamiltonian matrix is $H = \begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix}$.

(a) Is $|\lambda\rangle = \begin{pmatrix} i \\ 7i \\ -2 \end{pmatrix}$ an eigenstate of H? Is H Hermitian?

(b) Find the energy eigenvalues, a_1, a_2, and a_3, and the normalized energy eigenvectors, $|a_1\rangle$, $|a_2\rangle$, and $|a_3\rangle$, of H.

(c) Find the matrix corresponding to the operator obtained from the ket-bra product of the first eigenvector $P = |a_1\rangle\langle a_1|$. Is P a projection operator? Calculate the commutator $[P,\ H]$ firstly by using commutator algebra and then by using matrix products.

Solution

(a) The ket $|\lambda\rangle$ is an eigenstate of H only if the action of the Hamiltonian on $|\lambda\rangle$ is of the form $H|\lambda\rangle = b|\lambda\rangle$, where b is constant. This is not the case here:

$$H|\lambda\rangle = \begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} i \\ 7i \\ -2 \end{pmatrix} = \begin{pmatrix} -7+2i \\ -1+7i \\ 7i \end{pmatrix}. \tag{2.417}$$

Using the definition of the Hermitian adjoint of matrices (2.188), it is easy to ascertain that H is Hermitian:

$$H^\dagger = \begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} = H. \tag{2.418}$$

(b) The energy eigenvalues can be obtained by solving the secular equation

$$\begin{aligned} 0 &= \begin{vmatrix} 2-a & i & 0 \\ -i & 1-a & 1 \\ 0 & 1 & -a \end{vmatrix} = (2-a)\left[(1-a)(-a)-1\right] - i(-i)(-a) \\ &= -(a-1)(a-1-\sqrt{3})(a-1+\sqrt{3}), \end{aligned} \tag{2.419}$$

which leads to

$$a_1 = 1, \quad a_2 = 1 - \sqrt{3}, \quad a_3 = 1 + \sqrt{3}. \tag{2.420}$$

To find the eigenvector corresponding to the first eigenvalue, $a_1 = 1$, we need to solve the matrix equation

$$\begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Longrightarrow \begin{array}{rcl} x + iy & = & 0 \\ -ix + z & = & 0 \\ y - z & = & 0 \end{array} \tag{2.421}$$

which yields $x = 1$, $y = z = i$. So the eigenvector corresponding to $a_1 = 1$ is

$$| \, a_1 \rangle = \begin{pmatrix} 1 \\ i \\ i \end{pmatrix}. \tag{2.422}$$

This eigenvector is not normalized since $\langle a_1 \mid a_1 \rangle = 1 + (i^*)(i) + (i^*)(i) = 3$. The normalized $| \, a_1 \rangle$ is therefore

$$| \, a_1 \rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ i \\ i \end{pmatrix}. \tag{2.423}$$

Solving (2.421) for the other two energy eigenvalues, $a_2 = 1 - \sqrt{3}$, $a_3 = 1 + \sqrt{3}$, and normalizing, we end up with

$$| \, a_2 \rangle = \frac{1}{\sqrt{6(2 - \sqrt{3})}} \begin{pmatrix} i(2 - \sqrt{3}) \\ 1 - \sqrt{3} \\ 1 \end{pmatrix}, \qquad | \, a_3 \rangle = \frac{1}{\sqrt{6(2 + \sqrt{3})}} \begin{pmatrix} i(2 + \sqrt{3}) \\ 1 + \sqrt{3} \\ 1 \end{pmatrix}. \tag{2.424}$$

(c) The operator P is given by

$$P = | \, a_1 \rangle \langle a_1 \, | = \frac{1}{3} \begin{pmatrix} 1 \\ i \\ i \end{pmatrix} \begin{pmatrix} 1 & -i & -i \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix}. \tag{2.425}$$

Since this matrix is Hermitian and since the square of P is equal to P,

$$P^2 = \frac{1}{9} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix} = P, \tag{2.426}$$

so P is a projection operator. Using the relations $H \mid a_1 \rangle = \mid a_1 \rangle$ and $\langle a_1 \mid H = \langle a_1 \mid$ (because H is Hermitian), and since $P = \mid a_1 \rangle \langle a_1 \mid$, we can evaluate algebraically the commutator $[P, \, H]$ as follows:

$$[P, \, H] = PH - HP = | \, a_1 \rangle \langle a_1 \mid H - H \mid a_1 \rangle \langle a_1 \, | = | \, a_1 \rangle \langle a_1 \, | - | \, a_1 \rangle \langle a_1 \, | = 0. \tag{2.427}$$

We can reach the same result by using the matrices of H and P:

$$\begin{aligned} [P, \, H] &= \frac{1}{3} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix} \begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \frac{1}{3} \begin{pmatrix} 2 & i & 0 \\ -i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & -i & -i \\ i & 1 & 1 \\ i & 1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{2.428}$$

Problem 2.11

Consider the matrices $A = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix}$.

(a) Check if A and B are Hermitian and find the eigenvalues and eigenvectors of A. Any degeneracies?

(b) Verify that $\text{Tr}(AB) = \text{Tr}(BA)$, $\det(AB) = \det(A)\det(B)$, and $\det(B^\dagger) = (\det(B))^*$.

(c) Calculate the commutator $[A, B]$ and the anticommutator $\{A, B\}$.

(d) Calculate the inverses A^{-1}, B^{-1}, and $(AB)^{-1}$. Verify that $(AB)^{-1} = B^{-1}A^{-1}$.

(e) Calculate A^2 and infer the expressions of A^{2n} and A^{2n+1}. Use these results to calculate the matrix of e^{xA}.

Solution

(a) The matrix A is Hermitian but B is not. The eigenvalues of A are $a_1 = -1$ and $a_2 = a_3 = 1$ and its normalized eigenvectors are

$$\mid a_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}, \qquad \mid a_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix}, \qquad \mid a_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{2.429}$$

Note that the eigenvalue 1 is doubly degenerate, since the two eigenvectors $\mid a_2\rangle$ and $\mid a_3\rangle$ correspond to the same eigenvalue $a_2 = a_3 = 1$.

(b) A calculation of the products (AB) and (BA) reveals that the traces $\text{Tr}(AB)$ and $\text{Tr}(BA)$ are equal:

$$\begin{aligned} \text{Tr}(AB) &= \text{Tr}\begin{pmatrix} 0 & 1 & -2i \\ 3 & 1 & 5 \\ -2i & 1 & 0 \end{pmatrix} = 1, \\ \text{Tr}(BA) &= \text{Tr}\begin{pmatrix} 0 & i & 2i \\ -5i & 1 & 3i \\ 2i & -i & 0 \end{pmatrix} = 1 = \text{Tr}(AB). \end{aligned} \tag{2.430}$$

From the matrices A and B, we have $\det(A) = i(i) = -1$, $\det(B) = -4 + 16i$. We can thus write

$$\det(AB) = \det\begin{pmatrix} 0 & 1 & -2i \\ 3 & 1 & 5 \\ -2i & 1 & 0 \end{pmatrix} = 4 - 16i = (-1)(-4 + 16i) = \det(A)\det(B). \tag{2.431}$$

On the other hand, since $\det(B) = -4 + 16i$ and $\det(B^\dagger) = -4 - 16i$, we see that $\det(B^\dagger) = -4 - 16i = (-4 + 16i)^* = (\det(B))^*$.

