Chapter 9

Operations on States

We have seen in the preceding Chapter that the appropriate mathematical language for describing the states of a physical system is that of vectors belonging to a complex vector space. But the state space by itself is insufficient to fully describe the properties of a physical system. Describing such basic physical processes as how the state of a system evolves in time, or how to represent such basic physical quantities as position, momentum or energy, requires making use of further developments in the mathematics of vector spaces. These developments involve introducing a new mathematical entity known as an operator whose role it is to 'operate' on vectors and map them into other vectors. In fact, the earliest version of modern quantum mechanics, that put forward by Heisenberg, was formulated by him in terms of operators represented by matrices, at that time a not particularly well known (even to Heisenberg) development in pure mathematics. It was Born who recognized, and pointed out to Heisenberg, that he was using matrices in his work – another example of a purely mathematical construct that has proven to be of immediate value in describing the physical world.

Operators play many different roles in quantum mechanics. They can be used to represent physical processes that result in the change of state of the system, such as the evolution of the state of a system in time, or the creation or destruction of particles such as occurs, for instance in the emission or absorption of photons – particles of light – by matter. But operators have a further role, the one recognized by Heisenberg, which is to represent the physical properties of a system that can be, in principle, experimentally measured, such as energy, momentum, position and so on, so-called observable properties of a system. It is the aim of this Chapter to introduce the mathematical concept of an operator, and to show what the physical significance is of operators in quantum mechanics.

9.1 Definition and Properties of Operators

9.1.1 Definition of an Operator

An operator acting on the state of a system acts to map this state into some other state. If we represent an operator by a symbol $\widehat{A}$ – note the presence of the $\widehat{\ }$ – and suppose that the system is in a state $|\psi\rangle$, then the outcome of $\widehat{A}$ acting on $|\psi\rangle$, written $\widehat{A}|\psi\rangle$, (*not* $|\psi\rangle\widehat{A}$, which is not a combination of symbols that has been assigned any meaning) defines a new state $|\phi\rangle$ say, so that

$$\widehat{A}|\psi\rangle = |\phi\rangle. \tag{9.1}$$

An operator is fully characterized by specifying its effect on *every* state of the system. This could be done, for instance, in terms of some sort of rule that enables $|\phi\rangle$ to be determined for any given $|\psi\rangle$.

Example 9.1 Consider the operator $\widehat{A}$ acting on the states of a spin half system, and suppose, for the arbitrary state $|S\rangle = a|+\rangle + b|-\rangle$, that the action of the operator $\widehat{A}$ is such that $\widehat{A}|S\rangle = b|+\rangle + a|-\rangle$, i.e. the action of the operator $\widehat{A}$ on the state $|S\rangle$ is to exchange the coefficients $\langle\pm|S\rangle \leftrightarrow \langle\mp|S\rangle$. This rule is then enough to define the result of $\widehat{A}$ acting on any state of the system, i.e. the operator is fully specified.

Example 9.2 A slightly more complicated example is one for which the action of an operator $\widehat{N}$ on the state $|S\rangle$ is given by $\widehat{N}|S\rangle = a^2|+\rangle + b^2|-\rangle$. As we shall see below, the latter operator is of a kind not usually encountered in quantum mechanics, that is, it is non-linear, see Section 9.1.2 below.

9.1.2 Properties of Operators

Below, some of the basic properties of operators are summarized. Here a general perspective is adopted, but the properties will be encountered again and in a more concrete fashion when we look at representations of operators by matrices.

Equality of Operators

If two operators, $\widehat{A}$ and $\widehat{B}$ say, are such that

$$\widehat{A}|\psi\rangle = \widehat{B}|\psi\rangle \tag{9.2}$$

for all state vectors $|\psi\rangle$ belonging to the state space of the system then the two operators are said to be equal, written

$$\widehat{A} = \widehat{B}. \tag{9.3}$$

Linear and Antilinear Operators

There is essentially no limit to the way in which operators could be defined, but of particular importance are operators that have the following property. If $\widehat{A}$ is an operator such that for any arbitrary pair of states $|\psi_1\rangle$ and $|\psi_2\rangle$ and for any complex numbers c_1 and c_2:

$$\widehat{A}\big[c_1|\psi_1\rangle + c_2|\psi_2\rangle\big] = c_1\widehat{A}|\psi_1\rangle + c_2\widehat{A}|\psi_2\rangle, \tag{9.4}$$

then $\widehat{A}$ is said to be a *linear* operator. In quantum mechanics, operators are, with one exception, linear. The exception is the time reversal operator $\widehat{T}$ which has the property

$$\widehat{T}\big[c_1|\psi_1\rangle + c_2|\psi_2\rangle\big] = c_1^*\widehat{T}|\psi_1\rangle + c_2^*\widehat{T}|\psi_2\rangle \tag{9.5}$$

which is said to be *anti-linear*. We will not have any need to concern ourselves with the time reversal operator, so any operator that we will be encountering here will be tacitly assumed to be linear.

Example 9.3 Consider the operator $\widehat{A}$ acting on the states of a spin half system, such that for the arbitrary state $|S\rangle = a|+\rangle + b|-\rangle$, $\widehat{A}|S\rangle = b|+\rangle + a|-\rangle$. Show that this operator is linear. Introduce another state $|S'\rangle = a'|+\rangle + b'|-\rangle$ and consider

$$\begin{aligned}\widehat{A}\big[\alpha|S\rangle + \beta|S'\rangle\big] &= \widehat{A}\big[(\alpha a + \beta a')|+\rangle + (\alpha b + \beta b')|-\rangle\big]\\ &= (\alpha b + \beta b')|+\rangle + (\alpha a + \beta a')|-\rangle\\ &= \alpha\big(b|+\rangle + a|-\rangle\big) + \beta\big(b'|+\rangle + a'|-\rangle\big)\\ &= \alpha\widehat{A}|S\rangle + \beta\widehat{A}|S'\rangle.\end{aligned}$$

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Example 9.4 Consider the operator $\widehat{N}$ defined such that if $|S\rangle = a|+\rangle + b|-\rangle$ then $\widehat{N}|S\rangle = a^2|+\rangle + b^2|-\rangle$. It is straightforward to show that this operator is non-linear. Thus, if we have another state $|S'\rangle = a'|+\rangle + b'|-\rangle$, then

$$\widehat{N}\big[|S\rangle + |S'\rangle\big] = \widehat{N}\big[(a+a')|+\rangle + (b+b')|-\rangle\big] = (a+a')^2|+\rangle + (b+b')^2|-\rangle.$$

But

$$\widehat{N}|S\rangle + \widehat{N}|S'\rangle = (a^2 + a'^2)|+\rangle + (b^2 + b'^2)|-\rangle$$

which is certainly not equal to $\widehat{N}\big[|S\rangle + |S'\rangle\big]$. Thus the operator $\widehat{N}$ is non-linear. ■

The importance of linearity lies in the fact that since any state vector $|\psi\rangle$ can be written as a linear combination of a complete set of basis states, $\{|\varphi_n\rangle, n = 1, 2, \ldots\}$:

$$|\psi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle$$

then

$$\widehat{A}|\psi\rangle = \widehat{A}\sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum_n \widehat{A}|\varphi_n\rangle\langle\varphi_n|\psi\rangle \tag{9.6}$$

so that provided we know what an operator $\widehat{A}$ does to each basis state, we can determine what $\widehat{A}$ does to any vector belonging to the state space.

