

Chapter 13

Observables and Measurements in Quantum Mechanics

TILL now, almost all attention has been focussed on discussing the *state* of a quantum system. As we have seen, this is most succinctly done by treating the package of information that defines a state as if it were a vector in an abstract Hilbert space. Doing so provides the mathematical machinery that is needed to capture the physically observed properties of quantum systems. A method by which the state space of a physical system can be set up was described in Section 8.4.2 wherein an essential step was to associate a set of basis states of the system with the exhaustive collection of results obtained when measuring some physical property, or observable, of the system. This linking of particular states with particular measured results provides a way that the observable properties of a quantum system can be described in quantum mechanics, that is in terms of Hermitean operators. It is the way in which this is done that is the main subject of this Chapter.

13.1 Measurements in Quantum Mechanics

One of the most difficult and controversial problems in quantum mechanics is the so-called measurement problem. Opinions on the significance of this problem vary widely. At one extreme the attitude is that there is in fact no problem at all, while at the other extreme the view is that the measurement problem is one of the great unsolved puzzles of quantum mechanics. The issue is that quantum mechanics only provides probabilities for the different possible outcomes in an experiment – it provides no mechanism by which the actual, finally observed result, comes about. Of course, probabilistic outcomes feature in many areas of classical physics as well, but in that case, probability enters the picture simply because there is insufficient information to make a definite prediction. In principle, that missing information is there to be found, it is just that accessing it may be a practical impossibility. In contrast, there is no ‘missing information’ for a quantum system, what we see is all that we can get, even in principle, though there are theories that say that this missing information resides in so-called ‘hidden variables’. But in spite of these concerns about the measurement problem, there are some features of the measurement process that are commonly accepted as being essential parts of the final story. What is clear is that performing a measurement always involves a piece of equipment that

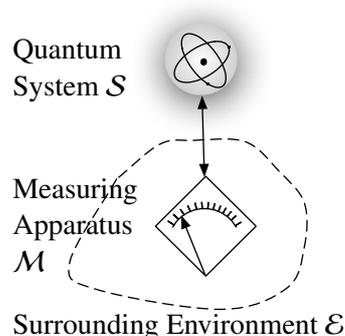


Figure 13.1: System S interacting with measuring apparatus M in the presence of the surrounding environment E . The outcome of the measurement is registered on the dial on the measuring apparatus.

is macroscopic in size, and behaves according to the laws of classical physics. In Section 8.5, the process of decoherence was mentioned as playing a crucial role in giving rise to the observed classical behaviour of macroscopic systems, and so it is not surprising to find that decoherence plays an important role in the formulation of most modern theories of quantum measurement. Any quantum measurement then appears to require three components: the system, typically a microscopic system, whose properties are to be measured, the measuring apparatus itself, which interacts with the system under observation, and the environment surrounding the apparatus whose presence supplies the decoherence needed so that, ‘for all practical purposes (FAPP)’, the apparatus behaves like a classical system, whose output can be, for instance, a pointer on the dial on the measuring apparatus coming to rest, pointing at the final result of the measurement, that is, a number on the dial. Of course, the apparatus could produce an electrical signal registered on an oscilloscope, or bit of data stored in a computer memory, or a flash of light seen by the experimenter as an atom strikes a fluorescent screen, but it is often convenient to use the simple picture of a pointer.

The experimental apparatus would be designed according to what physical property it is of the quantum system that is to be measured. Thus, if the system were a single particle, the apparatus could be designed to measure its energy, or its position, or its momentum or its spin, or some other property. These measurable properties are known as *observables*, a concept that we have already encountered in Section 8.4.1. But how do we know what it is that a particular experimental setup would be measuring? The design would be ultimately based on classical physics principles, i.e., if the apparatus were intended to measure the energy of a quantum system, then it would also measure the energy of a classical system if a classical system were substituted for the quantum system. In this way, the macroscopic concepts of classical physics can be transferred to quantum systems. We will not be examining the details of the measurement process in any great depth here. Rather, we will be more concerned with some of the general characteristics of the outputs of a measurement procedure and how these general features can be incorporated into the mathematical formulation of the quantum theory.

13.2 Observables and Hermitean Operators

So far we have consistently made use of the idea that if we know something definite about the state of a physical system, say that we know the z component of the spin of a spin half particle is $S_z = \frac{1}{2}\hbar$, then we assign to the system the state $|S_z = \frac{1}{2}\hbar\rangle$, or, more simply, $|+\rangle$. It is at this point that we need to look a little more closely at this idea, as it will lead us to associating an operator with the physical concept of an observable. Recall that an observable is, roughly speaking, any measurable property of a physical system: position, spin, energy, momentum Thus, we talk about the position x of a particle as an observable for the particle, or the z component of spin, S_z as a further observable and so on.

