Chapter 3

Linear Algebra In Dirac Notation

3.1 Hilbert Space and Inner Product

In Ch. 2 it was noted that quantum wave functions form a linear space in the sense that multiplying a function by a complex number or adding two wave functions together produces another wave function. It was also pointed out that a particular quantum state can be represented either by a wave function $\psi(x)$ which depends upon the position variable x, or by an alternative function $\hat{\psi}(p)$ of the momentum variable p. It is convenient to employ the Dirac symbol $|\psi\rangle$, known as a "ket", to denote a quantum state without referring to the particular function used to represent it. The kets, which we shall also refer to as *vectors* to distinguish them from *scalars*, which are complex numbers, are the elements of the quantum Hilbert space $\mathcal{H}$. (The real numbers form a subset of the complex numbers, so that when a scalar is referred to as a "complex number", this includes the possibility that it might be a real number.)

If α is any scalar (complex number), the ket corresponding to the wave function $\alpha\psi(x)$ is denoted by $\alpha|\psi\rangle$, or sometimes by $|\psi\rangle\alpha$, and the ket corresponding to $\phi(x) + \psi(x)$ is denoted by $|\phi\rangle + |\psi\rangle$ or $|\psi\rangle + |\phi\rangle$, and so forth. This correspondence could equally well be expressed using momentum wave functions, because the Fourier transform, (2.15) or (2.16), is a linear relationship between $\psi(x)$ and $\hat{\psi}(p)$, so that $\alpha\phi(x)+\beta\psi(x)$ and $\alpha\hat{\phi}(p)+\beta\hat{\psi}(p)$ correspond to the same quantum state $\alpha|\psi\rangle+\beta|\phi\rangle$. The addition of kets and multiplication by scalars obey some fairly obvious rules:

$$\begin{aligned} \alpha\big(\beta|\psi\rangle\big) = (\alpha\beta)|\psi\rangle, \quad (\alpha+\beta)|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle, \\ \alpha\big(|\phi\rangle + |\psi\rangle\big) = \alpha|\phi\rangle + \alpha|\psi\rangle, \quad 1|\psi\rangle = |\psi\rangle. \end{aligned} \tag{3.1}$$

Multiplying any ket by the number 0 yields the unique *zero vector* or *zero ket*, which will, because there is no risk of confusion, also be denoted by 0.

The linear space $\mathcal{H}$ is equipped with an *inner product*

$$\mathcal{I}\big(|\omega\rangle, |\psi\rangle\big) = \langle\omega|\psi\rangle \tag{3.2}$$

which assigns to any pair of kets $|\omega\rangle$ and $|\psi\rangle$ a complex number. While the Dirac notation $\langle\omega|\psi\rangle$, already employed in Ch. 2, is more compact than the one based on $\mathcal{I}\big(,\big)$, it is, for purposes of exposition, useful to have a way of writing the inner product which clearly indicates how it depends on two different ket vectors.

An inner product must satisfy the following conditions:

1. Interchanging the two arguments results in the complex conjugate of the original expression:

$$\mathcal{I}\big(|\psi\rangle, |\omega\rangle\big) = \big[\mathcal{I}\big(|\omega\rangle, |\psi\rangle\big)\big]^*. \tag{3.3}$$

2. The inner product is *linear* as a function of its second argument:

$$\mathcal{I}\big(|\omega\rangle, \alpha|\phi\rangle + \beta|\psi\rangle\big) = \alpha\mathcal{I}\big(|\omega\rangle, |\phi\rangle\big) + \beta\mathcal{I}\big(|\omega\rangle, |\psi\rangle\big). \tag{3.4}$$

3. The inner product is an *antilinear* function of its first argument:

$$\mathcal{I}\big(\alpha|\phi\rangle + \beta|\psi\rangle, |\omega\rangle\big) = \alpha^*\mathcal{I}\big(|\phi\rangle, |\omega\rangle\big) + \beta^*\mathcal{I}\big(|\psi\rangle, |\omega\rangle\big). \tag{3.5}$$

4. The inner product of a ket with itself,

$$\mathcal{I}\big(|\psi\rangle, |\psi\rangle\big) = \langle\psi|\psi\rangle = \||\psi\rangle\|^2 \tag{3.6}$$

is a positive (greater than zero) real number unless $|\psi\rangle$ is the zero vector, in which case $\langle\psi|\psi\rangle = 0$.

The term "antilinear" in the third condition refers to the fact that the *complex conjugates* of α and β appear on the right side of (3.5), rather than α and β themselves, as would be the case for a linear function. Actually, (3.5) is an immediate consequence of (3.3) and (3.4)—simply take the complex conjugate of both sides of (3.4), and then apply (3.3)—but it is of sufficient importance that it is worth stating separately. The reader can check that the inner products defined in (2.3) and (2.24) satisfy these conditions. (There are some subtleties associated with $\psi(x)$ when x is a continuous real number, but we must leave discussion of these matters to books on functional analysis.)

The positive square root $\||\psi\rangle\|$ of $\||\psi\rangle\|^2$ in (3.6) is called the *norm* of $|\psi\rangle$. As already noted in Ch. 2, $\alpha|\psi\rangle$ and $|\psi\rangle$ have exactly the same physical significance if α is a non-zero complex number. Consequently, as far as the quantum physicist is concerned, the actual norm, as long as it is positive, is a matter of indifference. By multiplying a non-zero ket by a suitable constant, one can always make its norm equal to 1. This process is called *normalizing* the ket, and a ket with norm equal to 1 is said to be *normalized*. Normalizing does not produce a unique result, because $e^{i\phi}|\psi\rangle$, where ϕ is an arbitrary real number or *phase*, has precisely the same norm as $|\psi\rangle$. Two kets $|\phi\rangle$ and $|\psi\rangle$ are said to be *orthogonal* if $\langle\phi|\psi\rangle = 0$, which by (3.3) implies that $\langle\psi|\phi\rangle = 0$.