Example 9.5 Consider the spin states $|+\rangle$ and $|-\rangle$, basis states for a spin half system, and suppose an operator $\widehat{A}$ has the properties

$$\begin{aligned}\widehat{A}|+\rangle &= \tfrac{1}{2}i\hbar|-\rangle\\ \widehat{A}|-\rangle &= -\tfrac{1}{2}i\hbar|+\rangle.\end{aligned}$$

Then if a spin half system is in the state

$$|S\rangle = \frac{1}{\sqrt{2}}\big[|+\rangle + |-\rangle\big]$$

then

$$\begin{aligned}\widehat{A}|S\rangle &= \frac{1}{\sqrt{2}}\widehat{A}|+\rangle + \frac{1}{\sqrt{2}}\widehat{A}|-\rangle\\ &= \tfrac{1}{2}\hbar\frac{i}{\sqrt{2}}\big[|-\rangle - |+\rangle\big]\\ &= -\tfrac{1}{2}i\hbar\frac{1}{\sqrt{2}}\big[|+\rangle - |-\rangle\big].\end{aligned}$$

So the state vector $|S\rangle = \frac{1}{\sqrt{2}}\big[|+\rangle + |-\rangle\big]$ is mapped into the state vector $-\frac{1}{2}i\hbar\frac{1}{\sqrt{2}}\big[|+\rangle - |-\rangle\big]$, which represents a different physical state, and one which, incidentally, is not normalized to unity. ■

Example 9.6 Suppose an operator $\widehat{B}$ is defined so that

$$\widehat{B}|+\rangle = \tfrac{1}{2}\hbar|-\rangle$$
$$\widehat{B}|-\rangle = \tfrac{1}{2}\hbar|+\rangle.$$

If we let $\widehat{B}$ act on the state $|S\rangle = \big[|+\rangle + |-\rangle\big]/\sqrt{2}$ then we find that

$$\widehat{B}|S\rangle = \tfrac{1}{2}\hbar|S\rangle \tag{9.7}$$

i.e. in this case, we regain the same state vector $|S\rangle$, though multiplied by a factor $\frac{1}{2}\hbar$. This last equation is an example of an eigenvalue equation: $|S\rangle$ is said to be an eigenvector of the operator $\widehat{B}$, and $\frac{1}{2}\hbar$ is its eigenvalue. The concept of an eigenvalue and eigenvector is very important in quantum mechanics, and much more will be said about it later. ■

Linearity also makes it possible to set up a direct way of proving the equality of two operators. Above it was stated that two operators, $\widehat{A}$ and $\widehat{B}$ say, will be equal if $\widehat{A}|\psi\rangle = \widehat{B}|\psi\rangle$ for all states $|\psi\rangle$. However, it is sufficient to note that if for all the basis vectors $\{|\varphi_n\rangle, n = 1, 2, \ldots\}$

$$\widehat{A}|\varphi_n\rangle = \widehat{B}|\varphi_n\rangle \tag{9.8}$$

then we immediately have, for any arbitrary state $|\psi\rangle$ that

$$\begin{aligned}
\widehat{A}|\psi\rangle &= \widehat{A}\sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \\
&= \sum_n \widehat{A}|\varphi_n\rangle\langle\varphi_n|\psi\rangle \\
&= \sum_n \widehat{B}|\varphi_n\rangle\langle\varphi_n|\psi\rangle \\
&= \widehat{B}\sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \\
&= \widehat{B}|\psi\rangle
\end{aligned} \tag{9.9}$$

so that $\widehat{A} = \widehat{B}$. Thus, to prove the equality of two operators, it is sufficient to show that the action of the operators on each member of a basis set gives the same result.

The Unit Operator and the Zero Operator

Of all the operators that can be defined, there are two whose properties are particularly simple – the unit operator $\widehat{1}$ and the zero operator $\widehat{0}$. The unit operator is the operator such that

$$\widehat{1}|\psi\rangle = |\psi\rangle \tag{9.10}$$

for all states $|\psi\rangle$, and the zero operator is such that

$$\widehat{0}|\psi\rangle = 0 \tag{9.11}$$

for all kets $|\psi\rangle$.

Addition of Operators

The sum of two operators $\widehat{A}$ and $\widehat{B}$, written $\widehat{A}+\widehat{B}$ is defined in the obvious way, that is

$$(\widehat{A}+\widehat{B})|\psi\rangle = \widehat{A}|\psi\rangle + \widehat{B}|\psi\rangle \tag{9.12}$$

for all vectors $|\psi\rangle$. The sum of two operators is, of course, another operator, $\widehat{S}$ say, written $\widehat{S}=\widehat{A}+\widehat{B}$, such that

$$\widehat{S}|\psi\rangle = (\widehat{A}+\widehat{B})|\psi\rangle = \widehat{A}|\psi\rangle + \widehat{B}|\psi\rangle \tag{9.13}$$

for all states $|\psi\rangle$.

Example 9.7 Consider the two operators $\widehat{A}$ and $\widehat{B}$ defined by

$$\begin{aligned} \widehat{A}|+\rangle &= \tfrac{1}{2}i\hbar|-\rangle & \widehat{B}|+\rangle &= \tfrac{1}{2}\hbar|-\rangle \\ \widehat{A}|-\rangle &= -\tfrac{1}{2}i\hbar|+\rangle & \widehat{B}|-\rangle &= \tfrac{1}{2}\hbar|+\rangle. \end{aligned} \tag{9.14}$$

Their sum $\widehat{S}$ will then be such that

$$\begin{aligned} \widehat{S}|+\rangle &= \tfrac{1}{2}(1+i)\hbar|-\rangle \\ \widehat{S}|-\rangle &= \tfrac{1}{2}(1-i)\hbar|+\rangle. \end{aligned} \tag{9.15}$$

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Multiplication of an Operator by a Complex Number

This too is defined in the obvious way. Thus, if $\widehat{A}|\psi\rangle = |\phi\rangle$ then we can define the operator $\lambda\widehat{A}$ where λ is a complex number to be such that

$$(\lambda\widehat{A})|\psi\rangle = \lambda(\widehat{A}|\psi\rangle) = \lambda|\phi\rangle. \tag{9.16}$$

Combining this with the previous definition of the sum of two operators, we can then make say that in general

$$(\lambda\widehat{A}+\mu\widehat{B})|\psi\rangle = \lambda(\widehat{A}|\psi\rangle) + \mu(\widehat{B}|\psi\rangle) \tag{9.17}$$

where λ and μ are both complex numbers.

Multiplication of Operators

Given that an operator $\widehat{A}$ say, acting on a ket vector $|\psi\rangle$ maps it into another ket vector $|\phi\rangle$, then it is possible to allow a second operator, $\widehat{B}$ say, to act on $|\phi\rangle$, producing yet another ket vector $|\xi\rangle$ say. This we can write as

$$\widehat{B}\{\widehat{A}|\psi\rangle\} = \widehat{B}|\phi\rangle = |\xi\rangle. \tag{9.18}$$

This can be written

$$\widehat{B}\{\widehat{A}|\psi\rangle\} = \widehat{B}\widehat{A}|\psi\rangle \tag{9.19}$$

i.e. without the braces $\{\dots\}$, with the understanding that the term on the right hand side is to be interpreted as meaning that first $\widehat{A}$ acts on the state to its right, and then $\widehat{B}$, in the sense specified in Eq. (9.18). The combination $\widehat{B}\widehat{A}$ is said to be the product of the two operators $\widehat{A}$ and $\widehat{B}$. The product of two operators is, of course, another operator. Thus we can write $\widehat{C}=\widehat{B}\widehat{A}$ where the operator $\widehat{C}$ is such that

$$\widehat{C}|\psi\rangle = \widehat{B}\widehat{A}|\psi\rangle \tag{9.20}$$

for all states $|\psi\rangle$.