(c) The commutator $[A,\ B]$ is given by

$$AB - BA = \begin{pmatrix} 0 & 1 & -2i \\ 3 & 1 & 5 \\ -2i & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & i & 2i \\ -5i & 1 & 3i \\ 2i & -i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1-i & -4i \\ 3+5i & 0 & 5-3i \\ -4i & 1+i & 0 \end{pmatrix} \tag{2.432}$$

and the anticommutator $\{A, B\}$ by

$$AB + BA = \begin{pmatrix} 0 & 1 & -2i \\ 3 & 1 & 5 \\ -2i & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & i & 2i \\ -5i & 1 & 3i \\ 2i & -i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1+i & 0 \\ 3-5i & 2 & 5+3i \\ 0 & 1-i & 0 \end{pmatrix}. \tag{2.433}$$

(d) A calculation similar to (2.200) leads to the inverses of A, B, and AB:

$$A^{-1} = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}, \qquad B^{-1} = \frac{1}{68}\begin{pmatrix} 22+3i & 8-2i & 20-5i \\ -6-24i & 4+16i & 10+40i \\ -12+3i & 8-2i & -14-5i \end{pmatrix}, \tag{2.434}$$

$$(AB)^{-1} = \frac{1}{68}\begin{pmatrix} -5-20i & 8-2i & -3+22i \\ 40-10i & 4+16i & 24-6i \\ -5+14i & 8-2i & -3-12i \end{pmatrix}. \tag{2.435}$$

From (2.434) it is now easy to verify that the product $B^{-1}A^{-1}$ is equal to $(AB)^{-1}$:

$$B^{-1}A^{-1} = \frac{1}{68}\begin{pmatrix} -5-20i & 8-2i & -3+22i \\ 40-10i & 4+16i & 24-6i \\ -5+14i & 8-2i & -3-12i \end{pmatrix} = (AB)^{-1}. \tag{2.436}$$

(e) Since

$$A^2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I, \tag{2.437}$$

we can write $A^3 = A$, $A^4 = I$, $A^5 = A$, and so on. We can generalize these relations to any value of n: $A^{2n} = I$ and $A^{2n+1} = A$:

$$A^{2n} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I, \qquad A^{2n+1} = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix} = A. \tag{2.438}$$

Since $A^{2n} = I$ and $A^{2n+1} = A$, we can write

$$e^{xA} = \sum_{n=0}^{\infty} \frac{x^n A^n}{n!} = \sum_{n=0}^{\infty} \frac{x^{2n} A^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{x^{2n+1} A^{2n+1}}{(2n+1)!} = I \sum_{n=0}^{\infty} \frac{x^{2n}}{(2n)!} + A \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!}. \tag{2.439}$$

The relations

$$\sum_{n=0}^{\infty} \frac{x^{2n}}{(2n)!} = \cosh x, \qquad \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!} = \sinh x, \tag{2.440}$$

lead to

$$\begin{aligned} e^{xA} &= I\cosh x + A\sinh x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\cosh x + \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}\sinh x \\ &= \begin{pmatrix} \cosh x & 0 & i\sinh x \\ 0 & \cosh x + \sinh x & 0 \\ -i\sinh x & 0 & \cosh x \end{pmatrix}. \end{aligned} \tag{2.441}$$

Problem 2.12

Consider two matrices: $A = \begin{pmatrix} 0 & i & 2 \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix}$. Calculate $A^{-1}\ B$ and $B\ A^{-1}$. Are they equal?

Solution

As mentioned above, a calculation similar to (2.200) leads to the inverse of A:

$$A^{-1} = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ 1/2 & -i/2 & 0 \end{pmatrix}. \tag{2.442}$$

The products $A^{-1}\ B$ and $B\ A^{-1}$ are given by

$$A^{-1}B = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ 1/2 & -i/2 & 0 \end{pmatrix} \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix} = \begin{pmatrix} 0 & 1 & -2i \\ 3 & 1 & 5 \\ 1-3i/2 & 0 & -5i/2 \end{pmatrix}, \tag{2.443}$$

$$BA^{-1} = \begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix} \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ 1/2 & -i/2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & i & 2i \\ 5/2 & 1-5i/2 & 3i \\ -1 & 0 & 0 \end{pmatrix}. \tag{2.444}$$

We see that $A^{-1}\ B$ and $B\ A^{-1}$ are not equal.

Remark

We should note that the quotient B/A of two matrices A and B is equal to the product BA^{-1} and not $A^{-1}B$; that is:

$$\frac{B}{A} = BA^{-1} = \frac{\begin{pmatrix} 2 & i & 0 \\ 3 & 1 & 5 \\ 0 & -i & -2 \end{pmatrix}}{\begin{pmatrix} 0 & i & 2 \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}} = \begin{pmatrix} 0 & i & 2i \\ 5/2 & 1-5i/2 & 3i \\ -1 & 0 & 0 \end{pmatrix}. \tag{2.445}$$

Problem 2.13

Consider the matrices $A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$.

(a) Find the eigenvalues and normalized eigenvectors of A and B. Denote the eigenvectors of A by $\mid a_1\rangle$, $\mid a_2\rangle$, $\mid a_3\rangle$ and those of B by $\mid b_1\rangle$, $\mid b_2\rangle$, $\mid b_3\rangle$. Are there any degenerate eigenvalues?

(b) Show that each of the sets $\mid a_1\rangle$, $\mid a_2\rangle$, $\mid a_3\rangle$ and $\mid b_1\rangle$, $\mid b_2\rangle$, $\mid b_3\rangle$ forms an orthonormal and complete basis, i.e., show that $\langle a_j \mid a_k\rangle = \delta_{jk}$ and $\sum_{j=1}^{3} \mid a_j\rangle\langle a_j \mid = I$, where I is the 3×3 unit matrix; then show that the same holds for $\mid b_1\rangle$, $\mid b_2\rangle$, $\mid b_3\rangle$.

(c) Find the matrix U of the transformation from the basis $\{\mid a\rangle\}$ to $\{\mid b\rangle\}$. Show that $U^{-1} = U^\dagger$. Verify that $U^\dagger U = I$. Calculate how the matrix A transforms under U, i.e., calculate $A' = UAU^\dagger$.

Solution

(a) It is easy to verify that the eigenvalues of A are $a_1 = 0$, $a_2 = \sqrt{2}$, $a_3 = -\sqrt{2}$ and their corresponding normalized eigenvectors are

$$| a_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \qquad | a_2\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \qquad | a_3\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}. \tag{2.446}$$

The eigenvalues of B are $b_1 = 1$, $b_2 = 0$, $b_3 = -1$ and their corresponding normalized eigenvectors are

$$| b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad | b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad | b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.447}$$

None of the eigenvalues of A and B are degenerate.

(b) The set $| a_1\rangle$, $| a_2\rangle$, $| a_3\rangle$ is indeed complete because the sum of $| a_1\rangle\langle a_1 |$, $| a_2\rangle\langle a_2 |$, and $| a_3\rangle\langle a_3 |$ as given by

$$| a_1\rangle\langle a_1 | = \frac{1}{2}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}\begin{pmatrix} -1 & 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \tag{2.448}$$

$$| a_2\rangle\langle a_2 | = \frac{1}{4}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}\begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}, \tag{2.449}$$

$$| a_3\rangle\langle a_3 | = \frac{1}{4}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}\begin{pmatrix} 1 & -\sqrt{2} & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}, \tag{2.450}$$

is equal to unity:

$$\begin{aligned} \sum_{j=1}^{3} | a_j\rangle\langle a_j | &= \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix} \\ &\quad + \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{2.451}$$

The states $| a_1\rangle$, $| a_2\rangle$, $| a_3\rangle$ are orthonormal, since $\langle a_1 | a_2\rangle = \langle a_1 | a_3\rangle = \langle a_3 | a_2\rangle = 0$ and $\langle a_1 | a_1\rangle = \langle a_2 | a_2\rangle = \langle a_3 | a_3\rangle = 1$. Following the same procedure, we can ascertain that

$$| b_1\rangle\langle b_1 | + | b_2\rangle\langle b_2 | + | b_3\rangle\langle b_3 | = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.452}$$

We can verify that the states $| b_1\rangle$, $| b_2\rangle$, $| b_3\rangle$ are orthonormal, since $\langle b_1 \mid b_2\rangle = \langle b_1 \mid b_3\rangle = \langle b_3 \mid b_2\rangle = 0$ and $\langle b_1 \mid b_1\rangle = \langle b_2 \mid b_2\rangle = \langle b_3 \mid b_3\rangle = 1$.