3.2 Linear Functionals and the Dual Space

Let $|\omega\rangle$ be some fixed element of $\mathcal{H}$. Then the function

$$\mathcal{J}\big(|\psi\rangle\big) = \mathcal{I}\big(|\omega\rangle, |\psi\rangle\big) \tag{3.7}$$

assigns to every $|\psi\rangle$ in $\mathcal{H}$ a complex number in a linear manner,

$$\mathcal{J}\big(\alpha|\phi\rangle + \beta|\psi\rangle\big) = \alpha\mathcal{J}\big(|\phi\rangle\big) + \beta\mathcal{J}\big(|\psi\rangle\big), \tag{3.8}$$

as a consequence of (3.4). Such a function is called a *linear functional*. There are many different linear functionals of this sort, one for every $|\omega\rangle$ in $\mathcal{H}$. In order to distinguish them we could place

a label on $\mathcal{J}$ and, for example, write it as $\mathcal{J}_{|\omega\rangle}\big(|\psi\rangle\big)$. The notation $\mathcal{J}_{|\omega\rangle}$ is a bit clumsy, even if its meaning is clear, and Dirac's $\langle\omega|$, called a "bra", provides a simpler way to denote the same object, so that (3.8) takes the form

$$\langle\omega|\big(\alpha|\phi\rangle + \beta|\psi\rangle\big) = \alpha\langle\omega|\phi\rangle + \beta\langle\omega|\psi\rangle, \tag{3.9}$$

if we also use the compact Dirac notation for inner products.

Among the advantages of (3.9) over (3.8) is that the former looks very much like the distributive law for multiplication if one takes the simple step of replacing $\langle\omega| \cdot |\psi\rangle$ by $\langle\omega|\psi\rangle$. Indeed, a principal virtue of Dirac notation is that many different operations of this general type become "automatic", allowing one to concentrate on issues of physics without getting overly involved in mathematical bookkeeping. However, if one is in doubt about what Dirac notation really means, it may be helpful to check things out by going back to the more awkward but also more familiar notation of functions, such as $\mathcal{I}\big(,\big)$ and $\mathcal{J}\big()$.

Linear functionals can themselves be added together and multiplied by complex numbers, and the rules are fairly obvious. Thus the right side of

$$\big[\,\alpha\langle\tau| + \beta\langle\omega|\,\big]\,\big(|\psi\rangle\big) = \alpha\langle\tau|\psi\rangle + \beta\langle\omega|\psi\rangle \tag{3.10}$$

gives the complex number obtained when the linear functional $\alpha\langle\tau| + \beta\langle\omega|$, formed by addition following multiplication by scalars, and placed inside square brackets for clarity, is applied to the ket $|\psi\rangle$. Thus linear functionals themselves form a linear space, called the *dual* of the space $\mathcal{H}$; we shall denote it by $\mathcal{H}^\dagger$.

Although $\mathcal{H}$ and $\mathcal{H}^\dagger$ are not identical spaces—the former is inhabited by kets and the latter by bras—the two are closely related. There is a one-to-one map from one to the other denoted by a dagger:

$$\langle\omega| = \big(|\omega\rangle\big)^\dagger, \quad |\omega\rangle = \big(\langle\omega|\big)^\dagger. \tag{3.11}$$

The parentheses may be omitted when it is obvious what the dagger operation applies to, but including them does no harm. The dagger map is *antilinear*,

$$\begin{aligned} \big(\alpha|\phi\rangle + \beta|\psi\rangle\big)^\dagger &= \alpha^*\langle\phi| + \beta^*\langle\psi|, \\ \big(\gamma\langle\tau| + \delta\langle\omega|\big)^\dagger &= \gamma^*|\tau\rangle + \delta^*|\omega\rangle, \end{aligned} \tag{3.12}$$

reflecting the fact that the inner product $\mathcal{I}$ is antilinear in its left argument, (3.5). When applied twice in a row, the dagger operation is the identity map:

$$\big(\big(|\omega\rangle\big)^\dagger\big)^\dagger = |\omega\rangle, \quad \big(\big(\langle\omega|\big)^\dagger\big)^\dagger = \langle\omega|. \tag{3.13}$$

There are occasions when the Dirac notation $\langle\omega|\psi\rangle$ is not convenient because it is too compact. In such cases the dagger operation can be useful, because $\big(|\omega\rangle\big)^\dagger|\psi\rangle$ means the same thing as $\langle\omega|\psi\rangle$. Thus, for example,

$$\big(\alpha|\tau\rangle + \beta|\omega\rangle\big)^\dagger|\psi\rangle = \big(\alpha^*\langle\tau| + \beta^*\langle\omega|\big)|\psi\rangle = \alpha^*\langle\tau|\psi\rangle + \beta^*\langle\omega|\psi\rangle \tag{3.14}$$

is one way to express the fact the inner product is antilinear in its first argument, (3.5), without having to employ $\mathcal{I}(,)$.

3.3 Operators, Dyads

A *linear operator*, or simply an *operator* A is a linear function which maps $\mathcal{H}$ into itself. That is, to each $|\psi\rangle$ in $\mathcal{H}$, A assigns another element $A\big(|\psi\rangle\big)$ in $\mathcal{H}$ in such a way that

$$A\big(\alpha|\phi\rangle + \beta|\psi\rangle\big) = \alpha A\big(|\phi\rangle\big) + \beta A\big(|\psi\rangle\big) \tag{3.15}$$

whenever $|\phi\rangle$ and $|\psi\rangle$ are any two elements of $\mathcal{H}$, and α and β are complex numbers. One customarily omits the parentheses and writes $A|\phi\rangle$ instead of $A\big(|\phi\rangle\big)$ where this will not cause confusion, as on the right (but not the left) side of (3.15). In general we shall use capital letters, A, B, and so forth, to denote operators. The letter I is reserved for the *identity operator* which maps every element of $\mathcal{H}$ to itself:

$$I|\psi\rangle = |\psi\rangle. \tag{3.16}$$

The *zero operator* which maps every element of $\mathcal{H}$ to the zero vector will be denoted by 0.

The inner product of some element $|\phi\rangle$ of $\mathcal{H}$ with the ket $A|\psi\rangle$ can be written as

$$\big(|\phi\rangle\big)^\dagger A|\psi\rangle = \langle\phi|A|\psi\rangle, \tag{3.17}$$

where the notation on the right side, the "sandwich" with the operator between a bra and a ket, is standard Dirac notation. It is often referred to as a "matrix element", even when no matrix is actually under consideration. (Matrices are discussed in Sec. 3.6.) One can write $\langle\phi|A|\psi\rangle$ as $\big(\langle\phi|A\big)\big(|\psi\rangle\big)$, and think of it as the linear functional or bra vector

$$\langle\phi|A \tag{3.18}$$

acting on or evaluated at $|\psi\rangle$. In this sense it is natural to think of a linear operator A on $\mathcal{H}$ as inducing a linear map of the dual space $\mathcal{H}^\dagger$ onto itself, which carries $\langle\phi|$ to $\langle\phi|A$. This map can also, without risk of confusion, be denoted by A, and while one could write it as $A\big(\langle\phi|\big)$, in Dirac notation $\langle\phi|A$ is more natural. Sometimes one speaks of "the operator A acting to the left".