Example 9.8 Consider the products of the two operators defined in Eq. (9.14). First $\widehat{C} = \widehat{B}\widehat{A}$:

$$\begin{aligned}\widehat{C}|+\rangle = \widehat{B}\widehat{A}|+\rangle &= \widehat{B}(\tfrac{1}{2}i\hbar|-\rangle) = \tfrac{1}{4}i\hbar^2|+\rangle \\ \widehat{C}|-\rangle = \widehat{B}\widehat{A}|-\rangle &= \widehat{B}(-\tfrac{1}{2}i\hbar|+\rangle) = -\tfrac{1}{4}i\hbar^2|-\rangle,\end{aligned} \tag{9.21}$$

and next $\widehat{D} = \widehat{A}\widehat{B}$:

$$\begin{aligned}\widehat{D}|+\rangle = \widehat{A}\widehat{B}|+\rangle &= \widehat{A}(\tfrac{1}{2}\hbar|-\rangle) = -\tfrac{1}{4}i\hbar^2|+\rangle \\ \widehat{D}|-\rangle = \widehat{A}\widehat{B}|-\rangle &= \widehat{A}(-\tfrac{1}{2}\hbar|+\rangle) = \tfrac{1}{4}i\hbar^2|-\rangle.\end{aligned} \tag{9.22}$$

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Apart from illustrating how to implement the definition of the product of two operators, this example also shows a further important result, namely that, in general, $\widehat{A}\widehat{B} \neq \widehat{B}\widehat{A}$. In other words, the order in which two operators are multiplied is important. The difference between the two, written

$$\widehat{A}\widehat{B} - \widehat{B}\widehat{A} = \big[\widehat{A}, \widehat{B}\big] \tag{9.23}$$

is known as the commutator of $\widehat{A}$ and $\widehat{B}$. If the commutator vanishes, the operators are said to commute. The commutator plays a fundamental role in the physical interpretation of quantum mechanics, being both a bridge between the classical description of a physical system and its quantum description, and important in describing the consequences of sequences of measurements performed on a quantum system.

Projection Operators

An operator $\widehat{P}$ that has the property

$$\widehat{P}^2 = \widehat{P} \tag{9.24}$$

is said to be a *projection operator*. An important example of a projection operator is the operator $\widehat{P}_n$ defined, for a given set of orthonormal basis states $\{|\varphi_n\rangle; n = 1, 2, 3 \ldots\}$ by

$$\widehat{P}_n|\varphi_m\rangle = \delta_{nm}|\varphi_n\rangle. \tag{9.25}$$

That this operator is a projection operator can be readily confirmed:

$$\widehat{P}_n^2|\varphi_m\rangle = \widehat{P}_n\{\widehat{P}_n|\phi_m\rangle\} = \delta_{nm}\widehat{P}_n|\varphi_m\rangle = \delta_{nm}^2|\phi_m\rangle. \tag{9.26}$$

But since $\delta_{nm}^2 = \delta_{nm}$, (recall that the Kronecker delta δ_{nm} is either unity for $n = m$ or zero for $n \neq m$) we immediately have that

$$\widehat{P}_n^2|\varphi_m\rangle = \delta_{nm}|\varphi_m\rangle = \widehat{P}_n|\varphi_m\rangle \tag{9.27}$$

from which we conclude that $\widehat{P}_n^2 = \widehat{P}_n$. The importance of this operator lies in the fact that if we let it act on an arbitrary vector $|\psi\rangle$, then we see that

$$\widehat{P}_n|\psi\rangle = \widehat{P}_n\sum_m |\varphi_m\rangle\langle\varphi_m|\psi\rangle = \sum_m \widehat{P}_n|\varphi_m\rangle\langle\varphi_m|\psi\rangle = \sum_m \delta_{nm}|\varphi_m\rangle\langle\varphi_m|\psi\rangle = |\varphi_n\rangle\langle\varphi_n|\psi\rangle \tag{9.28}$$

i.e. it 'projects' out the component of $|\psi\rangle$ in the direction of the basis state φ_n.

Functions of Operators

Having defined what is meant by adding and multiplying operators, we can now define the idea of a function of an operator. If we have a function $f(x)$ which we can expand as a power series in x:

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots = \sum_{n=0}^{\infty} a_n x^n \tag{9.29}$$

then we define $f(\widehat{A})$, a function of the operator $\widehat{A}$, to be also given by the same power series, i.e.

$$f(\widehat{A}) = a_0 + a_1 \widehat{A} + a_2 \widehat{A}^2 + \cdots = \sum_{n=0}^{\infty} a_n \widehat{A}^n. \tag{9.30}$$

Questions such as the convergence of such a series (if it is an infinite series) will not be addressed here.

Example 9.9 The most important example of a function of an operator that we will have to deal with here is the exponential function:

$$f(\widehat{A}) = e^{\widehat{A}} = 1 + \widehat{A} + \frac{1}{2!}\widehat{A}^2 + \dots. \tag{9.31}$$

Many important operators encountered in quantum mechanics, in particular the time evolution operator which specifies how the state of a system evolves in time, is given as an exponential function of an operator. ■

It is important to note that in general, the usual rules for manipulating exponential functions do not apply for exponentiated operators. In particular, it should be noted that in general

$$e^{\widehat{A}} e^{\widehat{B}} \neq e^{\widehat{A}+\widehat{B}} \tag{9.32}$$

unless $\widehat{A}$ commutes with $\widehat{B}$.

The Inverse of an Operator

If, for some operator $\widehat{A}$ there exists another operator $\widehat{B}$ with the property that

$$\widehat{A}\widehat{B} = \widehat{B}\widehat{A} = \widehat{1} \tag{9.33}$$

then $\widehat{B}$ is said to be the inverse of $\widehat{A}$ and is written

$$\widehat{B} = \widehat{A}^{-1}. \tag{9.34}$$

Example 9.10 An important example is the inverse of the operator $\exp(\widehat{A})$ defined by the power series in Eq. (9.31) above. The inverse of this operator is readily seen to be just $\exp(-\widehat{A})$. ■

9.2 Action of Operators on Bra Vectors

Given that an operator maps a ket vector into another ket, as summarized in the defining equation $\widehat{A}|\psi\rangle = |\phi\rangle$, we can then take the inner product of $|\phi\rangle$ with any other state vector $|\xi\rangle$ say to yield the complex number $\langle\xi|\phi\rangle$. This we can obviously also write as

$$\langle\xi|\phi\rangle = \langle\xi|(\widehat{A}|\psi\rangle). \tag{9.35}$$

This then raises the interesting question, since a bra vector is juxtaposed with an operator in Eq. (9.35), whether we could give a meaning to an operator acting on a bra vector. In other words, we can give a meaning to $\langle\xi|\widehat{A}$?

Presumably, the outcome of $\widehat{A}$ acting on a bra vector is to produce another bra vector, i.e. we can write $\langle\xi|\widehat{A} = \langle\chi|$, though as yet we have not specified how to determine what the bra vector $\langle\chi|$ might be. But since operators were originally defined above in terms of their action on ket vectors, it makes sense to define the action of an operator on a bra in a way that makes use of what we know about the action of an operator on any ket vector. So, we define $\langle\xi|\widehat{A}$ such that

$$(\langle\xi|\widehat{A})|\psi\rangle = \langle\xi|(\widehat{A}|\psi\rangle) \quad \text{for all ket vectors } |\psi\rangle. \tag{9.36}$$

The value of this definition, apart from the fact that it relates the action of operators on bra vectors back to the action of operators of operators on ket vectors, is that $\langle\xi|(\widehat{A}|\psi\rangle)$ will always give the same result as $\langle\xi|(\widehat{A}|\psi\rangle)$ i.e. it is immaterial whether we let $\widehat{A}$ act on the ket vector first, and then take the inner product with $|\xi\rangle$, or to let $\widehat{A}$ act on $\langle\xi|$ first, and then take the inner product with $|\psi\rangle$. Thus the brackets are not needed, and we can write:

$$(\langle\xi|\widehat{A})|\psi\rangle = \langle\xi|(\widehat{A}|\psi\rangle) = \langle\xi|\widehat{A}|\psi\rangle. \tag{9.37}$$