When we say that we ‘know’ the value of some physical observable of a quantum system, we are presumably implying that some kind of measurement has been made that provided us with this knowledge. It is furthermore assumed that in the process of acquiring this knowledge, the system, after the measurement has been performed, survives the measurement, and moreover if we were to immediately remeasure the same quantity, we would get the same result. This is certainly the situation with the measurement of spin in a Stern-Gerlach experiment. If an atom emerges from one such set of apparatus in a beam that indicates that $S_z = \frac{1}{2}\hbar$ for that atom, and we were to pass the atom through a second apparatus, also with its magnetic field oriented in the z direction, we would find the atom emerging in the $S_z = \frac{1}{2}\hbar$ beam once again. Under such circumstances, we would be justified in saying that the atom has been prepared in the state $|S_z = \frac{1}{2}\hbar\rangle$. However, the reality is that few measurements are of this kind, i.e. the system being subject to measurement is physically modified, if not destroyed, by the measurement process. An extreme example is a measurement designed to count the number of photons in a single mode

cavity field. Photons are typically counted by photodetectors whose mode of operation is to absorb a photon and create a pulse of current. So we may well be able to count the number of photons in the field, but in doing so, there is no field left behind after the counting is completed. All that we can conclude, regarding the state of the cavity field, is that it is left in the vacuum state $|0\rangle$ after the measurement is completed, but we can say nothing for certain about the state of the field before the measurement was undertaken. However, all is not lost. If we fiddle around with the process by which we put photons in the cavity in the first place, it will hopefully be the case that amongst all the experimental procedures that could be followed, there are some that result in the cavity field being in a state for which every time we then measure the number of photons in the cavity, we always get the result n . It is then not unreasonable to claim that the experimental procedure has prepared the cavity field in a state which the number of photons in the cavity is n , and we can assign the state $|n\rangle$ to the cavity field.

This procedure can be equally well applied to the spin half example above. The preparation procedure here consists of putting atoms through a Stern-Gerlach apparatus with the field oriented in the z direction, and picking out those atoms that emerge in the beam for which $S_z = \frac{1}{2}\hbar$. This has the result of preparing the atom in a state for which the z component of spin would always be measured to have the value $\frac{1}{2}\hbar$. Accordingly, the state of the system is identified as $|S_z = \frac{1}{2}\hbar\rangle$, i.e. $|+\rangle$. In a similar way, we can associate the state $|-\rangle$ with the atom being in a state for which the z component of spin is always measured to be $-\frac{1}{2}\hbar$. We can also note that these two states are mutually exclusive, i.e. if in the state $|+\rangle$, then the result $S_z = -\frac{1}{2}\hbar$ is never observed, and furthermore, we note that the two states cover all possible values for S_z . Finally, the fact that observation of the behaviour of atomic spin show evidence of both randomness and interference lead us to conclude that if an atom is prepared in an arbitrary initial state $|S\rangle$, then the probability amplitude of finding it in some other state $|S'\rangle$ is given by

$$\langle S'|S\rangle = \langle S'|+\rangle\langle +|S\rangle + \langle S'|-\rangle\langle -|S\rangle$$

which leads, by the cancellation trick to

$$|S\rangle = |+\rangle\langle +|S\rangle + |-\rangle\langle -|S\rangle$$

which tells us that *any* spin state of the atom is to be interpreted as a vector expressed as a linear combination of the states $|\pm\rangle$. The states $|\pm\rangle$ constitute a complete set of orthonormal basis states for the state space of the system. We therefore have at hand just the situation that applies to the eigenstates and eigenvectors of a Hermitean operator as summarized in the following table:

Properties of a Hermitean Operator	Properties of Observable S_z
The eigenvalues of a Hermitean operator are all real.	Value of observable S_z measured to be real numbers $\pm\frac{1}{2}\hbar$.
Eigenvectors belonging to different eigenvalues are orthogonal.	States $ \pm\rangle$ associated with different values of the observable are mutually exclusive.
The eigenstates form a complete set of basis states for the state space of the system.	The states $ \pm\rangle$ associated with all the possible values of observable S_z form a complete set of basis states for the state space of the system.