Dirac notation is particularly convenient in the case of a simple type of operator known as a *dyad*, written as a ket followed by a bra, $|\omega\rangle\langle\tau|$. Applied to some ket $|\psi\rangle$ in $\mathcal{H}$, it yields

$$|\omega\rangle\langle\tau|\big(|\psi\rangle\big) = |\omega\rangle\langle\tau|\psi\rangle = \langle\tau|\psi\rangle|\omega\rangle. \tag{3.19}$$

Just as in (3.9), the first equality is "obvious" if one thinks of the product of $\langle\tau|$ with $|\psi\rangle$ as $\langle\tau|\psi\rangle$, and since the latter is a scalar it can be placed either after or in front of the ket $|\omega\rangle$. Setting A in (3.17) equal to the dyad $|\omega\rangle\langle\tau|$ yields

$$\langle\phi|\big(|\omega\rangle\langle\tau|\big)|\psi\rangle = \langle\phi|\omega\rangle\langle\tau|\psi\rangle, \tag{3.20}$$

where the right side is the product of the two scalars $\langle\phi|\omega\rangle$ and $\langle\tau|\psi\rangle$. Once again the virtues of Dirac notation are evident in that this result is an almost automatic consequence of writing the symbols in the correct order.

The collection of all operators is itself a linear space, since a scalar times an operator is an operator, and the sum of two operators is also an operator. The operator $\alpha A + \beta B$ applied to an element $|\psi\rangle$ of $\mathcal{H}$ yields the result:

$$\big(\alpha A + \beta B\big)|\psi\rangle = \alpha\big(A|\psi\rangle\big) + \beta\big(B|\psi\rangle\big), \tag{3.21}$$

where the parentheses on the right side can be omitted, since $\big(\alpha A\big)|\psi\rangle$ is equal to $\alpha\big(A|\psi\rangle\big)$, and both can be written as $\alpha A|\psi\rangle$.

The *product* AB of two operators A and B is the operator obtained by first applying B to some ket, and then A to the ket which results from applying B:

$$AB\big(|\psi\rangle\big) = A\big(B\big(|\psi\rangle\big)\big). \tag{3.22}$$

Normally the parentheses are omitted, and one simply writes $AB|\psi\rangle$. However, it is very important to note that operator multiplication, unlike multiplication of scalars, is *not* commutative: in general, $AB \neq BA$, since there is no particular reason to expect that $A\big(B\big(|\psi\rangle\big)\big)$ will be the same element of $\mathcal{H}$ as $B\big(A\big(|\psi\rangle\big)\big)$.

In the exceptional case in which $AB = BA$, that is, $AB|\psi\rangle = BA|\psi\rangle$ for all $|\psi\rangle$, one says that these two operators *commute with each other*, or (simply) *commute*. The identity operator I commutes with every other operator, $IA = AI = A$, and the same is true of the zero operator, $A0 = 0A = 0$. The operators in a collection $\{A_1, A_2, A_3, \ldots\}$ are said to commute with each other provided

$$A_j A_k = A_k A_j \tag{3.23}$$

for every j and k.

Operator products follow the usual distributive laws, and scalars can be placed anywhere in a product, though one usually moves them to the left side:

$$\begin{aligned} A(\gamma C + \delta D) &= \gamma AC + \delta AD, \\ (\alpha A + \beta B)C &= \alpha AC + \beta BC. \end{aligned} \tag{3.24}$$

In working out such products it is important that the order of the operators, from left to right, be preserved: one cannot (in general) replace AC with CA. The operator product of two dyads $|\omega\rangle\langle\tau|$ and $|\psi\rangle\langle\phi|$ is fairly obvious if one uses Dirac notation:

$$|\omega\rangle\langle\tau| \cdot |\psi\rangle\langle\phi| = |\omega\rangle\langle\tau|\psi\rangle\langle\phi| = \langle\tau|\psi\rangle|\omega\rangle\langle\phi|, \tag{3.25}$$

where the final answer is a scalar $\langle\tau|\psi\rangle$ multiplying the dyad $|\omega\rangle\langle\phi|$. Multiplication in the reverse order will yield an operator proportional to $|\psi\rangle\langle\tau|$, so in general two dyads do not commute with each other.

Given an operator A, if one can find an operator B such that

$$AB = I = BA, \tag{3.26}$$

then B is called the *inverse* of the operator A, written as A^{-1}, and A is the inverse of the operator B. On a finite-dimensional Hilbert space one only needs to check one of the equalities in (3.26), as it implies the other, whereas on an infinite-dimensional space both must be checked. Many operators do not posses inverses, but if an inverse exists, it is unique.

The antilinear dagger operation introduced earlier, (3.11) and (3.12), can also be applied to operators. For a dyad one has:

$$\big(|\omega\rangle\langle\tau|\big)^\dagger = |\tau\rangle\langle\omega|. \tag{3.27}$$

Note that the right side is obtained by applying † separately to each term in the ket-bra "product" $|\omega\rangle\langle\tau|$ on the left, following the prescription in (3.11), and then writing the results in reverse order. When applying it to linear combinations of dyads, one needs to remember that the dagger operation is antilinear:

$$\big(\alpha|\omega\rangle\langle\tau| + \beta|\phi\rangle\langle\psi|\big)^\dagger = \alpha^*|\tau\rangle\langle\omega| + \beta^*|\psi\rangle\langle\phi|. \tag{3.28}$$

By generalizing (3.28) in an obvious way, one can apply the dagger operation to any sum of dyads, and thus to any operator on a finite-dimensional Hilbert space $\mathcal{H}$, since any operator can be written as a sum of dyads. However, the following definition is more useful. Given an operator A, its *adjoint* $(A)^\dagger$, usually written as $A^\dagger$, is the unique operator such that

$$\langle\psi|A^\dagger|\phi\rangle = \langle\phi|A|\psi\rangle^* \tag{3.29}$$

for any $|\phi\rangle$ and $|\psi\rangle$ in $\mathcal{H}$. Note that bra and ket are interchanged on the two sides of the equation. A useful mnemonic for expressions such as (3.29) is to think of complex conjugation as a special case of the dagger operation when that is applied to a scalar. Then the right side can be written and successively transformed,

$$\big(\langle\phi|A|\psi\rangle\big)^\dagger = \big(|\psi\rangle\big)^\dagger A^\dagger \big(\langle\phi|\big)^\dagger = \langle\psi|A^\dagger|\phi\rangle, \tag{3.30}$$

into the left side of (3.29) using the general rule that a dagger applied to a product is the product of the result of applying it to the individual factors, but written in the reverse order.