This way of defining the action of an operator on a bra vector, Eq. (9.37), is rather back-handed, so it is important to see that it does in fact do the job! To see that the definition actually works, we will look at the particular case of the spin half state space again. Suppose we have an operator $\widehat{A}$ defined such that

$$\begin{aligned} \widehat{A}|+\rangle &= |+\rangle + i|-\rangle \\ \widehat{A}|-\rangle &= i|+\rangle + |-\rangle \end{aligned} \tag{9.38}$$

and we want to determine $\langle+|\widehat{A}$ using the above definition. Let $\langle\chi|$ be the bra vector we are after, i.e. $\langle+|\widehat{A} = \langle\chi|$. We know that we can always write

$$\langle\chi| = \langle\chi|+\rangle\langle+| + \langle\chi|-\rangle\langle-| \tag{9.39}$$

so the problem becomes evaluating $\langle\chi|\pm\rangle$. It is at this point that we make use of the defining condition above. Thus, we write

$$\langle\chi|\pm\rangle = (\langle+|\widehat{A})|\pm\rangle = \langle+|(\widehat{A}|\pm\rangle). \tag{9.40}$$

Using Eq. (9.38) this gives

$$\langle\chi|+\rangle = \langle+|(\widehat{A}|+\rangle) = 1 \quad \text{and} \quad \langle\chi|-\rangle = \langle+|(\widehat{A}|-\rangle) = i \tag{9.41}$$

and hence

$$\langle\chi| = \langle+| + i\langle-|. \tag{9.42}$$

Consequently, we conclude that

$$\langle+|\widehat{A} = \langle+| + i\langle-|. \tag{9.43}$$

If we note that $\widehat{A}|+\rangle = |+\rangle + i|-\rangle$ we can see that $\langle+|\widehat{A} \neq \langle+| - i\langle-|$. This example illustrates the result that if $\widehat{A}|\psi\rangle = |\phi\rangle$ then, in general, $\langle\psi|\widehat{A} \neq \langle\phi|$.

This example shows that the above 'indirect' definition of the action of an operator on a bra vector in terms of the action of the operator on ket vectors does indeed give us the result of the operator acting on a bra vector. The general method used in this example can be extended to the general case. So suppose we have a state space for some system spanned by a complete orthonormal set of basis states $\{|\varphi_n\rangle; n = 1, 2, \dots\}$, and assume that we know the action of an operator $\widehat{A}$ on an arbitrary basis state $|\varphi_n\rangle$:

$$\widehat{A}|\varphi_n\rangle = \sum_m |\varphi_m\rangle A_{mn} \tag{9.44}$$

where the A_{mn} are complex numbers. This equation is analogous to Eq. (9.38) in the example above. Now suppose we allow $\widehat{A}$ to act on an arbitrary bra vector $\langle\xi|$:

$$\langle\xi|\widehat{A} = \langle\chi| \tag{9.45}$$

We can express $\langle\chi|$ in terms of the basis states introduced above:

$$\langle\chi| = \sum_n \langle\chi|\varphi_n\rangle\langle\varphi_n|. \tag{9.46}$$

Thus, the problem reduces to showing that we can indeed calculate the coefficients $\langle\chi|\varphi_n\rangle$. These coefficients are given by

$$\langle\chi|\varphi_n\rangle = (\langle\xi|\widehat{A})|\varphi_n\rangle = \langle\xi|(\widehat{A}|\varphi_n\rangle) \tag{9.47}$$

where we have used the defining condition Eq. (9.36) to allow $\widehat{A}$ to act on the basis state $|\varphi_n\rangle$. Using Eq. (9.44) we can write

$$\begin{aligned}\langle\chi|\varphi_n\rangle &= \langle\xi|(\widehat{A}|\varphi_n\rangle)\\ &= \langle\xi|\Big[\sum_m |\varphi_m\rangle A_{mn}\Big]\\ &= \sum_m A_{mn}\langle\xi|\varphi_m\rangle.\end{aligned} \tag{9.48}$$

If we substitute this into the expression Eq. (9.46) we find that

$$\langle\chi| = \langle\xi|\widehat{A} = \sum_n \Big[\sum_m \langle\xi|\varphi_m\rangle A_{mn}\Big]\langle\varphi_n|. \tag{9.49}$$

The quantity within the brackets is a complex number which we can always evaluate since we know the A_{mn} and can evaluate the inner product $\langle\xi|\varphi_m\rangle$. Thus, by use of the defining condition Eq. (9.36), we are able to calculate the result of an operator acting on a bra vector. Of particular interest is the case in which $\langle\xi| = \langle\varphi_k|$ for which

$$\langle\varphi_k|\widehat{A} = \sum_n \Big[\sum_m \langle\varphi_k|\varphi_m\rangle A_{mn}\Big]\langle\varphi_n|. \tag{9.50}$$

Since the basis states are orthonormal, i.e. $\langle\varphi_k|\varphi_m\rangle = \delta_{km}$, then

$$\begin{aligned}\langle\varphi_k|\widehat{A} &= \sum_n \Big[\sum_m \delta_{km} A_{mn}\Big]\langle\varphi_n|\\ &= \sum_n A_{kn}\langle\varphi_n|.\end{aligned} \tag{9.51}$$

It is useful to put compare this result with Eq. (9.44):

$$\begin{aligned}\widehat{A}|\varphi_n\rangle &= \sum_m |\varphi_m\rangle A_{mn}\\ \langle\varphi_n|\widehat{A} &= \sum_m A_{nm}\langle\varphi_m|.\end{aligned} \tag{9.52}$$

Either of these expressions lead to the result

$$A_{mn} = \langle \varphi_m | \widehat{A} | \varphi_n \rangle. \tag{9.53}$$

For reasons which will become clearer later, the quantities A_{mn} are known as the matrix elements of the operator $\widehat{A}$ with respect to the set of basis states $\{|\varphi_n\rangle; n = 1, 2, \ldots\}$.

A further consequence of the above definition of the action of operators on bra vectors, which is actually implicit in the derivation of the result Eq. (9.49) is the fact that an operator $\widehat{A}$ that is linear with respect to ket vectors, is also linear with respect to bra vectors i.e.

$$\big[\lambda\langle\psi_1| + \mu\langle\psi_2|\big]\widehat{A} = \lambda\langle\psi_1|\widehat{A} + \mu\langle\psi_2|\widehat{A} \tag{9.54}$$

which further emphasizes the symmetry between the action of operators on bras and kets.

Much of what has been presented above is recast in terms of matrices and column and row vectors in a later Section.

9.3 The Hermitean Adjoint of an Operator

We have seen above that if $\widehat{A}|\psi\rangle = |\phi\rangle$ then $\langle\psi|\widehat{A} \neq \langle\phi|$. This then suggests the possibility of introducing an operator related to $\widehat{A}$, which we will write $\widehat{A}^\dagger$ which is such that

$$\text{if } \widehat{A}|\psi\rangle = |\phi\rangle \quad \text{then } \langle\psi|\widehat{A}^\dagger = \langle\phi|. \tag{9.55}$$

The operator $\widehat{A}^\dagger$ so defined is known as the *Hermitean adjoint* of $\widehat{A}$. There are issues concerning the definition of the Hermitean adjoint that require careful consideration if the state space is of infinite dimension. We will not be concerning ourselves with these matters here.