It is therefore natural to associate with the observable S_z , a Hermitean operator which we will write as \hat{S}_z such that \hat{S}_z has eigenstates $|\pm\rangle$ and associate eigenvalues $\pm\frac{1}{2}\hbar$, i.e.

$$\hat{S}_z|\pm\rangle = \pm\frac{1}{2}\hbar|\pm\rangle \quad (13.1)$$

so that, in the $\{|-\rangle, |+\rangle\}$ basis

$$\hat{S}_z \doteq \begin{pmatrix} \langle +|\hat{S}_z|+\rangle & \langle +|\hat{S}_z|-\rangle \\ \langle -|\hat{S}_z|+\rangle & \langle -|\hat{S}_z|-\rangle \end{pmatrix} \quad (13.2)$$

$$= \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (13.3)$$

So, in this way, we actually *construct* a Hermitean operator to represent a particular measurable property of a physical system.

The term ‘observable’, while originally applied to the physical quantity of interest, is also applied to the associated Hermitean operator. Thus we talk, for instance, about the observable \hat{S}_z . To a certain extent we have used the mathematical construct of a Hermitean operator to draw together in a compact fashion ideas that we have been freely using in previous Chapters.

It is useful to note the distinction between a quantum mechanical observable and the corresponding classical quantity. The latter quantity, say the position x of a particle, represents a single possible value for that observable – though it might not be known, it in principle has a definite, single value at any instant in time. In contrast, a quantum observable such as S_z is an operator which, through its eigenvalues, carries with it *all* the values that the corresponding physical quantity could possibly have. In a certain sense, this is a reflection of the physical state of affairs that pertains to quantum systems, namely that when a measurement is made of a particular physical property of a quantum systems, the outcome can, in principle, be *any* of the possible values that can be associated with the observable, even if the experiment is repeated under identical conditions.

This procedure of associating a Hermitean operator with every observable property of a quantum system can be readily generalized. The generalization takes a slightly different form if the observable has a continuous range of possible values, such as position and momentum, as against an observable with only discrete possible results. We will consider the discrete case first.

13.3 Observables with Discrete Values

The discussion presented in the preceding Section can be generalized into a collection of postulates that are intended to describe the concept of an observable. So, to begin, suppose, through an exhaustive series of measurements, we find that a particular observable, call it Q , of a physical system, is found to have the values — all real numbers — q_1, q_2, \dots . Alternatively, we may have sound theoretical arguments that inform us as to what the possible values could be. For instance, we might be interested in the position of a particle free to move in one dimension, in which case the observable Q is just the position of the particle, which would be expected to have any value in the range $-\infty$ to $+\infty$. We now introduce the states $|q_1\rangle, |q_2\rangle, \dots$ these being states for which the observable Q definitely has the value q_1, q_2, \dots respectively. In other words, these are the states for which, if we were to measure Q , we would be guaranteed to get the results q_1, q_2, \dots respectively. We now have an interesting state of affairs summarized below.

1. We have an observable Q which, when measured, is found to have the values q_1, q_2, \dots that are all real numbers.
2. For each possible value of Q the system can be prepared in a corresponding state $|q_1\rangle, |q_2\rangle, \dots$ for which the values q_1, q_2, \dots will be obtained with certainty in any measurement of Q .

At this stage we are still not necessarily dealing with a quantum system. We therefore assume that this system exhibits the properties of intrinsic randomness and interference that characterizes quantum systems, and which allows the state of the system to be identified as vectors belonging to the state space of the system. This leads to the next property:

3. If prepared in this state $|q_n\rangle$, and we measure Q , we only ever get the result q_n , i.e. we never observe the result q_m with $q_m \neq q_n$. Thus we conclude $\langle q_n|q_m\rangle = \delta_{nm}$. The states $\{|q_n\rangle; n = 1, 2, 3, \dots\}$ are orthonormal.
4. The states $|q_1\rangle, |q_2\rangle, \dots$ cover all the possibilities for the system and so these states form a complete set of orthonormal basis states for the state space of the system.

That the states form a complete set of basis states means that any state $|\psi\rangle$ of the system can be expressed as

$$|\psi\rangle = \sum_n c_n |q_n\rangle \quad (13.4)$$

while orthonormality means that $\langle q_n|q_m\rangle = \delta_{nm}$ from which follows $c_n = \langle q_n|\psi\rangle$. The completeness condition can then be written as

$$\sum_n |q_n\rangle\langle q_n| = \hat{1} \quad (13.5)$$

5. For the system in state $|\psi\rangle$, the probability of obtaining the result q_n on measuring Q is $|\langle q_n|\psi\rangle|^2$ provided $\langle \psi|\psi\rangle = 1$.