The adjoint of a linear combination of operators is what one would expect,

$$(\alpha A + \beta B)^\dagger = \alpha^* A^\dagger + \beta^* B^\dagger, \tag{3.31}$$

in light of (3.28) and the fact that the dagger operation is antilinear. The adjoint of a product of operators is the product of the adjoints *in the reverse order*:

$$(AB)^\dagger = B^\dagger A^\dagger, \quad (ABC)^\dagger = C^\dagger B^\dagger A^\dagger, \tag{3.32}$$

and so forth. The dagger operation, see (3.11), applied to a ket of the form $A|\psi\rangle$ yields a linear functional or bra vector

$$\big(A|\psi\rangle\big)^\dagger = \langle\psi|A^\dagger, \tag{3.33}$$

where the right side should be interpreted in the same way as (3.18): the operator $A^\dagger$ on $\mathcal{H}$ induces a map, denoted by the same symbol $A^\dagger$, on the space $\mathcal{H}^\dagger$ of linear functionals, by "operating to the left". One can check that (3.33) is consistent with (3.29)

An operator which is equal to its adjoint, $A = A^\dagger$ is said to be *Hermitian* or *self-adjoint*. (The two terms mean the same thing for operators on finite-dimensional spaces, but have different meanings for infinite-dimensional spaces.) Given that the dagger operation is in some sense a generalization of complex conjugation, one will not be surprised to learn that Hermitian operators behave in many respects like real numbers, a point to which we shall return in Ch. 5.

3.4 Projectors and Subspaces

A particular type of Hermitian operator called a *projector* plays a central role in quantum theory. A projector is any operator P which satisfies the two conditions

$$P^2 = P, \quad P^\dagger = P. \tag{3.34}$$

The first of these, $P^2 = P$, defines a *projection operator* which need not be Hermitian. Hermitian projection operators are also called *orthogonal projection operators*, but we shall call them projectors. Associated with a projector P is a linear subspace $\mathcal{P}$ of $\mathcal{H}$ consisting of all kets which are left unchanged by P, that is, those $|\psi\rangle$ for which $P|\psi\rangle = |\psi\rangle$. We shall say that P *projects onto* $\mathcal{P}$, or is the *projector onto* $\mathcal{P}$. The projector P acts like the identity operator on the subspace $\mathcal{P}$. The identity operator I is a projector, and it projects onto the entire Hilbert space $\mathcal{H}$. The zero operator 0 is a projector which projects onto the subspace consisting of nothing but the zero vector.

Any non-zero ket $|\phi\rangle$ generates a one-dimensional subspace $\mathcal{P}$, often called a *ray* or (by quantum physicists) a *pure state*, consisting of all scalar multiples of $|\phi\rangle$, that is to say, the collection of kets of the form $\{\alpha|\phi\rangle\}$, where α is any complex number. The projector onto $\mathcal{P}$ is the dyad

$$P = [\phi] = |\phi\rangle\langle\phi|/\langle\phi|\phi\rangle, \tag{3.35}$$

where the right side is simply $|\phi\rangle\langle\phi|$ if $|\phi\rangle$ is normalized, which we shall assume to be the case in the following discussion. The symbol $[\phi]$ for the projector projecting onto the ray generated by $|\phi\rangle$ is not part of standard Dirac notation, but it is very convenient, and will be used throughout this book. Sometimes, when it will not cause confusion, the square brackets will be omitted: ϕ will be used in place of $[\phi]$. It is straightforward to show that the dyad (3.35) satisfies the conditions in (3.34) and that

$$P(\alpha|\phi\rangle) = |\phi\rangle\langle\phi|(\alpha|\phi\rangle) = \alpha|\phi\rangle\langle\phi|\phi\rangle = \alpha|\phi\rangle, \tag{3.36}$$

so that P leaves the elements of $\mathcal{P}$ unchanged. When it acts on any vector $|\chi\rangle$ orthogonal to $|\phi\rangle$, $\langle\phi|\chi\rangle = 0$, P produces the zero vector:

$$P|\chi\rangle = |\phi\rangle\langle\phi|\chi\rangle = 0|\phi\rangle = 0. \tag{3.37}$$

The properties of P in (3.36) and (3.37) can be given a geometrical interpretation, or at least one can construct a geometrical analogy using real numbers instead of complex numbers. Consider the two dimensional plane shown in Fig. 3.1, with vectors labeled using Dirac kets. The line passing through $|\phi\rangle$ is the subspace $\mathcal{P}$. Let $|\omega\rangle$ be some vector in the plane, and suppose that its projection onto $\mathcal{P}$, along a direction perpendicular to $\mathcal{P}$, Fig. 3.1(a), falls at the point $\alpha|\phi\rangle$. Then

$$|\omega\rangle = \alpha|\phi\rangle + |\chi\rangle, \tag{3.38}$$

where $|\chi\rangle$ is a vector perpendicular (orthogonal) to $|\phi\rangle$, indicated by the dashed line. Applying P to both sides of (3.38), using (3.36) and (3.37), one finds that

$$P|\omega\rangle = \alpha|\phi\rangle. \tag{3.39}$$

That is, P on acting on any point $|\omega\rangle$ in the plane projects it onto $\mathcal{P}$ along a line perpendicular to $\mathcal{P}$, as indicated by the arrow in Fig. 3.1(a). Of course, such a projection applied to a point

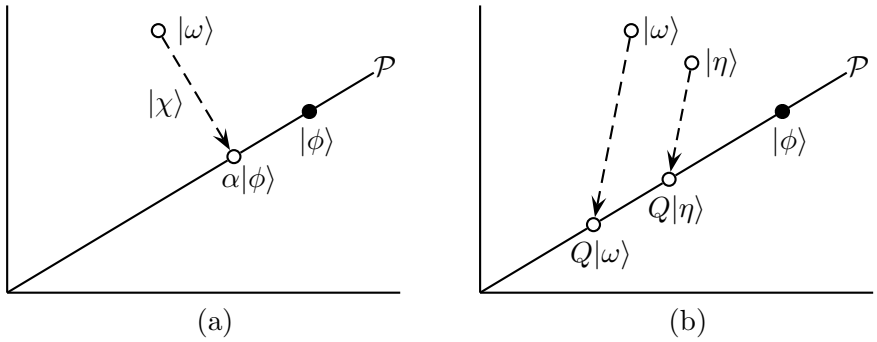

Figure 3.1: Illustrating (a) an orthogonal (perpendicular) projection onto $\mathcal{P}$; (b) a nonorthogonal projection represented by Q.

already on $\mathcal{P}$ leaves it unchanged, corresponding to the fact that P acts as the identity operation for elements of this subspace. For this reason, $P\big(P\big(|\omega\rangle\big)\big)$ is always the same as $P\big(|\omega\rangle\big)$, which is equivalent to the statement that $P^2 = P$. It is also possible to imagine projecting points onto $\mathcal{P}$ along a fixed direction which is *not* perpendicular to $\mathcal{P}$, as in Fig. 3.1(b). This defines a linear operator Q which is again a projection operator, since elements of $\mathcal{P}$ are mapped onto themselves, and thus $Q^2 = Q$. However, this operator is not Hermitian (in the terminology of real vector spaces, it is not symmetrical), so it is not an orthogonal ("perpendicular") projection operator.