Thus we see we have introduced a new operator which has been defined in terms of its actions on bra vectors. In keeping with our point of view that operators should be defined in terms of their action on ket vectors, it should be the case that this above definition unambiguaously tells us what the action of $\widehat{A}^\dagger$ will be on any ket vector. In other words, how do we evaluate $\widehat{A}^\dagger|\psi\rangle$ for any arbitrary ket vector $|\psi\rangle$? In order to do this, we need a useful property of the Hermitean adjoint which can be readily derived from the above definition. Thus, consider $\langle\xi|\widehat{A}|\psi\rangle$, which we recognize is simply a complex number given by

$$\langle\xi|\widehat{A}|\psi\rangle = \langle\xi|(\widehat{A}|\psi\rangle) = \langle\xi|\phi\rangle \tag{9.56}$$

where $\widehat{A}|\psi\rangle = |\phi\rangle$. Thus, if we take the complex conjugate. we have

$$\langle\xi|\widehat{A}|\psi\rangle^* = \langle\xi|\phi\rangle^* = \langle\phi|\xi\rangle. \tag{9.57}$$

But, since $\widehat{A}|\psi\rangle = |\phi\rangle$ then $\langle\psi|\widehat{A}^\dagger = \langle\phi|$ so we have

$$\langle\xi|\widehat{A}|\psi\rangle^* = (\langle\psi|\widehat{A}^\dagger)|\xi\rangle = \langle\psi|\widehat{A}^\dagger|\xi\rangle \tag{9.58}$$

where in the last step the brackets have been dropped since it does not matter whether an operator acts on the ket or the bra vector.

Thus, taking the complex conjugate of $\langle\xi|\widehat{A}|\psi\rangle$ amounts to reversing the order of the factors, and replacing the operator by its Hermitean conjugate. Using this it is then possible to determine the action of $\widehat{A}^\dagger$ on a ket vector. The situation here is analogous to that which was encountered in Section 9.2. Thus, suppose we are dealing with a state space spanned by a complete orthonormal set of basis states $\{|\varphi_n\rangle; n = 1, 2, \dots\}$, and suppose we know that action of an operator $\widehat{A}$ on each of the basis states:

$$\widehat{A}|\varphi_n\rangle = \sum_m |\varphi_m\rangle A_{mn} \tag{9.59}$$

and we want to determine $\widehat{A}^\dagger|\psi\rangle$ where $|\psi\rangle$ is an arbitrary ket vector. If we let $\widehat{A}^\dagger|\psi\rangle = |\zeta\rangle$, then we can, as usual, make the expansion:

$$|\zeta\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\zeta\rangle. \tag{9.60}$$

The coefficients $\langle\varphi_n|\zeta\rangle$ can then be written:

$$\begin{aligned}\langle\varphi_n|\zeta\rangle &= \langle\varphi_n|\widehat{A}^\dagger|\psi\rangle \\ &= \langle\psi|\widehat{A}|\varphi_n\rangle^* \\ &= \left(\langle\psi|\Big[\sum_m |\varphi_m\rangle A_{mn}\Big]\right)^* \\ &= \sum_m \langle\psi|\varphi_m\rangle^* A^*_{mn}\end{aligned} \tag{9.61}$$

so that

$$\begin{aligned}|\zeta\rangle &= \widehat{A}^\dagger|\psi\rangle \\ &= \sum_n\sum_m |\varphi_n\rangle\langle\psi|\varphi_m\rangle^* A^*_{mn} \\ &= \sum_n |n\rangle\Big[\sum_m A^*_{mn}\langle\varphi_m|\psi\rangle\Big].\end{aligned} \tag{9.62}$$

The quantity within the brackets is a complex number which we can always evaluate since we know the A_{mn} and can evaluate the inner product $\langle\varphi_m|\psi\rangle$. Thus, we have shown that the action of the Hermitean adjoint on a ket vector can be readily calculated.

Of particular interest is the case in which $|\psi\rangle = |\varphi_k\rangle$ so that

$$\widehat{A}^\dagger|\varphi_k\rangle = \sum_n |\varphi_n\rangle\Big[\sum_m A^*_{mn}\langle\varphi_m|\varphi_k\rangle\Big]. \tag{9.63}$$

Using the orthonormality of the basis states, i.e. $\langle\varphi_m|\varphi_k\rangle = \delta_{mk}$ we have

$$\begin{aligned}\widehat{A}^\dagger|\varphi_k\rangle &= \sum_n |n\rangle\Big[\sum_m A^*_{mn}\delta_{mk}\Big] \\ &= \sum_n |\varphi_n\rangle A^*_{kn}\end{aligned} \tag{9.64}$$

It is useful to compare this with Eq. (9.44):

$$\begin{aligned}\widehat{A}|\varphi_n\rangle &= \sum_m |\varphi_m\rangle A_{mn} \\ \widehat{A}^\dagger|\varphi_n\rangle &= \sum_m |\varphi_m\rangle A^*_{nm}\end{aligned} \tag{9.65}$$

From these two results, we see that

$$\langle\varphi_m|\widehat{A}|\varphi_n\rangle^* = A^*_{mn} = \langle\varphi_n|\widehat{A}^\dagger|\varphi_m\rangle. \tag{9.66}$$

Much of this discussion on Hermitean operators is recast in terms of matrices and column and row vectors in a later Section.

9.3.1 Hermitean and Unitary Operators

If an operator $\widehat{A}$ has the property that

$$\widehat{A} = \widehat{A}^\dagger \tag{9.67}$$

then the operator is said to be Hermitean. If $\widehat{A}$ is Hermitean, then

$$\langle\psi|\widehat{A}|\phi\rangle^* = \langle\phi|\widehat{A}|\psi\rangle \tag{9.68}$$

Hermitean operators place a central role in quantum mechanics in that the observable properties of a physical system such as position, momentum, spin, energy and so on are represented by Hermitean operators in a way that will be described in the following Chapter.

If the operator $\widehat{A}$ is such that

$$\widehat{A}^\dagger = \widehat{A}^{-1} \tag{9.69}$$

then the operator is said to be unitary. Unitary operators also play a central role in quantum mechanics in that such operators represent performing actions on a system, such as displacing the system in space or time. The time evolution operator with which the evolution in time of the state of a quantum system can be determined is an important example of a unitary operator.

9.4 Eigenvalues and Eigenvectors

It can happen that, for some operator $\widehat{A}$, there exists a state vector $|\phi\rangle$ that has the property

$$\widehat{A}|\phi\rangle = a_\phi|\phi\rangle \tag{9.70}$$

where a_ϕ is, in general, a complex number. We have seen an example of such a situation in Eq. (9.7). If a situation such as that presented in Eq. (9.70) occurs, then the state $|\phi\rangle$ is said to be an eigenstate or eigenket of the operator $\widehat{A}$ with a_ϕ the associated eigenvalue. Often the notation

$$\widehat{A}|a\rangle = a|a\rangle \tag{9.71}$$

is used in which the eigenvector is labelled by its associated eigenvalue. This notation will be used almost exclusively here.

Determining the eigenvalues and eigenvectors of a given operator $\widehat{A}$, occasionally referred to as solving the eigenvalue problem for the operator, amounts to finding solutions to the eigenvalue equation Eq. (9.70). If the vector space is of finite dimension, then this can be done by matrix methods, while if the state space is of infinite dimension, then solving the eigenvalue problem can require solving a differential equation. Examples of both possibilities will be looked at later.

An operator $\widehat{A}$ may have

1. no eigenstates;
2. a discrete collection of eigenvalues a_1, a_2, ... and associated eigenvectors $|a_1\rangle$, $|a_2\rangle$, ...;
3. a continuous range of eigenvalues and associated eigenvectors, e.g. $\alpha_1 < a < \alpha_2$ (if the eigenvalues are real);

4. a combination of both discrete and continuous eigenvalues.

The collection of all the eigenvalues of an operator is called the *eigenvalue spectrum* of the operator. Note also that more than one eigenvector can have the same eigenvalue. Such an eigenvalue is said to be *degenerate*.

For the present we will be confining our attention to to operators that have discrete eigenvalue spectra. Modifications needed to handle continuous eigenvalues will be introduced later.