(c) The elements of the matrix U, corresponding to the transformation from the basis $\{| a\rangle\}$ to $\{| b\rangle\}$, are given by $U_{jk} = \langle b_j \mid a_k\rangle$ where $j,\ k = 1, 2, 3$:

$$U = \begin{pmatrix} \langle b_1 \mid a_1\rangle & \langle b_1 \mid a_2\rangle & \langle b_1 \mid a_3\rangle \\ \langle b_2 \mid a_1\rangle & \langle b_2 \mid a_2\rangle & \langle b_2 \mid a_3\rangle \\ \langle b_3 \mid a_1\rangle & \langle b_3 \mid a_2\rangle & \langle b_3 \mid a_3\rangle \end{pmatrix}, \tag{2.453}$$

where the elements $\langle b_j \mid a_k\rangle$ can be calculated from (2.446) and (2.447):

$$U_{11} = \langle b_1 \mid a_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = -\frac{\sqrt{2}}{2}, \tag{2.454}$$

$$U_{12} = \langle b_1 \mid a_2\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}, \tag{2.455}$$

$$U_{13} = \langle b_1 \mid a_3\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}, \tag{2.456}$$

$$U_{21} = \langle b_2 \mid a_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = 0, \tag{2.457}$$

$$U_{22} = \langle b_2 \mid a_2\rangle = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{\sqrt{2}}{2}, \tag{2.458}$$

$$U_{23} = \langle b_2 \mid a_3\rangle = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = -\frac{\sqrt{2}}{2}, \tag{2.459}$$

$$U_{31} = \langle b_3 \mid a_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = \frac{\sqrt{2}}{2}, \tag{2.460}$$

$$U_{32} = \langle b_3 \mid a_2\rangle = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}, \tag{2.461}$$

$$U_{33} = \langle b_3 \mid a_3\rangle = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}. \tag{2.462}$$

Collecting these elements, we obtain

$$U = \frac{1}{2} \begin{pmatrix} -\sqrt{2} & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ \sqrt{2} & 1 & 1 \end{pmatrix}. \tag{2.463}$$

Calculating the inverse of U as we did in (2.200), we see that it is equal to its Hermitian adjoint:

$$U^{-1} = \frac{1}{2}\begin{pmatrix} -\sqrt{2} & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \\ 1 & -\sqrt{2} & 1 \end{pmatrix} = U^{\dagger}. \tag{2.464}$$

This implies that the matrix U is unitary. The matrix A transforms as follows:

$$\begin{aligned} A' &= UAU^{\dagger} = \frac{1}{4}\begin{pmatrix} -\sqrt{2} & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ \sqrt{2} & 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} -\sqrt{2} & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 1-\sqrt{2} & -1 & 1 \\ -1 & -2 & 1 \\ 1 & 1 & 1+\sqrt{2} \end{pmatrix}. \end{aligned} \tag{2.465}$$

Problem 2.14

Calculate the following expressions involving Dirac's delta function:

(a) $\int_{-5}^{5} \cos(3x)\delta(x-\pi/3)\,dx$

(b) $\int_0^{10} \left[e^{2x-7}+4\right]\delta(x+3)\,dx$

(c) $\left[2\cos^2(3x) - \sin(x/2)\right]\delta(x+\pi)$

(d) $\int_0^{\pi} \cos(3\theta)\delta'''(\theta-\pi/2)\,d\theta$

(e) $\int_2^9 \left(x^2-5x+2\right)\delta[2(x-4)]\,dx$.

Solution

(a) Since $x=\pi/3$ lies within the interval $(-5,\ 5)$, equation (2.281) yields

$$\int_{-5}^{5} \cos(3x)\delta(x-\pi/3)\,dx = \cos\left(3\frac{\pi}{3}\right) = -1. \tag{2.466}$$

(b) Since $x=-3$ lies outside the interval $(0,\ 10)$, Eq (2.281) yields at once

$$\int_0^{10} \left[e^{2x-7}+4\right]\delta(x+3)\,dx = 0. \tag{2.467}$$

(c) Using the relation $f(x)\delta(x-a) = f(a)\delta(x-a)$ which is listed in Appendix A, we have

$$\begin{aligned} \left[2\cos^2(3x) - \sin(x/2)\right]\delta(x+\pi) &= \left[2\cos^2(3(-\pi)) - \sin((-\pi)/2)\right]\delta(x+\pi) \\ &= 3\delta(x+\pi). \end{aligned} \tag{2.468}$$

(d) Inserting $n=3$ into Eq (2.282) and since $\cos'''(3\theta) = 27\sin(3\theta)$, we obtain

$$\begin{aligned} \int_0^{\pi} \cos(3\theta)\delta'''(\theta-\pi/2)\,d\theta &= (-1)^3\cos'''(3\pi/2) = (-1)^3\,27\sin(3\pi/2) \\ &= 27. \end{aligned} \tag{2.469}$$

(e) Since $\delta[2(x-4)] = (1/2)\delta(x-4)$, we have

$$\begin{aligned} \int_2^9 \left(x^2 - 5x + 2\right) \delta[2(x-4)], dx &= \frac{1}{2}\int_2^9 \left(x^2 - 5x + 2\right) \delta(x-4)\, dx \\ &= \frac{1}{2}\left(4^2 - 5\times 4 + 2\right) = -1. \end{aligned} \quad (2.470)$$

Problem 2.15

Consider a system whose Hamiltonian is given by $\hat{H} = \alpha\left(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|\right)$, where α is a real number having the dimensions of energy and $|\,\phi_1\rangle$, $|\,\phi_2\rangle$ are normalized eigenstates of a Hermitian operator $\hat{A}$ that has no degenerate eigenvalues.

(a) Is $\hat{H}$ a projection operator? What about $\alpha^{-2}\hat{H}^2$?

(b) Show that $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ are not eigenstates of $\hat{H}$.

(c) Calculate the commutators $[\hat{H},\ |\,\phi_1\rangle\langle\phi_1\,|]$ and $[\hat{H},\ |\,\phi_2\rangle\langle\phi_2\,|]$ then find the relation that may exist between them.

(d) Find the normalized eigenstates of $\hat{H}$ and their corresponding energy eigenvalues.

(e) Assuming that $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ form a complete and orthonormal basis, find the matrix representing $\hat{H}$ in the basis. Find the eigenvalues and eigenvectors of the matrix and compare the results with those derived in (d).

Solution

(a) Since $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ are eigenstates of $\hat{A}$ and since $\hat{A}$ is Hermitian, they must be orthogonal, $\langle\phi_1\,|\,\phi_2\rangle = 0$ (instance of Theorem 2.1). Now, since $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ are both normalized and since $\langle\phi_1\,|\,\phi_2\rangle = 0$, we can reduce $\hat{H}^2$ to

$$\begin{aligned} \hat{H}^2 &= \alpha^2\left(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|\right)\left(|\,\phi_1\rangle\langle\phi_1\,| + |\,\phi_2\rangle\langle\phi_2\,|\right) \\ &= \alpha^2\left(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|\right), \end{aligned} \quad (2.471)$$

which is different from $\hat{H}$; hence $\hat{H}$ is not a projection operator. The operator $\alpha^{-2}\hat{H}^2$ is a projection operator since it is both Hermitian and equal to its own square. Using (2.471) we can write

$$\begin{aligned} (\alpha^{-2}\hat{H}^2)^2 &= \left(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|\right)\left(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|\right) \\ &= |\,\phi_1\rangle\langle\phi_1\,| + |\,\phi_2\rangle\langle\phi_2\,| = \alpha^{-2}\hat{H}^2. \end{aligned} \quad (2.472)$$

(b) Since $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ are both normalized, and since $\langle\phi_1\,|\,\phi_2\rangle = 0$, we have

$$\hat{H}\,|\,\phi_1\rangle = \alpha\,|\,\phi_1\rangle\langle\phi_2\,|\,\phi_1\rangle + \alpha\,|\,\phi_2\rangle\langle\phi_1\,|\,\phi_1\rangle = \alpha\,|\,\phi_2\rangle, \quad (2.473)$$

$$\hat{H}\,|\,\phi_2\rangle = \alpha\,|\,\phi_1\rangle; \quad (2.474)$$

hence $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ are not eigenstates of $\hat{H}$. In addition, we have

$$\langle\phi_1\,|\,\hat{H}\,|\,\phi_1\rangle = \langle\phi_2\,|\,\hat{H}\,|\,\phi_2\rangle = 0. \quad (2.475)$$