Given a projector P, we define its *complement*, written as $\sim P$ or $\tilde{P}$, also called the *negation* of P (see Sec. 4.4), to be the projector defined by

$$\tilde{P} = I - P. \tag{3.40}$$

It is easy to show that $\tilde{P}$ satisfies the conditions for a projector in (3.34), and that

$$P\tilde{P} = 0 = \tilde{P}P. \tag{3.41}$$

From (3.40) it is obvious that P is, in turn, the complement (or negation) of $\tilde{P}$. Let $\mathcal{P}$ and $\mathcal{P}^\perp$ be the subspaces of $\mathcal{H}$ onto which P and $\tilde{P}$ project. Any element $|\omega\rangle$ of $\mathcal{P}^\perp$ is orthogonal to any element $|\phi\rangle$ of $\mathcal{P}$:

$$\langle\omega|\phi\rangle = \big(|\omega\rangle\big)^\dagger|\phi\rangle = \big(\tilde{P}|\omega\rangle\big)^\dagger\big(P|\phi\rangle\big) = \langle\omega|\tilde{P}P|\phi\rangle = 0, \tag{3.42}$$

because $\tilde{P}P = 0$. Here we have used the fact that P and $\tilde{P}$ act as identity operators on their respective subspaces, and the third equality makes use of (3.33). As a consequence, any element $|\psi\rangle$ of $\mathcal{H}$ can be written as the sum of two orthogonal kets, one belonging to $\mathcal{P}$ and one to $\mathcal{P}^\perp$:

$$|\psi\rangle = I|\psi\rangle = P|\psi\rangle + \tilde{P}|\psi\rangle. \tag{3.43}$$

Using (3.43), one can show that $\mathcal{P}^\perp$ is the *orthogonal complement* of $\mathcal{P}$, the collection of all elements of $\mathcal{H}$ which are orthogonal to *every* ket in $\mathcal{P}$. Similarly, $\mathcal{P}$ is the orthogonal complement $(\mathcal{P}^\perp)^\perp$ of $\mathcal{P}^\perp$.

3.5 Orthogonal Projectors and Orthonormal Bases

Two projectors P and Q are said to be (mutually) *orthogonal* if

$$PQ = 0. \tag{3.44}$$

By taking the adjoint of this equation, one can show that $QP = 0$, so that the order of the operators in the product does not matter. An *orthogonal collection of projectors*, or a *collection of (mutually) orthogonal projectors* is a set of *non-zero* projectors $\{P_1, P_2, \ldots\}$ with the property that

$$P_j P_k = 0 \text{ for } j \neq k. \tag{3.45}$$

The zero operator never plays a useful role in such collections, and excluding it simplifies various definitions.

Using (3.34) one can show that the sum $P + Q$ of two orthogonal projectors P and Q is a projector, and, more generally, the sum

$$R = \sum_j P_j \tag{3.46}$$

of the members of an orthogonal collection of projectors is a projector. When a projector R is written as a sum of projectors in an orthogonal collection, we shall say that this collection constitutes a *decomposition* or *refinement* of R. In particular, if R is the identity operator I, the collection is a *decomposition (refinement) of the identity*:

$$I = \sum_j P_j. \tag{3.47}$$

We shall often write down a sum in the form (3.47) and refer to it as a "decomposition of the identity." However, it is important to note that the decomposition is not the sum itself, but rather it is the set of summands, the collection of projectors which enter the sum. Whenever a *projector* R can be written as a sum of projectors in the form (3.46), it is necessarily the case that these projectors form an *orthogonal* collection, meaning that (3.45) is satisfied (see the bibliography). Nonetheless it does no harm to consider (3.45) as part of the definition of a decomposition of the identity, or of some other projector.

If two non-zero kets $|\omega\rangle$ and $|\phi\rangle$ are orthogonal, the same is true of the corresponding projectors $[\omega]$ and $[\phi]$, as is obvious from the definition in (3.35). An *orthogonal collection* of kets is a set $\{|\phi_1\rangle, |\phi_2\rangle, \ldots\}$ of *non-zero* elements of $\mathcal{H}$ such that $\langle\phi_j|\phi_k\rangle = 0$ when j is unequal to k. If in addition the kets in such a collection are normalized, so that

$$\langle\phi_j|\phi_k\rangle = \delta_{jk}, \tag{3.48}$$

we shall say that it is an *orthonormal collection*; the word "orthonormal" combines "orthogonal" and "normalized". The corresponding projectors $\{[\phi_1], [\phi_2], \ldots\}$ form an orthogonal collection, and

$$[\phi_j]\,|\phi_k\rangle = |\phi_j\rangle\langle\phi_j|\phi_k\rangle = \delta_{jk}|\phi_j\rangle. \tag{3.49}$$

Let $\mathcal{R}$ be the subspace of $\mathcal{H}$ consisting of all linear combinations of kets belonging to an orthonormal collection $\{|\phi_j\rangle\}$, that is, all elements of the form

$$|\psi\rangle = \sum_j \sigma_j |\phi_j\rangle, \tag{3.50}$$

where the σ_j are complex numbers. Then the projector R onto $\mathcal{R}$ is the sum of the corresponding dyad projectors:

$$R = \sum_j |\phi_j\rangle\langle\phi_j| = \sum_j [\phi_j]. \tag{3.51}$$

This follows from the fact that, in light of (3.49), R acts as the identity operator on a sum of the form (3.50), whereas $R|\omega\rangle = 0$ for every $|\omega\rangle$ which is orthogonal to every $|\phi_j\rangle$ in the collection, and thus to every $|\psi\rangle$ of the form (3.50)

If every element of $\mathcal{H}$ can be written in the form (3.50), the orthonormal collection is said to form an *orthonormal basis* of $\mathcal{H}$, and the corresponding decomposition of the identity is

$$I = \sum_j |\phi_j\rangle\langle\phi_j| = \sum_j [\phi_j]. \tag{3.52}$$

A *basis* of $\mathcal{H}$ is a collection of linearly independent kets which span $\mathcal{H}$ in the sense that any element of $\mathcal{H}$ can be written as a linear combination of kets in the collection. Such a collection need not consist of normalized states, nor do they have to be mutually orthogonal. However, in this book we shall for the most part use orthonormal bases, and for this reason the adjective "orthonormal" will sometimes be omitted when doing so will not cause confusion.