The completeness of the states $|q_1\rangle, |q_2\rangle, \dots$ means that there is *no* state $|\psi\rangle$ of the system for which $\langle q_n|\psi\rangle = 0$ for *every* state $|q_n\rangle$. In other words, we must have

$$\sum_n |\langle q_n|\psi\rangle|^2 \neq 0. \quad (13.6)$$

Thus there is a non-zero probability for at least *one* of the results q_1, q_2, \dots to be observed – if a measurement is made of Q , a result has to be obtained!

6. The observable Q is represented by a Hermitean operator \hat{Q} whose eigenvalues are the possible results q_1, q_2, \dots of a measurement of Q , and the associated eigenstates are the states $|q_1\rangle, |q_2\rangle, \dots$, i.e. $\hat{Q}|q_n\rangle = q_n|q_n\rangle$. The name ‘observable’ is often applied to the operator \hat{Q} itself.

The spectral decomposition of the observable \hat{Q} is then

$$\hat{Q} = \sum_n q_n |q_n\rangle\langle q_n|. \quad (13.7)$$

Apart from anything else, the eigenvectors of an observable constitute a set of basis states for the state space of the associated quantum system.

For state spaces of finite dimension, the eigenvalues of any Hermitean operator are discrete, and the eigenvectors form a complete set of basis states. For state spaces of infinite dimension, it is possible for a Hermitean operator not to have a complete set of eigenvectors, so that it is possible for a system to be in a state which cannot be represented as a linear combination of the eigenstates of such an operator. In this case, the operator cannot be understood as being an observable as it would appear to be the case that the system could be placed in a state for which a measurement of the associated observable yielded no value! To put it another way, if a Hermitean operator could be constructed whose eigenstates did not form a complete set, then we can rightfully claim that such an operator cannot represent an observable property of the system.

It should also be pointed out that it is quite possible to construct all manner of Hermitean operators to be associated with any given physical system. Such operators would have all the mathematical

properties to be associated with their being Hermitian, but it is not necessarily the case that these represent either any readily identifiable physical feature of the system at least in part because it might not be at all apparent how such ‘observables’ could be measured. The same is at least partially true classically — the quantity px^2 where p is the momentum and x the position of a particle does not immediately suggest a useful, familiar or fundamental property of a single particle.

13.3.1 The Von Neumann Measurement Postulate

Finally, we add a further postulate concerning the state of the system immediately after a measurement is made. This is the von Neumann projection postulate:

7. If on measuring Q for a system in state $|\psi\rangle$, a result q_n is obtained, then the state of the system immediately after the measurement is $|q_n\rangle$.

This postulate can be rewritten in a different way by making use of the projection operators introduced in Section 11.1.3. Thus, if we write

$$\hat{P}_n = |q_n\rangle\langle q_n| \quad (13.8)$$

then the state of the system after the measurement, for which the result q_n was obtained, is

$$\frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} = \frac{\hat{P}_n|\psi\rangle}{\sqrt{|\langle q_n|\psi\rangle|^2}} \quad (13.9)$$

where the term in the denominator is there to guarantee that the state after the measurement is normalized to unity.

This postulate is almost stating the obvious in that we *name* a state according to the information that we obtain about it as a result of a measurement. But it can also be argued that if, after performing a measurement that yields a particular result, we immediately repeat the measurement, it is reasonable to expect that there is a 100% chance that the same result be regained, which tells us that the system must have been in the associated eigenstate. This was, in fact, the main argument given by von Neumann to support this postulate. Thus, von Neumann argued that the fact that the value has a stable result upon repeated measurement indicates that the system really has that value after measurement.

This postulate regarding the effects of measurement has always been a source of discussion and disagreement. This postulate is satisfactory in that it is consistent with the manner in which the idea of an observable was introduced above, but it is not totally clear that it is a postulate that can be applied to all measurement processes. The kind of measurements wherein this postulate is satisfactory are those for which the system ‘survives’ the measuring process, which is certainly the case in the Stern-Gerlach experiments considered here. But this is not at all what is usually encountered in practice. For instance, measuring the number of photons in an electromagnetic field inevitably involves detecting the photons by absorbing them, i.e. the photons are destroyed. Thus we may find that if n photons are absorbed, then we can say that there *were* n photons in the cavity, i.e. the photon field *was* in state $|n\rangle$, but after the measuring process is over, it is in the state $|0\rangle$. To cope with this fairly typical state of affairs it is necessary to generalize the notion of measurement to allow for this – so-called generalized measurement theory. But even here, it is found that the generalized measurement process being described can be understood as a von Neumann-type projection made on a larger system of which the system of interest is a part. This larger system could include, for instance, the measuring apparatus itself, so that instead of making a projective measurement on the system itself, one is made on the measuring apparatus. We will not be discussing these aspects of measurement theory here.