Example 9.11 If $|a\rangle$ is an eigenstate of $\widehat{A}$ with eigenvalue a, then a function $f(\widehat{A})$ of $\widehat{A}$ (where the function can be expanded as a power series) will also have $|a\rangle$ as an eigenstate with eigenvalue $f(a)$. This can be reasily shown by first noting that

$$\widehat{A}^n|a\rangle = \widehat{A}^{(n-1)}\widehat{A}|a\rangle = \widehat{A}^{(n-1)}a|a\rangle = a\widehat{A}^{(n-1)}|a\rangle.$$

Repeating this a further $n-1$ times then yields

$$\widehat{A}^n|a\rangle = a^n|a\rangle.$$

If we then apply this to

$$f(\widehat{A})|a\rangle$$

where $f(\widehat{A})$ has the power series expansion

$$f(\widehat{A}) = c_0 + c_1\widehat{A} + c_2\widehat{A}^2 + \ldots$$

then

$$\begin{aligned} f(\widehat{A})|a\rangle &= (c_0 + c_1\widehat{A} + c_2\widehat{A}^2 + \ldots)|a\rangle \\ &= c_0|a\rangle + c_1 a|a\rangle + c_2 a^2|a\rangle + \ldots \\ &= (c_0 + c_1 a + c_2 a^2 + \ldots)|a\rangle \\ &= f(a)|a\rangle. \end{aligned} \tag{9.72}$$

This turns out to be a very valuable result as we will often encounter functions of operators when we deal, in particular, with the time evolution operator. The time evolution operator is expressed as an exponential function of another operator (the Hamiltonian) whose eigenvalues and eigenvectors are central to the basic formalism of quantum mechanics. ∎

9.4.1 Eigenstates and Eigenvalues of Hermitean Operators

If an operator is Hermitean then its eigenstates and eigenvalues are found to possess a number of mathematical properties that are of substantial significance in quantum mechanics. So, if we suppose that an operator $\widehat{A}$ is Hermitean i.e. $\widehat{A} = \widehat{A}^\dagger$ then the following three properties hold true.

1. The eigenvalues of $\widehat{A}$ are all real.

The proof is as follows. Since

$$\widehat{A}|a\rangle = a|a\rangle$$

then

$$\langle a|\widehat{A}|a\rangle = a\langle a|a\rangle.$$

Taking the complex conjugate then gives

$$\langle a|\widehat{A}|a\rangle^* = a^*\langle a|a\rangle.$$

Now, using the facts that $\langle\phi|\widehat{A}|\psi\rangle = \langle\psi|\widehat{A}|\phi\rangle^*$ (Eq. (9.58)), and that $\langle a|a\rangle$ is real, we have

$$\langle a|\widehat{A}^\dagger|a\rangle = a^*\langle a|a\rangle.$$

Now using the fact that $\widehat{A} = \widehat{A}^\dagger$ then gives

$$\langle a|\widehat{A}|a\rangle = a^*\langle a|a\rangle = a\langle a|a\rangle$$

and hence

$$(a^* - a)\langle a|a\rangle = 0.$$

And so, finally, since $\langle a|a\rangle \neq 0$,

$$a^* = a.$$

This property is of central importance in the physical interpretation of quantum mechanics in that all physical observable properties of a system are represented by Hermitean operators, with the eigenvalues of the operators representing all the possible values that the physical property can be observed to have.

2. Eigenvectors belonging to different eigenvalues are orthogonal, i.e. if $\widehat{A}|a\rangle = a|a\rangle$ and $\widehat{A}|a'\rangle = a'|a'\rangle$ where $a \neq a'$, then $\langle a|a'\rangle = 0$.

The proof is as follows. Since

$$\widehat{A}|a\rangle = a|a\rangle$$

then

$$\langle a'|\widehat{A}|a\rangle = a\langle a'|a\rangle.$$

But

$$\widehat{A}|a'\rangle = a'|a'\rangle$$

so that

$$\langle a|\widehat{A}|a'\rangle = a'\langle a|a'\rangle$$

and hence on taking the complex conjugate

$$\langle a'|\widehat{A}^\dagger|a\rangle = a'^*\langle a'|a\rangle = a'\langle a'|a\rangle$$

where we have used the fact that the eigenvalues of $\widehat{A}$ are real, and hence $a' = a'^*$. Overall then,

$$\langle a'|\widehat{A}|a\rangle = a'\langle a'|a\rangle = a\langle a'|a\rangle$$

and hence

$$(a' - a)\langle a'|a\rangle = 0$$

so finally, if $a' \neq a$, then

$$\langle a'|a\rangle = 0.$$

The importance of this result lies in the fact that it makes it possible to construct a set of orthonormal states that define a basis for the state space of the system. To do this, we need the next property of Hermitean operators.

3. The eigenstates form a complete set of basis states for the state space of the system.

This can be proven to be always true if the state space is of finite dimension. If the state space is of infinite dimension, then completeness of the eigenstates of a Hermitean operator is not guaranteed. However, as we will see later, it is always assumed in quantum mechanics that the eigenstates of a Hermitean operator form a complete set. This assumption is based on physical considerations, and will be discussed later.

We can also always assume, *if the eigenvalue spectrum is discrete*, that these eigenstates are normalized to unity. If we were to suppose that they were not so normalized, for instance if the eigenstate $|a\rangle$ of the operator $\widehat{A}$ is such that $\langle a|a\rangle \neq 1$, then we simply define a new state vector by

$$\widetilde{|a\rangle} = \frac{|a\rangle}{\sqrt{\langle a|a\rangle}} \tag{9.73}$$

which is normalized to unity. This new state $\widetilde{|a\rangle}$ is still an eigenstate of $\widehat{A}$ with eigenvalue a – in fact it represents the same physical state as $|a\rangle$ – so we might as well have assumed from the very start that $|a\rangle$ was normalized to unity. Thus, provided the eigenvalue spectrum is discrete, then as well as the eigenstates forming a complete set of basis states, they also form an orthonormal set.

Thus, if the operator $\widehat{A}$ is Hermitean, and has an (assumed) complete set of eigenstates $\{|a_n\rangle; n = 1, 2, 3\ldots\}$, then these eigenstates form an orthonormal basis for the system. Any arbitrary state $|\psi\rangle$ can therefore be written as

$$|\psi\rangle = \sum_n |a_n\rangle\langle a_n|\psi\rangle. \tag{9.74}$$

If the eigenvalue spectrum of an operator is continuous, then it is not possible to assume that the eigenstates can be normalized to unity. A different normalization scheme is required, as will be discussed in the next section.

9.4.2 Continuous Eigenvalues

Far from being the exception, Hermitean operators with continuous eigenvaues are basic to quantum mechanics. So in the following, consider a Hermitean operator $\widehat{A}$ with continuous eigenvalues a lying in some range, between α_1 and α_2 say:

$$\widehat{A}|a\rangle = a|a\rangle \qquad \alpha_1 < a < \alpha_2. \tag{9.75}$$

That there is a difficulty in dealing with eigenstates associated with a continuous range of eigenvalues can be seen if we make use of the (assumed) completeness of the eigenstates of a Hermitean operator, Eq. (9.74). It seems reasonable to postulate that in the case of continuous eigenvalues, this completeness relation would become an integral over the continuous range of eigenvalues:

$$|\psi\rangle = \int_{\alpha_1}^{\alpha_2} |a\rangle\langle a|\psi\rangle da. \tag{9.76}$$

The probability amplitude $\langle a|\psi\rangle$ are functions of the continuous variable a, and is often written $\langle a|\psi\rangle = \psi(a)$. If we now consider the inner product

$$\langle a'|\psi\rangle = \int_{\alpha_1}^{\alpha_2} \langle a'|a\rangle\langle a|\psi\rangle da \tag{9.77}$$

or

$$\psi(a') = \int_{\alpha_1}^{\alpha_2} \langle a'|a\rangle \psi(a) da \tag{9.78}$$

we now see that we have an interesting difficulty. We know that $\langle a'|a\rangle = 0$ if $a' \neq a$, so if $\langle a|a\rangle$ is assigned a finite value, the integral on the right hand side will vanish, so that $\psi(a) = 0$ for all a!! But if $\psi(a)$ is to be a non-trivial quantity, i.e. if it is not to be zero for all a, then it cannot be the case that $\langle a|a\rangle$ is finite. In other words, $\langle a'|a\rangle$ must be infinite for $a = a'$ in some sense in order to guarantee a non-zero integral. The way in which this can be done involves introducing a new 'function', the Dirac delta function, which has some rather unusual properties.