(c) Using the relations derived above, $\hat{H}\,|\,\phi_1\rangle = \alpha\,|\,\phi_2\rangle$ and $\hat{H}\,|\,\phi_2\rangle = \alpha\,|\,\phi_1\rangle$, we can write

$$[\hat{H}, |\,\phi_1\rangle\langle\phi_1\,|] = \alpha\left(|\,\phi_2\rangle\langle\phi_1\,| - |\,\phi_1\rangle\langle\phi_2\,|\right), \quad (2.476)$$

$$[\hat{H}, |\,\phi_2\rangle\langle\phi_2\,|] = \alpha\,(|\,\phi_1\rangle\langle\phi_2\,| - |\,\phi_2\rangle\langle\phi_1\,|)\,; \tag{2.477}$$

hence

$$[\hat{H}, |\,\phi_1\rangle\langle\phi_1\,|] = -[\hat{H}, |\,\phi_2\rangle\langle\phi_2\,|]. \tag{2.478}$$

(d) Consider a general state $|\,\psi\rangle = \lambda_1\,|\,\phi_1\rangle + \lambda_2\,|\,\phi_2\rangle$. Applying $\hat{H}$ to this state, we get

$$\begin{aligned}\hat{H}\,|\,\psi\rangle &= \alpha\,(|\,\phi_1\rangle\langle\phi_2\,| + |\,\phi_2\rangle\langle\phi_1\,|)\,(\lambda_1\,|\,\phi_1\rangle + \lambda_2\,|\,\phi_2\rangle) \\ &= \alpha\,(\lambda_2\,|\,\phi_1\rangle + \lambda_1\,|\,\phi_2\rangle)\,. \end{aligned} \tag{2.479}$$

Now, since $|\,\psi\rangle$ is normalized, we have

$$\langle\psi\,|\,\psi\rangle = |\,\lambda_1\,|^2 + |\,\lambda_2\,|^2 = 1. \tag{2.480}$$

The previous two equations show that $|\,\lambda_1\,| = |\,\lambda_2\,| = 1/\sqrt{2}$ and that $\lambda_1 = \pm\lambda_2$. Hence the eigenstates of the system are:

$$|\,\psi_\pm\rangle = \frac{1}{\sqrt{2}}\,(|\,\phi_1\rangle \pm |\,\phi_2\rangle)\,. \tag{2.481}$$

The corresponding eigenvalues are $\pm\alpha$:

$$\hat{H}\,|\,\psi_\pm\rangle = \pm\alpha\,|\,\psi_\pm\rangle. \tag{2.482}$$

(e) Since $\langle\phi_1\,|\,\phi_2\rangle = \langle\phi_2\,|\,\phi_1\rangle = 0$ and $\langle\phi_1\,|\,\phi_1\rangle = \langle\phi_2\,|\,\phi_2\rangle = 1$, we can verify that $H_{11} = \langle\phi_1\,|\,\hat{H}\,|\,\phi_1\rangle = 0$, $H_{22} = \langle\phi_2\,|\,\hat{H}\,|\,\phi_2\rangle = 0$, $H_{12} = \langle\phi_1\,|\,\hat{H}\,|\,\phi_2\rangle = \alpha$, $H_{21} = \langle\phi_2\,|\,\hat{H}\,|\,\phi_1\rangle = \alpha$. The matrix of $\hat{H}$ is thus given by

$$H = \alpha\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.483}$$

The eigenvalues of this matrix are equal to $\pm\alpha$ and the corresponding eigenvectors are $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$. These results are indeed similar to those derived in (d).

Problem 2.16

Consider the matrices $A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 7 & -3i \\ 0 & 3i & 5 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & -i & 3i \\ -i & 0 & i \\ 3i & i & 0 \end{pmatrix}$.

(a) Check the hermiticity of A and B.

(b) Find the eigenvalues of A and B; denote the eigenvalues of A by a_1, a_2, and a_3. Explain why the eigenvalues of A are real and those of B are imaginary.

(c) Calculate $\mathrm{Tr}(A)$ and $\det(A)$. Verify $\mathrm{Tr}(A) = a_1 + a_2 + a_3$, $\det(A) = a_1 a_2 a_3$.

Solution

(a) Matrix A is Hermitian but B is anti-Hermitian:

$$A^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 7 & -3i \\ 0 & 3i & 5 \end{pmatrix} = A, \qquad B^\dagger = \begin{pmatrix} 0 & i & -3i \\ i & 0 & -i \\ -3i & -i & 0 \end{pmatrix} = -B. \tag{2.484}$$

(b) The eigenvalues of A are $a_1 = 6 - \sqrt{10}$, $a_2 = 1$, and $a_3 = 6 + \sqrt{10}$ and those of B are $b_1 = -i\left(3 + \sqrt{17}\right)/2$, $b_2 = 3i$, and $b_3 = i\left(-3 + \sqrt{17}\right)/2$. The eigenvalues of A are real and those of B are imaginary. This is expected since, as shown in (2.74) and (2.75), the expectation values of Hermitian operators are real and those of anti-Hermitian operators are imaginary.

(c) A direct calculation of the trace and the determinant of A yields $\mathrm{Tr}(A) = 1+7+5 = 13$ and $\det(A) = (7)(5)-(3i)(-3i) = 26$. Adding and multiplying the eigenvalues $a_1 = 6-\sqrt{10}$, $a_2 = 1$, $a_3 = 6 + \sqrt{10}$, we have $a_1 + a_2 + a_3 = 6 - \sqrt{10} + 1 + 6 + \sqrt{10} = 13$ and $a_1a_2a_3 = (6 - \sqrt{10})(1)(6 + \sqrt{10}) = 26$. This confirms the results (2.260) and (2.261):

$$\mathrm{Tr}(A) = a_1 + a_2 + a_3 = 13, \qquad \det(A) = a_1a_2a_3 = 26. \tag{2.485}$$

Problem 2.17

Consider a one-dimensional particle which moves along the x-axis and whose Hamiltonian is $\hat{H} = -\mathcal{E}d^2/dx^2 + 16\mathcal{E}\hat{X}^2$, where $\mathcal{E}$ is a real constant having the dimensions of energy.

(a) Is $\psi(x) = Ae^{-2x^2}$, where A is a normalization constant that needs to be found, an eigenfunction of $\hat{H}$? If yes, find the energy eigenvalue.

(b) Calculate the probability of finding the particle anywhere along the negative x-axis.

(c) Find the energy eigenvalue corresponding to the wave function $\phi(x) = 2x\psi(x)$.

(d) Specify the parities of $\phi(x)$ and $\psi(x)$. Are $\phi(x)$ and $\psi(x)$ orthogonal?

Solution

(a) The integral $\int_{-\infty}^{+\infty} e^{-4x^2}dx = \sqrt{\pi}/2$ allows us to find the normalization constant:

$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = A^2\int_{-\infty}^{+\infty} e^{-4x^2}dx = A^2\frac{\sqrt{\pi}}{2}; \tag{2.486}$$

this leads to $A = \sqrt{2/\sqrt{\pi}}$ and hence $\psi(x) = \sqrt{2/\sqrt{\pi}}e^{-2x^2}$. Since the first and second derivatives of $\psi(x)$ are given by

$$\psi'(x) = \frac{d\psi(x)}{dx} = -4x\psi(x), \qquad \psi''(x) = \frac{d^2\psi(x)}{dx^2} = (16x^2 - 4)\psi(x), \tag{2.487}$$

we see that $\psi(x)$ is an eigenfunction of $\hat{H}$ with an energy eigenvalue equal to $4\mathcal{E}$:

$$\hat{H}\psi(x) = -\mathcal{E}\frac{d^2\psi(x)}{dx^2}+16\mathcal{E}x^2\psi(x) = -\mathcal{E}(16x^2-4)\psi(x)+16\mathcal{E}x^2\psi(x) = 4\mathcal{E}\psi(x). \tag{2.488}$$

(b) Since $\int_{-\infty}^{0} e^{-4x^2}dx = \sqrt{\pi}/4$, the probability of finding the particle anywhere along the negative x-axis is equal to $\frac{1}{2}$:

$$\int_{-\infty}^{0} |\psi(x)|^2\,dx = \frac{2}{\sqrt{\pi}}\int_{-\infty}^{0} e^{-4x^2}dx = \frac{1}{2}. \tag{2.489}$$

This is expected, since this probability is half the total probability, which in turn is equal to one.