13.4 The Collapse of the State Vector

The von Neumann postulate is quite clearly stating that as a consequence of a measurement, the state of the system undergoes a discontinuous change of state, i.e. $|\psi\rangle \rightarrow |q_n\rangle$ if the result q_n is obtained on performing a measurement of an observable Q . This instantaneous change in state is known as ‘the collapse of the state vector’. This conjures up the impression that the process of measurement necessarily involves a physical interaction with the system, that moreover, results in a major physical disruption of the state of a system – one moment the system is in a state $|\psi\rangle$, the next it is forced into a state $|q_n\rangle$. However, if we return to the quantum eraser example considered in Section 4.3.2 we see that there need not be any actual physical interaction with a system at all in order to obtain information about it. The picture that emerges is that the change of state is nothing more benign than being an updating, through observation, of the knowledge we have of the state of a system as a consequence of the outcome of a measurement. While obtaining this information must necessarily involve some kind of physical interaction involving a measuring apparatus, this interaction may or may not be associated with any physical disruption to the system of interest itself. This emphasizes the notion that quantum states are as much states of knowledge as they are physical states.

13.4.1 Sequences of measurements

Having on hand a prescription by which we can specify the state of a system after a measurement has been performed makes it possible to study the outcome of alternating measurements of different observables being performed on a system. We have already seen an indication of the sort of result to be found in the study of the measurement of different spin components of a spin half particle in Section 6.4.3. For instance, if a measurement of, say, S_x is made, giving a result $\frac{1}{2}\hbar$, and then S_z is measured, giving, say, $\frac{1}{2}\hbar$, and then S_x remeasured, there is an equal chance that either of the results $\pm\frac{1}{2}\hbar$ will be obtained, i.e. the formerly precisely known value of S_x is ‘randomly scrambled’ by the intervening measurement of S_z . The two observables are said to be incompatible: it is not possible to have exact knowledge of both S_x and S_z at the same time. This behaviour was presented in Section 6.4.3 as an experimentally observed fact, but we can now see how this kind of behaviour comes about within the formalism of the theory.

If we let \hat{S}_x and \hat{S}_z be the associated Hermitean operators, we can analyze the above observed behaviour as follows. The first measurement of S_x , which yielded the outcome $\frac{1}{2}\hbar$, results in the spin half system ending up in the state $|S_x = \frac{1}{2}\hbar\rangle$, an eigenstate of \hat{S}_x with eigenvalue $\frac{1}{2}\hbar$. The second measurement, of S_z , results in the system ending up in the state $|S_z = \frac{1}{2}\hbar\rangle$, the eigenstate of \hat{S}_z with eigenvalue $\frac{1}{2}\hbar$. However, this latter state cannot be an eigenstate of \hat{S}_x . If it were, we would not get the observed outcome, that is, on the remeasurement of S_x , we would not get a random scatter of results (i.e. the two results $S_x = \pm\frac{1}{2}\hbar$ occurring randomly but equally likely). In the same way we can conclude that $|S_x = -\frac{1}{2}\hbar\rangle$ is also not an eigenstate of \hat{S}_z , and likewise, the eigenstates $|S_z = \pm\frac{1}{2}\hbar\rangle$ of \hat{S}_z cannot be eigenstates of \hat{S}_x . Thus we see that the two incompatible observables S_x and S_z do not share the same eigenstates.