The Dirac Delta Function

What we are after is a 'function' $\delta(x - x_0)$ with the property that

$$f(x_0) = \int_{-\infty}^{+\infty} \delta(x - x_0) f(x) dx \tag{9.79}$$

for all (reasonable) functions $f(x)$.

So what is $\delta(x-x_0)$? Perhaps the simplest way to get at what this function looks like is to examine beforehand a sequence of functions defined by

$$\begin{aligned} D(\epsilon, x) &= \epsilon^{-1} \quad -\epsilon/2 < x < \epsilon/2 \\ &= 0 \qquad x < -\epsilon, x > \epsilon. \end{aligned} \tag{9.80}$$

What we first notice about this function is that it defines a rectangle whose area is always unity for any (non-zero) value of ϵ, i.e.

$$\int_{-\infty}^{+\infty} D(\epsilon, x) dx = 1. \tag{9.81}$$

Secondly, we note that as ϵ is made smaller, the rectangle becomes taller and narrower. Thus, if we look at an integral

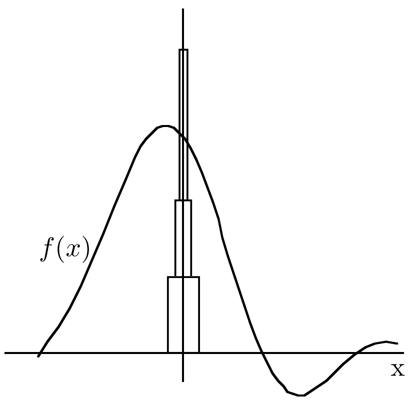

Figure 9.1: A sequence of rectangles of decreasing width but increasing height, maintaining a constant area of unity approaches an infinitely high 'spike' at $x = 0$.

$$\int_{-\infty}^{+\infty} D(\epsilon, x) f(x) dx = \epsilon^{-1} \int_{-\epsilon/2}^{\epsilon/2} f(x) dx \tag{9.82}$$

where $f(x)$ is a reasonably well behaved function (i.e. it is continuous in the neighbourhood of $x = 0$), we see that as $\epsilon \to 0$, this tends to the limit $f(0)$. We can summarize this by the equation

$$\lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} D(\epsilon, x) f(x) dx = f(0). \tag{9.83}$$

Taking the limit inside the integral sign (an illegal mathematical operation, by the way), we can write this as

$$\int_{-\infty}^{+\infty} \lim_{\epsilon \to 0} D(\epsilon, x) f(x) dx = \int_{-\infty}^{+\infty} \delta(x) f(x) = f(0) \tag{9.84}$$

where we have introduced the 'Dirac delta function' $\delta(x)$ defined as the limit

$$\delta(x) = \lim_{\epsilon \to 0} D(\epsilon, x), \tag{9.85}$$

a function with the unusual property that it is zero everywhere except for $x = 0$, where it is infinite.

The above defined function $D(\epsilon, x)$ is but one 'representation' of the Dirac delta function. There are in effect an infinite number of different functions that in an appropriate limit behave as the rectangular function here. Some examples are

$$\begin{aligned} \delta(x - x_0) &= \lim_{L \to \infty} \frac{1}{\pi} \frac{\sin L(x - x_0)}{x - x_0} \\ &= \lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{(x - x_0)^2 + \epsilon^2} \\ &= \lim_{\lambda \to \infty} \lambda e^{-\lambda |x - x_0|}. \end{aligned} \tag{9.86}$$

In all cases, the function on the right hand side becomes narrower and taller as the limit is taken, while the area under the various curves remains the same, that is, unity.

The delta function is not to be thought of as a function as it is usually defined in pure mathematics, but rather it is to be understood that a limit of the kind outlined above is implied whenever the delta function appears in an integral. However, such mathematical niceties do not normally need to be a source of concern in most instances. It is usually sufficient to be aware of the basic property Eq. (9.79) and a few other rules that can be proven using the limiting process, such as

$$\begin{aligned} \delta(x) &= \delta(-x) \\ \delta(ax) &= \frac{1}{|a|} \delta(x) \\ \int_{-\infty}^{+\infty} \delta(x - x_0)\delta(x - x_1) &= \delta(x_0 - x_1) \\ \int_{-\infty}^{+\infty} f(x)\delta'(x - x_0)dx &= -f'(x_0). \end{aligned}$$

The limiting process should be employed if there is some doubt about any result obtained. For instance, it can be shown that the square of a delta function cannot be given a satisfactory meaning.

Delta Function Normalization of Eigenstates

Returning to the result

$$\psi(a') = \int_{\alpha_1}^{\alpha_2} \langle a'|a\rangle \psi(a) da \tag{9.87}$$

we see that the inner product $\langle a'|a\rangle$, must be interpreted as a delta function:

$$\langle a'|a\rangle = \delta(a - a'). \tag{9.88}$$

The states $|a\rangle$ are said to be delta function normalized, in contrast to the orthonormal property of discrete eigenstates.

One result of this is that states such as $|a\rangle$ are of infinite norm and so cannot be normalized to unity. Such states states cannot represent possible physical states of a system, though it is often convenient, with caution, to speak of such states as if they were physically realizable. Mathematical (and physical) paradoxes can arise if care is not taken. However, linear combinations of these states can be normalized to unity, as this following example illustrates.

If we consider a state $|\psi\rangle$ given by

$$|\psi\rangle = \int_{\alpha_1}^{\alpha_2} |a\rangle\langle a|\psi\rangle da, \tag{9.89}$$

then

$$\langle\psi|\psi\rangle = \int_{\alpha_1}^{\alpha_2} \langle\psi|a\rangle\langle a|\psi\rangle da. \tag{9.90}$$

But $\langle a|\psi\rangle = \psi(a)$ and $\langle\psi|a\rangle = \psi(a)^*$, so that

$$\langle\psi|\psi\rangle = \int_{\alpha_1}^{\alpha_2} |\psi(a)|^2 da. \tag{9.91}$$

Provided $|\psi(a)|^2$ is a well behaved function, this integral will converge to a finite result, so that the state $|\psi\rangle$ can indeed be normalized to unity.

9.5 Dirac Notation for Operators

The above discussion of the properties of operators was based on making direct use of the defining properties of an operator, that is, in terms of their actions on ket vectors, in particular the vectors belonging to a set of basis states. All of these properties can be represented in a very succinct way that makes explicit use of the Dirac notation. The essential idea is to give a meaning to the symbol $|\phi\rangle\langle\psi|$. The interpretation that is given is defined as follows:

$$\begin{aligned}\big(|\phi\rangle\langle\psi|\big)|\alpha\rangle &= |\phi\rangle\langle\psi|\alpha\rangle\\ \langle\alpha|\big(|\phi\rangle\langle\psi|\big) &= \langle\alpha|\phi\rangle\langle\psi|\end{aligned} \tag{9.92}$$

i.e. it maps kets into kets and bras into bras, exactly as an operator is supposed to.

If we further require $|\phi\rangle\langle\psi|$ to have the linear property

$$\begin{aligned}|\phi\rangle\langle\psi|\big(c_1|\psi_1\rangle + c_2|\psi_2\rangle\big) &= c_1\big(|\phi\rangle\langle\psi|\big)|\psi_1\rangle + c_2\big(|\phi\rangle\langle\psi|\big)|\psi_2\rangle\\ &= |\phi\rangle\big(c_1\langle\psi|\psi_1\rangle + c_2\langle\psi|\psi_2\rangle\big)\end{aligned} \tag{9.93}$$

and similarly for the operator acting on bra vectors, we have given the symbol the properties of a *linear operator*.