(c) Since the second derivative of $\phi(x) = 2x\psi(x)$ is $\phi''(x) = 4\psi'(x) + 2x\psi''(x) = 8x(-3+4x^2)\psi(x) = 4(-3+4x^2)\phi(x)$, we see that $\phi(x)$ is an eigenfunction of $\hat{H}$ with an energy eigenvalue equal to $12\mathcal{E}$:

$$\hat{H}\phi(x) = -\mathcal{E}\frac{d^2\phi(x)}{dx^2} + 16\mathcal{E}x^2\phi(x) = -4\mathcal{E}(-3+4x^2)\phi(x) + 16\mathcal{E}x^2\phi(x) = 12\mathcal{E}\phi(x). \tag{2.490}$$

(d) The wave functions $\psi(x)$ and $\phi(x)$ are even and odd, respectively, since $\psi(-x) = \psi(x)$ and $\phi(-x) = -\phi(x)$; hence their product is an odd function. Therefore, they are orthogonal, since the symmetric integration of an odd function is zero:

$$\begin{aligned}\langle \phi \mid \psi \rangle &= \int_{-\infty}^{+\infty} \phi^*(x)\psi(x)\,dx = \int_{-\infty}^{+\infty} \phi(x)\psi(x)\,dx = \int_{+\infty}^{-\infty} \phi(-x)\psi(-x)(-dx) \\ &= -\int_{-\infty}^{+\infty} \phi(x)\psi(x)\,dx = 0. \end{aligned} \tag{2.491}$$

Problem 2.18

(a) Find the eigenvalues and the eigenfunctions of the operator $\hat{A} = -d^2/dx^2$; restrict the search for the eigenfunctions to those complex functions that vanish everywhere except in the region $0 < x < a$.

(b) Normalize the eigenfunction and find the probability in the region $0 < x < a/2$.

Solution

(a) The eigenvalue problem for $-d^2/dx^2$ consists of solving the differential equation

$$-\frac{d^2\psi(x)}{dx^2} = \alpha\psi(x) \tag{2.492}$$

and finding the eigenvalues α and the eigenfunction $\psi(x)$. The most general solution to this equation is

$$\psi(x) = Ae^{ibx} + Be^{-ibx}, \tag{2.493}$$

with $\alpha = b^2$. Using the boundary conditions of $\psi(x)$ at $x = 0$ and $x = a$, we have

$$\psi(0) = A + B = 0 \implies B = -A, \qquad \psi(a) = Ae^{iba} + Be^{-iba} = 0. \tag{2.494}$$

A substitution of $B = -A$ into the second equation leads to $A\left(e^{iba} - e^{-iba}\right) = 0$ or $e^{iba} = e^{-iba}$ which leads to $e^{2iba} = 1$. Thus, we have $\sin 2ba = 0$ and $\cos 2ba = 1$, so $ba = n\pi$. The eigenvalues are then given by $\alpha_n = n^2\pi^2/a^2$ and the corresponding eigenvectors by $\psi_n(x) = A\left(e^{in\pi x/a} - e^{-in\pi x/a}\right)$; that is,

$$\alpha_n = \frac{n^2\pi^2}{a^2}, \qquad \psi_n(x) = C_n \sin\left(\frac{n\pi x}{a}\right). \tag{2.495}$$

So the eigenvalue spectrum of the operator $\hat{A} = -d^2/dx^2$ is discrete, because the eigenvalues and eigenfunctions depend on a discrete number n.

(b) The normalization of $\psi_n(x)$,

$$1 = C_n^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{C_n^2}{2}\int_0^a \left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx = \frac{C_n^2}{2}a, \tag{2.496}$$

yields $C_n = \sqrt{2/a}$ and hence $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$. The probability in the region $0 < x < a/2$ is given by

$$\frac{2}{a}\int_0^{a/2}\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{1}{a}\int_0^{a/2}\left[1-\cos\left(\frac{2n\pi x}{a}\right)\right]dx = \frac{1}{2}. \tag{2.497}$$

This is expected since the total probability is 1: $\int_0^a \mid \psi_n(x) \mid^2 dx = 1$.

2.10 Exercises

Exercise 2.1
Consider the two states $\mid \psi\rangle = i \mid \phi_1\rangle + 3i \mid \phi_2\rangle - \mid \phi_3\rangle$ and $\mid \chi\rangle = \mid \phi_1\rangle - i \mid \phi_2\rangle + 5i \mid \phi_3\rangle$, where $\mid \phi_1\rangle$, $\mid \phi_2\rangle$ and $\mid \phi_3\rangle$ are orthonormal.

(a) Calculate $\langle\psi \mid \psi\rangle$, $\langle\chi \mid \chi\rangle$, $\langle\psi \mid \chi\rangle$, $\langle\chi \mid \psi\rangle$, and infer $\langle\psi + \chi \mid \psi + \chi\rangle$. Are the scalar products $\langle\psi \mid \chi\rangle$ and $\langle\chi \mid \psi\rangle$ equal?

(b) Calculate $\mid \psi\rangle\langle\chi \mid$ and $\mid \chi\rangle\langle\psi \mid$. Are they equal? Calculate their traces and compare them.

(c) Find the Hermitian conjugates of $\mid \psi\rangle$, $\mid \chi\rangle$, $\mid \psi\rangle\langle\chi \mid$, and $\mid \chi\rangle\langle\psi \mid$.

Exercise 2.2
Consider two states $|\psi_1\rangle = |\phi_1\rangle + 4i|\phi_2\rangle + 5|\phi_3\rangle$ and $|\psi_2\rangle = b|\phi_1\rangle + 4|\phi_2\rangle - 3i|\phi_3\rangle$, where $|\phi_1\rangle$, $|\phi_2\rangle$, and$|\phi_3\rangle$ are orthonormal kets, and where b is a constant. Find the value of b so that $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal.

Exercise 2.3
If $\mid \phi_1\rangle$, $\mid \phi_2\rangle$, and $\mid \phi_3\rangle$ are orthonormal, show that the states $\mid \psi\rangle = i \mid \phi_1\rangle + 3i \mid \phi_2\rangle - \mid \phi_3\rangle$ and $\mid \chi\rangle = \mid \phi_1\rangle - i \mid \phi_2\rangle + 5i \mid \phi_3\rangle$ satisfy

(a) the triangle inequality and

(b) the Schwarz inequality.

Exercise 2.4
Find the constant α so that the states $\mid \psi\rangle = \alpha \mid \phi_1\rangle + 5 \mid \phi_2\rangle$ and $\mid \chi\rangle = 3\alpha \mid \phi_1\rangle - 4 \mid \phi_2\rangle$ are orthogonal; consider $\mid \phi_1\rangle$ and $\mid \phi_2\rangle$ to be orthonormal.

Exercise 2.5
If $\mid \psi\rangle = \mid \phi_1\rangle + \mid \phi_2\rangle$ and $\mid \chi\rangle = \mid \phi_1\rangle - \mid \phi_2\rangle$, prove the following relations (note that $\mid \phi_1\rangle$ and $\mid \phi_2\rangle$ are not orthonormal):

(a) $\langle\psi \mid \psi\rangle + \langle\chi \mid \chi\rangle = 2\langle\phi_1 \mid \phi_1\rangle + 2\langle\phi_2 \mid \phi_2\rangle$,

(b) $\langle\psi \mid \psi\rangle - \langle\chi \mid \chi\rangle = 2\langle\phi_1 \mid \phi_2\rangle + 2\langle\phi_2 \mid \phi_1\rangle$.

Exercise 2.6
Consider a state which is given in terms of three orthonormal vectors $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ as follows:

$$|\psi\rangle = \frac{1}{\sqrt{15}}|\phi_1\rangle + \frac{1}{\sqrt{3}}|\phi_2\rangle + \frac{1}{\sqrt{5}}|\phi_3\rangle,$$

where $|\phi_n\rangle$ are eigenstates to an operator $\hat{B}$ such that: $\hat{B}|\phi_n\rangle = (3n^2 - 1)|\phi_n\rangle$ with $n = 1, 2, 3$.