3.6 Column Vectors, Row Vectors, and Matrices

Consider a Hilbert space $\mathcal{H}$ of dimension n, and a particular orthonormal basis. To make the notation a bit less cumbersome, let us label the basis kets as $|j\rangle$ rather than $|\phi_j\rangle$. Then (3.48) and (3.52) take the form

$$\langle j|k\rangle = \delta_{jk}, \tag{3.53}$$

$$I = \sum_j |j\rangle\langle j|, \tag{3.54}$$

and any element $|\psi\rangle$ of $\mathcal{H}$ can be written as

$$|\psi\rangle = \sum_j \sigma_j |j\rangle. \tag{3.55}$$

By taking the inner product of both sides of (3.55) with $|k\rangle$, one sees that

$$\sigma_k = \langle k|\psi\rangle, \tag{3.56}$$

and therefore (3.55) can be written as

$$|\psi\rangle = \sum_j \langle j|\psi\rangle|j\rangle = \sum_j |j\rangle\langle j|\psi\rangle. \tag{3.57}$$

The form on the right side with the scalar coefficient $\langle j|\psi\rangle$ following rather than preceding the ket $|j\rangle$ provides a convenient way of deriving or remembering this result since (3.57) is the obvious equality $|\psi\rangle = I|\psi\rangle$ with I replaced with the dyad expansion in (3.54).

Using the basis $\{|j\rangle\}$, the ket $|\psi\rangle$ can be conveniently represented as a *column vector* of the coefficients in (3.57):

$$\begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \cdots \\ \langle n|\psi\rangle \end{pmatrix}. \tag{3.58}$$

Because of (3.57), this column vector uniquely determines the ket $|\psi\rangle$, so as long as the basis is held fixed there is a one-to-one correspondence between kets and column vectors. (Of course, if the basis is changed, the same ket will be represented by a different column vector.) If one applies the dagger operation to both sides of (3.57), the result is

$$\langle\psi| = \sum_j \langle\psi|j\rangle\langle j|, \tag{3.59}$$

which could also be written down immediately using (3.54) and the fact that $\langle\psi| = \langle\psi|I$. The numerical coefficients on the right side of (3.59) form a *row vector*

$$\Big(\langle\psi|1\rangle, \langle\psi|2\rangle, \ldots \langle\psi|n\rangle\Big) \tag{3.60}$$

which uniquely determines $\langle\psi|$, and vice versa. This row vector is obtained by "transposing" the column vector in (3.58)—i.e., laying it on its side—and taking the complex conjugate of each element, which is the vector analog of $\langle\psi| = \big(|\psi\rangle\big)^\dagger$. An inner product can be written as a row vector times a column vector, in the sense of matrix multiplication:

$$\langle\phi|\psi\rangle = \sum_j \langle\phi|j\rangle\langle j|\psi\rangle. \tag{3.61}$$

This can be thought of as $\langle\phi|\psi\rangle = \langle\phi|I|\psi\rangle$ interpreted with the help of (3.54).

Given an operator A on $\mathcal{H}$, its jk *matrix element* is

$$A_{jk} = \langle j|A|k\rangle, \tag{3.62}$$

where the usual subscript notation is on the left, and the corresponding Dirac notation, see (3.17), is on the right. The matrix elements can be arranged to form a square matrix

$$\begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \cdots & \langle 1|A|n\rangle \\ \langle 2|A|1\rangle & \langle 2|A|2\rangle & \cdots & \langle 2|A|n\rangle \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \langle n|A|1\rangle & \langle n|A|2\rangle & \cdots & \langle n|A|n\rangle \end{pmatrix} \tag{3.63}$$

with the first or left index j of $\langle j|A|k\rangle$ labeling the rows, and the second or right index k labeling the columns. It is sometimes helpful to think of such a matrix as made up of a collection of n

row vectors of the form (3.60), or, alternatively, n column vectors of the type (3.58). The matrix elements of the adjoint $A^\dagger$ of the operator A are given by

$$\langle j|A^\dagger|k\rangle = \langle k|A|j\rangle^*, \tag{3.64}$$

which is a particular case of (3.29). Thus the matrix of $A^\dagger$ is the complex conjugate of the transpose of the matrix of A. If the operator $A = A^\dagger$ is Hermitian, (3.64) implies that its diagonal matrix elements $\langle j|A|j\rangle$ are real.

Let us suppose that the result of A operating on $|\psi\rangle$ is a ket

$$|\phi\rangle = A|\psi\rangle. \tag{3.65}$$

By multiplying this on the left with the bra $\langle k|$, and writing A as AI with I in the form (3.54), one obtains

$$\langle k|\phi\rangle = \sum_j \langle k|A|j\rangle\langle j|\psi\rangle. \tag{3.66}$$

That is, the column vector for $|\phi\rangle$ is obtained by multiplying the matrix for A times the column vector for $|\psi\rangle$, following the usual rule for matrix multiplication. This shows, incidentally, that the operator A is uniquely determined by its matrix (given a fixed orthonormal basis), since this matrix determines how A maps any $|\psi\rangle$ of the Hilbert space onto $A|\psi\rangle$. Another way to see that the matrix determines A is to write A as a sum of dyads, starting with $A = IAI$ and using (3.54):

$$A = \sum_j \sum_k |j\rangle\langle j|A|k\rangle\langle k| = \sum_j \sum_k \langle j|A|k\rangle\, |j\rangle\langle k|. \tag{3.67}$$

The matrix of the product AB of two operators is the matrix product of the two matrices, in the same order:

$$\langle j|AB|k\rangle = \sum_i \langle j|A|i\rangle\langle i|B|k\rangle, \tag{3.68}$$

an expression easily derived by writing $AB = AIB$ and invoking the invaluable (3.54).