We can further generalize this to include sums of such bra-ket combinations, e.g.

$$c_1|\phi_1\rangle\langle\psi_1| + c_2|\phi_2\rangle\langle\psi_2|$$

where c_1 and c_2 are complex numbers, is an operator such that

$$\big(c_1|\phi_1\rangle\langle\psi_1| + c_2|\phi_2\rangle\langle\psi_2|\big)|\xi\rangle = c_1|\phi_1\rangle\langle\psi_1|\xi\rangle + c_2|\phi_2\rangle\langle\psi_2|\xi\rangle \tag{9.94}$$

and similarly for the action on bra vectors.

Below we describe a number of important properties and examples that illustrate the usefulness of this notation.

Projection Operators In this notation, a projection operator $\widehat{P}$ will be simply given by

$$\widehat{P} = |\psi\rangle\langle\psi| \tag{9.95}$$

provided $|\psi\rangle$ is normalized to unity, since we have

$$\widehat{P}^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \widehat{P} \tag{9.96}$$

as required for a projection operator.

Completeness Relation This new notation also makes it possible to express the completeness relation in a particularly compact form. Recall that if the set of ket vectors $\{|\varphi_n\rangle; n = 1, 2, 3 \ldots\}$ is a complete set of orthonormal basis states for the state space of a system, then any state $|\psi\rangle$ can be written

$$|\psi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \tag{9.97}$$

which in our new notation can be written

$$|\psi\rangle = \Big(\sum_n |\varphi_n\rangle\langle\varphi_n|\Big)|\psi\rangle \tag{9.98}$$

so that we must conclude that

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = \widehat{1} \tag{9.99}$$

where $\widehat{1}$ is the unit operator. We can see that the individual terms in the sum, that is the $|\varphi_n\rangle\langle\varphi_n|$, are just projection operators, so that we have shown that the competeness relation can be expressed as a sum over a set of projection operators defined in terms of the basis states $\{|\varphi_n\rangle; n = 1, 2, 3 \ldots\}$. It is often referred to as a *decomposition of unity.*

In the case of continuous eigenvalues, the same argument as above can be followed through. Thus, if we suppose that a Hermitean operator $\widehat{A}$ has a set of eigenstates $\{|a\rangle; \alpha_1 < a < \alpha_2\}$, then we can readily show that

$$\int_{\alpha_1}^{\alpha_2} |a\rangle\langle a|da = \widehat{1}. \tag{9.100}$$

Note that, in practice, it is often the case that an operator can have both discrete and continuous eigenvalues, in which case the completeness relation can be written

$$\sum_n |\varphi_n\rangle\langle\varphi_n| + \int_{\alpha_1}^{\alpha_2} |a\rangle\langle a|da = \widehat{1} \tag{9.101}$$

The completeness relation experssed in this fashion (in both the discrete and continuous cases) is extremely important and has widespread use in calculational work, as illustrated in the following examples.

Example 9.12 Show that any operator can be expressed in terms of this Dirac notation.

We can see this for an operator A by writing

$$\widehat{A} = \widehat{1}\widehat{A}\widehat{1} \tag{9.102}$$

and using the decomposition of unity twice over to give

$$\begin{aligned}\widehat{A} &= \sum_m \sum_n |\varphi_m\rangle\langle\varphi_m|\widehat{A}|\varphi_n\rangle\langle\varphi_n| \\ &= \sum_m \sum_n |\varphi_m\rangle\langle\varphi_n|A_{mn}\end{aligned} \tag{9.103}$$

where $A_{mn} = \langle\varphi_m|\widehat{A}|\varphi_n\rangle$. ■

Example 9.13 Using the decomposition of unity in terms of the basis states $\{|\varphi_n\rangle; n = 1, 2, 3\ldots\}$, expand $\widehat{A}|\varphi_m\rangle$ in terms of these basis states.

This calculation proceeds by inserting the unit operator in a convenient place:

$$\begin{aligned}\widehat{A}|\varphi_m\rangle = \widehat{1}\widehat{A}|\varphi_m\rangle &= \Big(\sum_n |\varphi_n\rangle\langle\varphi_n|\Big)\widehat{A}|\varphi_m\rangle \\ &= \sum_n |\varphi_n\rangle\langle\varphi_n|\widehat{A}|\varphi_m\rangle \\ &= \sum_n A_{nm}|\varphi_n\rangle\end{aligned} \tag{9.104}$$

where $A_{nm} = \langle\varphi_n|\widehat{A}|\varphi_m\rangle$. ■

Example 9.14 Using the decomposition of unity, we can insert the unit operator between the two operators in the quantity $\langle\psi|\widehat{A}\widehat{B}|\phi\rangle$ to give

$$\langle\psi|\widehat{A}\widehat{B}|\phi\rangle = \langle\psi|\widehat{A}\widehat{1}\widehat{B}|\phi\rangle = \sum_n \langle\psi|\widehat{A}|\varphi_n\rangle\langle\varphi_n|\widehat{B}|\phi\rangle. \tag{9.105}$$

■

Hermitean conjugate of an operator It is straightforward to write down the Hermitean conjugate of an operator. Thus, for the operator $\widehat{A}$ given by

$$\widehat{A} = \sum_n c_n|\phi_n\rangle\langle\psi_n| \tag{9.106}$$

we have

$$\langle\phi|\widehat{A}|\psi\rangle = \sum_n c_n\langle\phi|\phi_n\rangle\langle\psi_n|\psi\rangle \tag{9.107}$$

so that taking the complex conjugate we get

$$\langle\psi|\widehat{A}^\dagger|\phi\rangle = \sum_n c_n^*\langle\psi|\psi_n\rangle\langle\phi_n|\phi\rangle = \langle\psi|\Big(\sum_n c_n^*|\psi_n\rangle\langle\phi_n|\Big)|\phi\rangle. \tag{9.108}$$

We can then extract from this the result

$$\widehat{A}^\dagger = \sum_n c_n^*|\psi_n\rangle\langle\phi_n|. \tag{9.109}$$

Spectral decomposition of an operator As a final important example, we can look at the case of expressing an Hermitean operator in terms of projectors onto its basis states. Thus, if we suppose that $\widehat{A}$ has the eigenstates $\{|a_n\rangle; n = 1, 2, 3 \ldots\}$ and associated eigenvalues $a_n, n = 1, 2, 3 \ldots$, so that

$$\widehat{A}|a_n\rangle = a_n|a_n\rangle \tag{9.110}$$

then by noting that the eigenstates of $\widehat{A}$ form a complete orthonormal set of basis states we can write the decomposition of unity in terms of the eigenstates of $\widehat{A}$ as

$$\sum_n |a_n\rangle\langle a_n| = \widehat{1}. \tag{9.111}$$

Thus we find that

$$\widehat{A} = \widehat{A}\,\widehat{1} = \widehat{A}\sum_n |a_n\rangle\langle a_n| = \sum_n \widehat{A}|a_n\rangle\langle a_n| = \sum_n a_n|a_n\rangle\langle a_n|. \tag{9.112}$$

so that

$$\widehat{A} = \sum_n a_n|a_n\rangle\langle a_n|. \tag{9.113}$$

The analogous result for continuous eigenstates is then

$$\widehat{A} = \int_{\alpha_1}^{\alpha_2} a|a\rangle\langle a|da \tag{9.114}$$

while if the operator has both continuous and discrete eigenvalues, the result is

$$\widehat{A} = \sum_n a_n|a_n\rangle\langle a_n| + \int_{\alpha_1}^{\alpha_2} a|a\rangle\langle a|da. \tag{9.115}$$

This is known as the spectral decomposition of the operator $\widehat{A}$, the name coming, in part, from the fact that the collection of eigenvalues of an operator is known as its eigenvalue spectrum.