(a) Find the norm of the state $|\psi\rangle$.

(b) Find the expectation value of $\hat{B}$ for the state $|\psi\rangle$.

(c) Find the expectation value of $\hat{B}^2$ for the state $|\psi\rangle$.

Exercise 2.7
Are the following sets of functions linearly independent or dependent?
(a) $4e^x$, e^x, $5e^x$
(b) $\cos x$, e^{ix}, $3\sin x$
(c) 7, x^2, $9x^4$, e^{-x}

Exercise 2.8
Are the following sets of functions linearly independent or dependent on the positive x-axis?
(a) x, $x+2$, $x+5$
(b) $\cos x$, $\cos 2x$, $\cos 3x$
(c) $\sin^2 x$, $\cos^2 x$, $\sin 2x$
(d) x, $(x-1)^2$, $(x+1)^2$
(e) $\sinh^2 x$, $\cosh^2 x$, 1

Exercise 2.9
Are the following sets of vectors linearly independent or dependent over the complex field?
(a) $(2, -3, 0)$, $(0, 0, 1)$, $(2i, i, -i)$
(b) $(0, 4, 0)$, $(i, -3i, i)$, $(2, 0, 1)$
(c) $(i, 1, 2)$, $(3, i, -1)$, $(-i, 3i, 5i)$

Exercise 2.10
Are the following sets of vectors (in the three-dimensional Euclidean space) linearly independent or dependent?
(a) $(4, 5, 6)$, $(1, 2, 3)$, $(7, 8, 9)$
(b) $(1, 0, 0)$, $(0, -5, 0)$, $(0, 0, \sqrt{7})$
(c) $(5, 4, 1)$, $(2, 0, -2)$, $(0, 6, -1)$

Exercise 2.11
Show that if $\hat{A}$ is a projection operator, the operator $1 - \hat{A}$ is also a projection operator.

Exercise 2.12
Show that $|\psi\rangle\langle\psi| / \langle\psi|\psi\rangle$ is a projection operator, regardless of whether $|\psi\rangle$ is normalized or not.

Exercise 2.13
In the following expressions, where $\hat{A}$ is an operator, specify the nature of each expression (i.e., specify whether it is an operator, a bra, or a ket); then find its Hermitian conjugate.
(a) $\langle\phi|\hat{A}|\psi\rangle\langle\psi|$
(b) $\hat{A}|\psi\rangle\langle\phi|$
(c) $\langle\phi|\hat{A}|\psi\rangle\,|\psi\rangle\langle\phi|\hat{A}$
(d) $\langle\psi|\hat{A}|\phi\rangle\,|\phi\rangle + i\hat{A}|\psi\rangle$
(e) $\left(|\phi\rangle\langle\phi|\hat{A}\right) - i\left(\hat{A}|\psi\rangle\langle\psi|\right)$

Exercise 2.14
Consider a two-dimensional space where a Hermitian operator $\hat{A}$ is defined by $\hat{A}|\phi_1\rangle = |\phi_1\rangle$ and $\hat{A}|\phi_2\rangle = -|\phi_2\rangle$; $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthonormal.
(a) Do the states $|\phi_1\rangle$ and $|\phi_2\rangle$ form a basis?
(b) Consider the operator $\hat{B} = |\phi_1\rangle\langle\phi_2|$. Is $\hat{B}$ Hermitian? Show that $\hat{B}^2 = 0$.

(c) Show that the products $\hat{B}\hat{B}^\dagger$ and $\hat{B}^\dagger\hat{B}$ are projection operators.
(d) Show that the operator $\hat{B}\hat{B}^\dagger - \hat{B}^\dagger\hat{B}$ is unitary.
(e) Consider $\hat{C} = \hat{B}\hat{B}^\dagger + \hat{B}^\dagger\hat{B}$. Show that $\hat{C} \mid \phi_1\rangle = \mid \phi_1\rangle$ and $\hat{C} \mid \phi_2\rangle = \mid \phi_2\rangle$.

Exercise 2.15
Prove the following two relations:
(a) $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{[\hat{A},\hat{B}]/2}$,
(b) $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \cdots$.
Hint: To prove the first relation, you may consider defining an operator function $\hat{F}(t) = e^{\hat{A}t}e^{\hat{B}t}$, where t is a parameter, $\hat{A}$ and $\hat{B}$ are t-independent operators, and then make use of $[\hat{A}, G(\hat{B})] = [\hat{A}, \hat{B}]dG(\hat{B})/d\hat{B}$, where $G(\hat{B})$ is a function depending on the operator $\hat{B}$.

Exercise 2.16
(a) Verify that the matrix

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

is unitary.
(b) Find its eigenvalues and the corresponding normalized eigenvectors.

Exercise 2.17
Consider the following three matrices:

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(a) Calculate the commutators $[A, B]$, $[B, C]$, and $[C, A]$.
(b) Show that $A^2 + B^2 + 2C^2 = 4I$, where I is the unity matrix.
(c) Verify that $\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB)$.

Exercise 2.18
Consider the following two matrices:

$$A = \begin{pmatrix} 3 & i & 1 \\ -1 & -i & 2 \\ 4 & 3i & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 2i & 5 & -3 \\ -i & 3 & 0 \\ 7i & 1 & i \end{pmatrix}.$$

Verify the following relations:
(a) $\det(AB) = \det(A)\det(B)$,
(b) $\det(A^T) = \det(A)$,
(c) $\det(A^\dagger) = (\det(A))^*$, and
(d) $\det(A^*) = (\det(A))^*$.

Exercise 2.19
Consider the matrix

$$A = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

(a) Find the eigenvalues and the normalized eigenvectors for the matrix A.

(b) Do these eigenvectors form a basis (i.e., is this basis complete and orthonormal)?

(c) Consider the matrix U which is formed from the normalized eigenvectors of A. Verify that U is unitary and that it satisfies

$$U^\dagger A U = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix},$$

where λ_1 and λ_2 are the eigenvalues of A.

(d) Show that $e^{xA} = \cosh x + A \sinh x$.

Exercise 2.20

Using the bra-ket algebra, show that $\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{C}\hat{A})$ where $\hat{A}, \hat{B}, \hat{C}$ are operators.

Exercise 2.21

For any two kets $| \psi\rangle$ and $| \phi\rangle$ that have finite norm, show that $\text{Tr}\,(| \psi\rangle\langle\phi |) = \langle\phi | \psi\rangle$.

Exercise 2.22

Consider the matrix $A = \begin{pmatrix} 0 & 0 & -1+i \\ 0 & 3 & 0 \\ -1-i & 0 & 0 \end{pmatrix}$.

(a) Find the eigenvalues and normalized eigenvectors of A. Denote the eigenvectors of A by $| a_1\rangle, | a_2\rangle, | a_3\rangle$. Any degenerate eigenvalues?

(b) Show that the eigenvectors $| a_1\rangle, | a_2\rangle, | a_3\rangle$ form an orthonormal and complete basis, i.e., show that $\sum_{j=1}^{3} | a_j\rangle\langle a_j | = I$, where I is the 3×3 unit matrix, and that $\langle a_j | a_k\rangle = \delta_{jk}$.

(c) Find the matrix corresponding to the operator obtained from the ket-bra product of the first eigenvector $P = | a_1\rangle\langle a_1 |$. Is P a projection operator?

Exercise 2.23

In a three-dimensional vector space, consider the operator whose matrix, in an orthonormal basis $\{| 1\rangle, | 2\rangle, | 3\rangle\}$, is

$$A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

(a) Is A Hermitian? Calculate its eigenvalues and the corresponding normalized eigenvectors. Verify that the eigenvectors corresponding to the two nondegenerate eigenvalues are orthonormal.

(b) Calculate the matrices representing the projection operators for the two nondegenerate eigenvectors found in part (a).

Exercise 2.24

Consider two operators $\hat{A}$ and $\hat{B}$ whose matrices are

$$A = \begin{pmatrix} 1 & 3 & 0 \\ 1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & -2 \\ 0 & 0 & 0 \\ -2 & 0 & 4 \end{pmatrix}.$$

(a) Are $\hat{A}$ and $\hat{B}$ Hermitian?