3.7 Diagonalization of Hermitian Operators

Books on linear algebra show that if $A = A^\dagger$ is Hermitian, it is always possible to find a particular orthonormal basis $\{|\alpha_j\rangle\}$ such that in this basis the matrix of A is *diagonal*, that is $\langle\alpha_j|A|\alpha_k\rangle = 0$ whenever $j \neq k$. The diagonal elements $a_j = \langle\alpha_j|A|\alpha_j\rangle$ must be real numbers in view of (3.64). By using (3.67) one can write A in the form

$$A = \sum_j a_j|\alpha_j\rangle\langle\alpha_j| = \sum_j a_j[\alpha_j], \tag{3.69}$$

a sum of real numbers times projectors drawn from an orthogonal collection. The ket $|\alpha_j\rangle$ is an *eigenvector* or *eigenket* of the operator A with *eigenvalue* a_j:

$$A|\alpha_j\rangle = a_j|\alpha_j\rangle. \tag{3.70}$$

An eigenvalue is said to be *degenerate* if it occurs more than once in (3.69), and its *multiplicity* is the number of times it occurs in the sum. An eigenvalue which only occurs once (multiplicity of one) is called *nondegenerate*. The identity operator has only one eigenvalue, equal to 1, whose multiplicity is the dimension n of the Hilbert space. A projector has only two distinct eigenvalues: 1 with multiplicity equal to the dimension m of the subspace onto which it projects, and 0 with multiplicity $n - m$.

The basis which diagonalizes A is unique only if all its eigenvalues are non-degenerate. Otherwise this basis is not unique, and it is sometimes more convenient to rewrite (3.69) in an alternative form in which each eigenvalue appears just once. The first step is to suppose that, as is always possible, the kets $|\alpha_j\rangle$ have been indexed in such a fashion that the eigenvalues are a non-decreasing sequence:

$$a_1 \leq a_2 \leq a_3 \leq \cdots . \tag{3.71}$$

The next step is best explained by means of an example. Suppose that $n = 5$, and that $a_1 = a_2 < a_3 < a_4 = a_5$. That is, the multiplicity of a_1 is two, that of a_3 is one, and that of a_4 is two. Then (3.69) can be written in the form

$$A = a_1 P_1 + a_3 P_2 + a_4 P_3, \tag{3.72}$$

where the three projectors

$$\begin{aligned} &P_1 = |\alpha_1\rangle\langle\alpha_1| + |\alpha_2\rangle\langle\alpha_2|, \quad P_2 = |\alpha_3\rangle\langle\alpha_3|, \\ &P_3 = |\alpha_4\rangle\langle\alpha_4| + |\alpha_5\rangle\langle\alpha_5| \end{aligned} \tag{3.73}$$

form a decomposition of the identity. By relabeling the eigenvalues as

$$a'_1 = a_1, \quad a'_2 = a_3, \quad a'_3 = a_4, \tag{3.74}$$

it is possible to rewrite (3.72) in the form

$$A = \sum_j a'_j P_j, \tag{3.75}$$

where no two eigenvalues are the same:

$$a'_j \neq a'_k \text{ for } j \neq k. \tag{3.76}$$

Generalizing from this example, we see that it is always possible to write a Hermitian operator in the form (3.75) with eigenvalues satisfying (3.76). If all the eigenvalues of A are nondegenerate, each P_j projects onto a ray or pure state, and (3.75) is just another way to write (3.69).

One advantage of using the expression (3.75), in which the eigenvalues are unequal, in preference to (3.69), where some of them can be the same, is that the decomposition of the identity $\{P_j\}$ which enters (3.75) is uniquely determined by the operator A. On the other hand, if an eigenvalue of A is degenerate, the corresponding eigenvectors are not unique. In the example in (3.72) one could replace $|\alpha_1\rangle$ and $|\alpha_2\rangle$ by any two normalized and mutually orthogonal kets $|\alpha'_1\rangle$ and $|\alpha'_2\rangle$ belonging to the two-dimensional subspace onto which P_1 projects, and similar considerations apply to $|\alpha_4\rangle$ and $|\alpha_5\rangle$. We shall call the (unique) decomposition of the identity $\{P_j\}$which allows a Hermitian

operator A to be written in the form (3.75) with eigenvalues satisfying (3.76) the *decomposition corresponding to* or *generated by* the operator A.

If $\{A, B, C, \ldots\}$ is a collection of Hermitian operators which commute with each other, (3.23), they can be simultaneously diagonalized in the sense that there is a single orthonormal basis $|\phi_j\rangle$ such that

$$A = \sum_j a_j [\phi_j], \quad B = \sum_j b_j [\phi_j], \quad C = \sum_j c_j [\phi_j], \tag{3.77}$$

and so forth. If instead one writes the operators in terms of the decompositions which they generate, as in (3.75),

$$A = \sum_j a'_j P_j, \quad B = \sum_k b'_k Q_k, \quad C = \sum_l c'_l R_l, \tag{3.78}$$

and so forth, the projectors in each decomposition commute with the projectors in the other decompositions: $P_j Q_k = Q_k P_j$, etc.

3.8 Trace

The trace of an operator A is the sum of its diagonal matrix elements:

$$\mathrm{Tr}(A) = \sum_j \langle j|A|j\rangle. \tag{3.79}$$

While the individual diagonal matrix elements depend upon the orthonormal basis, their sum, and thus the trace, is independent of basis and depends only on the operator A. The trace is a linear operation in that if A and B are operators, and α and β are scalars,

$$\mathrm{Tr}(\alpha A + \beta B) = \alpha \mathrm{Tr}(A) + \beta \mathrm{Tr}(B). \tag{3.80}$$

The trace of a dyad is the corresponding inner product,

$$\mathrm{Tr}\big(|\phi\rangle\langle\tau|\big) = \sum_j \langle j|\phi\rangle\langle\tau|j\rangle = \langle\tau|\phi\rangle, \tag{3.81}$$

as is clear from (3.61).

The trace of the product of two operators A and B is independent of the order of the product,

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA), \tag{3.82}$$

and the trace of the product of three or more operators is not changed if one makes a *cyclic permutation* of the factors:

$$\begin{aligned} \mathrm{Tr}(ABC) &= \mathrm{Tr}(BCA) = \mathrm{Tr}(CAB), \\ \mathrm{Tr}(ABCD) &= \mathrm{Tr}(BCDA) = \mathrm{Tr}(CDAB) = \mathrm{Tr}(DABC), \end{aligned} \tag{3.83}$$

and so forth; the cycling is done by moving the operator from the first position in the product to the last, or vice versa. By contrast, $\mathrm{Tr}(ACB)$ is, in general, *not* the same as $\mathrm{Tr}(ABC)$, for

ACB is obtained from ABC by interchanging the second and third factor, and this is not a cyclic permutation.

The complex conjugate of the trace of an operator is equal to the trace of its adjoint, as is evident from (3.64), and a similar rule applies to products of operators, where one should remember to reverse the order, see (3.32):

$$\begin{aligned} \big(\mathrm{Tr}(A)\big)^* &= \mathrm{Tr}(A^\dagger), \\ \big(\mathrm{Tr}(ABC)\big)^* &= \mathrm{Tr}(C^\dagger B^\dagger A^\dagger), \end{aligned} \tag{3.84}$$

etc.; additional identities can be obtained using cyclic permutations, as in (3.83).