(b) Do $\hat{A}$ and $\hat{B}$ commute?

(c) Find the eigenvalues and eigenvectors of $\hat{A}$ and $\hat{B}$.
(d) Are the eigenvectors of each operator orthonormal?
(e) Verify that $\hat{U}^{\dagger}\hat{B}\hat{U}$ is diagonal, $\hat{U}$ being the matrix of the normalized eigenvectors of $\hat{B}$.
(f) Verify that $\hat{U}^{-1} = \hat{U}^{\dagger}$.

Exercise 2.25
Consider an operator $\hat{A}$ so that $[\hat{A}, \ \hat{A}^{\dagger}] = 1$.

(a) Evaluate the commutators $[\hat{A}^{\dagger}\hat{A}, \ \hat{A}]$ and $[\hat{A}^{\dagger}\hat{A}, \ \hat{A}^{\dagger}]$.

(b) If the actions of $\hat{A}$ and $\hat{A}^{\dagger}$ on the states $\{\mid a\rangle\}$ are given by $\hat{A} \mid a\rangle = \sqrt{a} \mid a-1\rangle$ and $\hat{A}^{\dagger} \mid a\rangle = \sqrt{a+1} \mid a+1\rangle$ and if $\langle a' \mid a\rangle = \delta_{a'a}$, calculate $\langle a \mid \hat{A} \mid a+1\rangle$, $\langle a+1 \mid \hat{A}^{\dagger} \mid a\rangle$ and $\langle a \mid \hat{A}^{\dagger}\hat{A} \mid a\rangle$ and $\langle a \mid \hat{A}\hat{A}^{\dagger} \mid a\rangle$.

(c) Calculate $\langle a \mid (\hat{A}+\hat{A}^{\dagger})^2 \mid a\rangle$ and $\langle a \mid (\hat{A}-\hat{A}^{\dagger})^2 \mid a\rangle$.

Exercise 2.26
Consider a 4×4 matrix

$$A = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

(a) Find the matrices of $A^{\dagger}$, $N = A^{\dagger}A$, $H = N + \frac{1}{2}I$ (where I is the unit matrix), $B = A + A^{\dagger}$, and $C = i(A - A^{\dagger})$.

(b) Find the matrices corresponding to the commutators $[A^{\dagger}, A]$, $[B, \ C]$, $[N, \ B]$, and $[N, \ C]$.

(c) Find the matrices corresponding to B^2, C^2, $[N, \ B^2 + C^2]$, $[H, \ A^{\dagger}]$, $[H, \ A]$, and $[H, \ N]$.

(d) Verify that $\det(ABC) = \det(A)\det(B)\det(C)$ and $\det(C^{\dagger}) = (\det(C))^*$.

Exercise 2.27
If $\hat{A}$ and $\hat{B}$ commute, and if $\mid \psi_1\rangle$ and $\mid \psi_2\rangle$ are two eigenvectors of $\hat{A}$ with different eigenvalues ($\hat{A}$ is Hermitian), show that

(a) $\langle \psi_1 \mid \hat{B} \mid \psi_2\rangle$ is zero and

(b) $\hat{B} \mid \psi_1\rangle$ is also an eigenvector to $\hat{A}$ with the same eigenvalue as $\mid \psi_1\rangle$; i.e., if $\hat{A} \mid \psi_1\rangle = a_1 \mid \psi_1\rangle$, show that $\hat{A}(\hat{B} \mid \psi_1\rangle) = a_1\hat{B} \mid \psi_1\rangle$.

Exercise 2.28
Let A and B be two $n \times n$ matrices. Assuming that B^{-1} exists, show that $[A, \ B^{-1}] = -B^{-1}[A, \ B]B^{-1}$.

Exercise 2.29
Consider a physical system whose Hamiltonian H and an operator A are given, in a three-dimensional space, by the matrices

$$H = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad A = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

(a) Are H and A Hermitian?
(b) Show that H and A commute. Give a basis of eigenvectors common to H and A.

Exercise 2.30
(a) Using $[\hat{X},\ \hat{P}] = i\hbar$, show that $[\hat{X}^2,\ \hat{P}] = 2i\hbar\hat{X}$ and $[\hat{X},\ \hat{P}^2] = 2i\hbar\hat{P}$.
(b) Show that $[\hat{X}^2,\ \hat{P}^2] = 2i\hbar(i\hbar + 2\hat{P}\hat{X})$.
(c) Calculate the commutator $[\hat{X}^2,\ \hat{P}^3]$.

Exercise 2.31
Discuss the hermiticity of the commutators $[\hat{X},\ \hat{P}]$, $[\hat{X}^2,\ \hat{P}]$ and $[\hat{X},\ \hat{P}^2]$.

Exercise 2.32
(a) Evaluate the commutator $[\hat{X}^2,\ d/dx]$ by operating it on a wave function.
(b) Using $[\hat{X},\ \hat{P}] = i\hbar$, evaluate the commutator $[\hat{X}\hat{P}^2,\ \hat{P}\hat{X}^2]$ in terms of a linear combination of $\hat{X}^2\hat{P}^2$ and $\hat{X}\hat{P}$.

Exercise 2.33
Show that $[\hat{X},\ \hat{P}^n] = i\hbar\hat{X}\hat{P}^{n-1}$.

Exercise 2.34
Evaluate the commutators $[e^{i\hat{X}},\ \hat{P}]$, $[e^{i\hat{X}^2},\ \hat{P}]$, and $[e^{i\hat{X}},\ \hat{P}^2]$.

Exercise 2.35
Consider the matrix

$$A = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

(a) Find the eigenvalues and the normalized eigenvectors of A.
(b) Do these eigenvectors form a basis (i.e., is this basis complete and orthonormal)?
(c) Consider the matrix U which is formed from the normalized eigenvectors of A. Verify that U is unitary and that it satisfies the relation

$$U^\dagger A U = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

where λ_1, λ_2, and λ_3 are the eigenvalues of A.
(d) Show that $e^{xA} = \cosh x + A \sinh x$.
Hint: $\cosh x = \sum_{n=0}^{\infty} x^{2n}/(2n)!$ and $\sinh x = \sum_{n=0}^{\infty} x^{2n+1}/(2n+1)!$.

Exercise 2.36
(a) If $[\hat{A},\ \hat{B}] = c$, where c is a number, prove the following two relations: $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + c$ and $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-c/2}$.
(b) Now if $[\hat{A},\ \hat{B}] = c\hat{B}$, where c is again a number, show that $e^{\hat{A}}\hat{B}e^{-\hat{A}} = e^c\hat{B}$.

Exercise 2.37
Consider the matrix

$$A = \frac{1}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{pmatrix}.$$

(a) Find the eigenvalues of A and their corresponding eigenvectors.

(b) Consider the basis which is constructed from the three eigenvectors of A. Using matrix algebra, verify that this basis is both orthonormal and complete.

Exercise 2.38

(a) Specify the condition that must be satisfied by a matrix A so that it is both unitary and Hermitian.

(b) Consider the three matrices

$$M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad M_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad M_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Calculate the inverse of each matrix. Do they satisfy the condition derived in (a)?

Exercise 2.39

Consider the two matrices

$$A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \qquad B = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}.$$

(a) Are these matrices Hermitian?

(b) Calculate the inverses of these matrices.

(c) Are these matrices unitary?

(d) Verify that the determinants of A and B are of the form $e^{i\theta}$. Find the corresponding values of θ.

Exercise 2.40

Show that the transformation matrix representing a 90° counterclockwise rotation about the z-axis of the basis vectors $(\vec{i}, \vec{j}, \vec{k})$ is given by

$$U = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Exercise 2.41

Show that the transformation matrix representing a 90° clockwise rotation about the y-axis of the basis vectors $(\vec{i}, \vec{j}, \vec{k})$ is given by

$$U = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Exercise 2.42

Show that the operator $(\hat{X}\hat{P} + \hat{P}\hat{X})^2$ is equal to $(\hat{X}^2\hat{P}^2 + \hat{P}^2\hat{X}^2)$ plus a term of the order of $\hbar^2$.

Exercise 2.43

Consider the two matrices $A = \begin{pmatrix} 4 & i & 7 \\ 1 & 0 & 1 \\ 0 & 1 & -i \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 1 & 1 \\ 0 & i & 0 \\ -i & 0 & i \end{pmatrix}$. Calculate the products $B^{-1} A$ and $A B^{-1}$. Are they equal? What is the significance of this result?

Exercise 2.44
Use the relations listed in Appendix A to evaluate the following integrals involving Dirac's delta function:

(a) $\int_0^{\pi} \sin(3x)\cos^2(4x)\delta(x-\pi/2)\,dx$.
(b) $\int_{-2}^{2} e^{7x+2}\delta(5x)\,dx$.
(c) $\int_{-2\pi}^{2\pi} \sin(\theta/2)\delta''(\theta+\pi)\,d\theta$.
(d) $\int_0^{2\pi} \cos^2\theta\delta[(\theta-\pi)/4]\,d\theta$.

Exercise 2.45
Use the relations listed in Appendix A to evaluate the following expressions:

(a) $\int_0^5 (3x^2+2)\delta(x-1)\,dx$.
(b) $(2x^5-4x^3+1)\delta(x+2)$.
(c) $\int_0^{\infty}(5x^3-7x^2-3)\delta(x^2-4)\,dx$.

Exercise 2.46
Use the relations listed in Appendix A to evaluate the following expressions:

(a) $\int_3^7 e^{6x-2}\delta(-4x)\,dx$.
(b) $\cos(2\theta)\sin(\theta)\delta(\theta^2-\pi^2/4)$.
(c) $\int_{-1}^{1} e^{5x-1}\delta'''(x)\,dx$.

Exercise 2.47
If the position and momentum operators are denoted by $\hat{\vec{R}}$ and $\hat{\vec{P}}$, respectively, show that $\hat{\mathcal{P}}^{\dagger}\hat{\vec{R}}^{\,n}\hat{\mathcal{P}} = (-1)^n\hat{\vec{R}}^{\,n}$ and $\hat{\mathcal{P}}^{\dagger}\hat{\vec{P}}^{\,n}\hat{\mathcal{P}} = (-1)^n\hat{\vec{P}}^{\,n}$, where $\hat{\mathcal{P}}$ is the parity operator and n is an integer.

Exercise 2.48
Consider an operator

$$\begin{aligned}\hat{A} \;=\; & \mid\phi_1\rangle\langle\phi_1\mid + \mid\phi_2\rangle\langle\phi_2\mid + \mid\phi_3\rangle\langle\phi_3\mid - i\mid\phi_1\rangle\langle\phi_2\mid \\ & - \mid\phi_1\rangle\langle\phi_3\mid + i\mid\phi_2\rangle\langle\phi_1\mid - \mid\phi_3\rangle\langle\phi_1\mid,\end{aligned}$$

where $\mid\phi_1\rangle$, $\mid\phi_2\rangle$, and $\mid\phi_3\rangle$ form a complete and orthonormal basis.

(a) Is $\hat{A}$ Hermitian? Calculate $\hat{A}^2$; is it a projection operator?
(b) Find the 3×3 matrix representing $\hat{A}$ in the $\mid\phi_1\rangle$, $\mid\phi_2\rangle$, $\mid\phi_3\rangle$ basis.
(c) Find the eigenvalues and the eigenvectors of the matrix.

Exercise 2.49
The Hamiltonian of a two-state system is given by

$$\hat{H} = E\left(\mid\phi_1\rangle\langle\phi_1\mid - \mid\phi_2\rangle\langle\phi_2\mid - i\mid\phi_1\rangle\langle\phi_2\mid + i\mid\phi_2\rangle\langle\phi_1\mid\right),$$

where $\mid\phi_1\rangle$, $\mid\phi_2\rangle$ form a complete and orthonormal basis; E is a real constant having the dimensions of energy.

(a) Is $\hat{H}$ Hermitian? Calculate the trace of $\hat{H}$.
(b) Find the matrix representing $\hat{H}$ in the $\mid\phi_1\rangle$, $\mid\phi_2\rangle$ basis and calculate the eigenvalues and the eigenvectors of the matrix. Calculate the trace of the matrix and compare it with the result you obtained in (a).
(c) Calculate $[\hat{H},\ \mid\phi_1\rangle\langle\phi_1\mid]$, $[\hat{H},\ \mid\phi_2\rangle\langle\phi_2\mid]$, and $[\hat{H},\ \mid\phi_1\rangle\langle\phi_2\mid]$.

Exercise 2.50
Consider a particle which is confined to move along the positive x-axis and whose Hamiltonian is $\hat{H} = \mathcal{E} d^2/dx^2$, where $\mathcal{E}$ is a positive real constant having the dimensions of energy.

(a) Find the wave function that corresponds to an energy eigenvalue of $9\mathcal{E}$ (make sure that the function you find is finite everywhere along the positive x-axis and is square integrable). Normalize this wave function.

(b) Calculate the probability of finding the particle in the region $0 \leq x \leq 15$.

(c) Is the wave function derived in (a) an eigenfunction of the operator $\hat{A} = d/dx - 7$?

(d) Calculate the commutator $[\hat{H},\ \hat{A}]$.

Exercise 2.51
Consider the wave functions:

$$\psi(x, y) = \sin 2x \ \cos 5x, \qquad \phi(x, y) = e^{-2(x^2+y^2)}, \qquad \chi(x, y) = e^{-i(x+y)}.$$

(a) Verify if any of the wave functions is an eigenfunction of $\hat{A} = \partial/\partial x + \partial/\partial y$.

(b) Find out if any of the wave functions is an eigenfunction of $\hat{B} = \partial^2/\partial x^2 + \partial^2/\partial y^2 + 1$.

(c) Calculate the actions of $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ on each one of the wave functions and infer $[\hat{A},\ \hat{B}]$.

Exercise 2.52

(a) Is the state $\psi(\theta, \phi) = e^{-3i\phi} \cos\theta$ an eigenfunction of $\hat{A}_\phi = \partial/\partial\phi$ or of $\hat{B}_\theta = \partial/\partial\theta$?

(b) Are $\hat{A}_\phi$ and $\hat{B}_\theta$ Hermitian?

(c) Evaluate the expressions $\langle\psi \mid \hat{A}_\phi \mid \psi\rangle$ and $\langle\psi \mid \hat{B}_\theta \mid \psi\rangle$.

(d) Find the commutator $[\hat{A}_\phi,\ \hat{B}_\theta]$.

Exercise 2.53
Consider an operator $\hat{A} = (\hat{X} d/dx + 2)$.

(a) Find the eigenfunction of $\hat{A}$ corresponding to a zero eigenvalue. Is this function normalizable?

(b) Is the operator $\hat{A}$ Hermitian?

(c) Calculate $[\hat{A},\ \hat{X}]$, $[\hat{A},\ d/dx]$, $[\hat{A},\ d^2/dx^2]$, $[\hat{X},\ [\hat{A},\ \hat{X}]]$, and $[d/dx,\ [\hat{A},\ d/dx]]$.

Exercise 2.54
If $\hat{A}$ and $\hat{B}$ are two Hermitian operators, find their respective eigenvalues such that $\hat{A}^2 = 2\hat{I}$ and $\hat{B}^4 = \hat{I}$, where $\hat{I}$ is the unit operator.

Exercise 2.55
Consider the Hilbert space of two-variable complex functions $\psi(x, y)$. A permutation operator is defined by its action on $\psi(x, y)$ as follows: $\hat{\pi}\,\psi(x, y) = \psi(y, x)$.

(a) Verify that the operator $\hat{\pi}$ is linear and Hermitian.

(b) Show that $\hat{\pi}^2 = \hat{I}$. Find the eigenvalues and show that the eigenfunctions of $\hat{\pi}$ are given by

$$\psi_+(x, y) = \frac{1}{2}\left[\psi(x, y) + \psi(y, x)\right] \quad \text{and} \quad \psi_-(x, y) = \frac{1}{2}\left[\psi(x, y) - \psi(y, x)\right].$$