If $A = A^\dagger$ is Hermitian, one can calculate the trace in the basis in which A is diagonal, with the result

$$\mathrm{Tr}(A) = \sum_{j=1}^{n} a_j. \tag{3.85}$$

That is, the trace is equal to the sum of the eigenvalues appearing in (3.69). In particular, the trace of a projector P is the dimension of the subspace onto which it projects.

3.9 Positive Operators and Density Matrices

A Hermitian operator A is said to be a *positive* operator provided

$$\langle\psi|A|\psi\rangle \geq 0 \tag{3.86}$$

holds for every $|\psi\rangle$ in the Hilbert space or, equivalently, if all its eigenvalues are non-negative:

$$a_j \geq 0 \text{ for all } j. \tag{3.87}$$

While (3.87) is easily shown to imply (3.86), and vice versa, memorizing both definitions is worthwhile, as sometimes one is more useful, and sometimes the other.

If A is a positive operator and a a positive real number, then aA is a positive operator. Also the sum of any collection of positive operators is a positive operator; this is an obvious consequence of (3.86). The *support* of a positive operator A is defined to be the projector A_s, or the subspace onto which it projects, given by the sum of those $[\alpha_j]$ in (3.69) with $a_j > 0$, or of the P_j in (3.75) with $a'_j > 0$. It follows from the definition that

$$A_s A = A. \tag{3.88}$$

An alternative definition is that the support of A is the smallest projector A_s, in the sense of minimizing $\mathrm{Tr}(A_s)$, which satisfies (3.88)

The trace of a positive operator is obviously a non-negative number, see (3.85) and (3.87), and is strictly positive unless the operator is the zero operator with all zero eigenvalues. A positive operator A which is not the zero operator can always be *normalized* by defining a new operator

$$\bar{A} = A/\mathrm{Tr}(A) \tag{3.89}$$

whose trace is equal to 1. In quantum physics a positive operator with trace equal to 1 is called a *density matrix*. The terminology is unfortunate, because a density matrix is an operator, not a matrix, and the matrix for this operator depends on the choice of orthonormal basis. However, by now the term is firmly embedded in the literature, and attempts to replace it with something more rational, such as "statistical operator", have not been successful.

If C is any operator, then $C^\dagger C$ is a positive operator, since for any $|\psi\rangle$,

$$\langle\psi|C^\dagger C|\psi\rangle = \langle\phi|\phi\rangle \geq 0, \tag{3.90}$$

where $|\phi\rangle = C|\psi\rangle$. Consequently, $\mathrm{Tr}(C^\dagger C)$ is non-negative. If $\mathrm{Tr}(C^\dagger C) = 0$, then $C^\dagger C = 0$, and $\langle\psi|C^\dagger C|\psi\rangle$ vanishes for every $|\psi\rangle$, which means that $C|\psi\rangle$ is zero for every $|\psi\rangle$, and therefore $C = 0$. Thus for any operator C it is the case that

$$\mathrm{Tr}(C^\dagger C) \geq 0, \tag{3.91}$$

with equality if and only if $C = 0$.

The product AB of two positive operators A and B is, in general, not Hermitian, and therefore not a positive operator. However, if A and B commute, AB is positive, as can be seen from the fact that there is an orthonormal basis in which the matrices of both A and B, and therefore also AB are diagonal. This result generalizes to the product of any collection of commuting positive operators. Whether or not A and B commute, the fact that they are both positive means that $\mathrm{Tr}(AB)$ is a real, non-negative number,

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) \geq 0, \tag{3.92}$$

equal to 0 if and only if $AB = BA = 0$. This result does not generalize to a product of three or more operators: if A, B, and C are positive operators that do not commute with each other, there is in general nothing one can say about $\mathrm{Tr}(ABC)$.

To derive (3.92) it is convenient to first define the square root $A^{1/2}$ of a positive operator A by means of the formula

$$A^{1/2} = \sum_j \sqrt{a_j}\,[\alpha_j], \tag{3.93}$$

where $\sqrt{a_j}$ is the positive square root of the eigenvalue a_j in (3.69). Then when A and B are both positive, one can write

$$\begin{aligned} \mathrm{Tr}(AB) &= \mathrm{Tr}(A^{1/2}A^{1/2}B^{1/2}B^{1/2}) \\ &= \mathrm{Tr}(A^{1/2}B^{1/2}B^{1/2}A^{1/2}) = \mathrm{Tr}(C^\dagger C) \geq 0, \end{aligned} \tag{3.94}$$

where $C = B^{1/2}A^{1/2}$. If $\mathrm{Tr}(AB) = 0$, then, see (3.91), $C = 0 = C^\dagger$, and both $BA = B^{1/2}CA^{1/2}$ and $AB = A^{1/2}C^\dagger B^{1/2}$ vanish.

3.10 Functions of Operators

Suppose that $f(x)$ is an ordinary numerical function, such as x^2 or e^x. It is sometimes convenient to define a corresponding function $f(A)$ of an operator A, so that the value of the function is also an operator. When $f(x)$ is a polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots a_p x^p, \tag{3.95}$$

one can write

$$f(A) = a_0 I + a_1 A + a_2 A^2 + \cdots a_p A^p, \tag{3.96}$$

since the square, cube, etc. of any operator is is itself an operator. When $f(x)$ is represented by a power series, as in $\log(1+x) = x - x^2/2 + \cdots$, the same procedure will work provided the series in powers of the operator A converges, but this is often not a trivial issue.

An alternative approach is possible in the case of operators which can be diagonalized in some orthonormal basis. Thus if A is written in the form (3.69), one can define $f(A)$ to be the operator

$$f(A) = \sum_j f(a_j)\,[\alpha_j], \tag{3.97}$$

where $f(a_j)$ on the right side is the value of the numerical function. This agrees with the previous definition in the case of polynomials, but allows the use of much more general functions. As an example, the square root $A^{1/2}$ of a positive operator A as defined in (3.93) is obtained by setting $f(x) = \sqrt{x}$ for $x \geq 0$ in (3.97). Note that in order to use (3.97), the numerical function $f(x)$ must be defined for any x which is an eigenvalue of A. For a Hermitian operator these eigenvalues are real, but in other cases, such as the unitary operators discussed in Sec. 7.2, the eigenvalues may be complex, so for such operators $f(x)$ will need to be defined for suitable complex values of x.