There is a more succinct way by which to determine whether two observables are incompatible or not. This involves making use of the concept of the commutator of two operators, $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ as discussed in Section 11.1.3. To this end, consider the commutator $[\hat{S}_x, \hat{S}_z]$ and let it act on the eigenstate $|S_z = \frac{1}{2}\hbar\rangle = |+\rangle$:

$$[\hat{S}_x, \hat{S}_z]|+\rangle = (\hat{S}_x\hat{S}_z - \hat{S}_z\hat{S}_x)|+\rangle = \hat{S}_x\left(\frac{1}{2}\hbar|+\rangle\right) - \hat{S}_z\left(\hat{S}_x|+\rangle\right) = \left(\frac{1}{2}\hbar - \hat{S}_z\right)\left(\hat{S}_x|+\rangle\right). \quad (13.10)$$

Now let $\hat{S}_x|+\rangle = |\psi\rangle$. Then we see that in order for this expression to vanish, we must have

$$\hat{S}_z|\psi\rangle = \frac{1}{2}\hbar|\psi\rangle. \quad (13.11)$$

In other words, $|\psi\rangle$ would have to be the eigenstate of \hat{S}_z with eigenvalue $\frac{1}{2}\hbar$, i.e. $|\psi\rangle \propto |+\rangle$, or

$$\hat{S}_x|+\rangle = \text{constant} \times |+\rangle \quad (13.12)$$

But we have just pointed out that this cannot be the case, so the expression $[\hat{S}_x, \hat{S}_z]|+\rangle$ cannot be zero, i.e. we must have

$$[\hat{S}_x, \hat{S}_z] \neq 0. \quad (13.13)$$

Thus, the operators \hat{S}_x and \hat{S}_z do not commute.

The commutator of two observables serves as a means by which it can be determined whether or not the observables are compatible. If they do not commute, then they are incompatible: the measurement of one of the observables will randomly scramble any preceding result known for the other. In contrast, if they do commute, then it is possible to know precisely the value of both observables at the same time. An illustration of this is given later in this Chapter (Section 13.5.4), while the importance of compatibility is examined in more detail later in Chapter 14.

13.5 Examples of Discrete Valued Observables

There are many observables of importance for all manner of quantum systems. Below, some of the important observables for a single particle system are described. As the eigenstates of any observable constitutes a set of basis states for the state space of the system, these basis states can be used to set up representations of the state vectors and operators as column vectors and matrices. These representations are named according to the observable which defines the basis states used. Moreover, since there are in general many observables associated with a system, there are correspondingly many possible basis states that can be so constructed. Of course, there are an infinite number of possible choices for the basis states of a vector space, but what this procedure does is pick out those basis states which are of most immediate physical significance.

The different possible representations are useful in different kinds of problems, as discussed briefly below. It is to be noted that the term ‘observable’ is used both to describe the physical quantity being measured as well as the operator itself that corresponds to the physical quantity.

13.5.1 Position of a particle (in one dimension)

The position x of a particle is a continuous quantity, with values ranging over the real numbers, and a proper treatment of such an observable raises mathematical and interpretational issues that are dealt with elsewhere. But for the present, it is very convenient to introduce an ‘approximate’ position operator via models of quantum systems in which the particle, typically an electron, can only be found to be at certain discrete positions. The simplest example of this is the O_2^- ion discussed in Section 8.4.2.

This system can be found in two states $|\pm a\rangle$, where $\pm a$ are the positions of the electron on one or the other of the oxygen atoms. Thus these states form a pair of basis states for the state space of the system, which hence has a dimension 2. The position operator \hat{x} of the electron is such that

$$\hat{x}|\pm a\rangle = \pm a|\pm a\rangle \quad (13.14)$$

which can be written in the position representation as a matrix:

$$\hat{x} \doteq \begin{pmatrix} \langle +a|\hat{x}|+a\rangle & \langle +a|\hat{x}|-a\rangle \\ \langle -a|\hat{x}|+a\rangle & \langle -a|\hat{x}|-a\rangle \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}. \quad (13.15)$$

The completeness relation for these basis states reads

$$|+a\rangle\langle +a| + |-a\rangle\langle -a| = \hat{1}. \quad (13.16)$$

which leads to

$$\hat{x} = a|+a\rangle\langle+a| - a|-a\rangle\langle-a|. \quad (13.17)$$

The state space of the system has been established as having dimension 2, so any other observable of the system can be represented as a 2×2 matrix. We can use this to construct the possible forms of other observables for this system, such as the momentum operator and the Hamiltonian.

This approach can be readily generalized to e.g. a CO_2^- ion, in which case there are three possible positions for the electron, say $x = \pm a, 0$ where $\pm a$ are the positions of the electron when on the oxygen atoms and 0 is the position of the electron when on the carbon atom. The position operator \hat{x} will then be such that

$$\hat{x}|\pm a\rangle = \pm a|\pm a\rangle \quad \hat{x}|0\rangle = 0|0\rangle. \quad (13.18)$$

13.5.2 Momentum of a particle (in one dimension)

As is the case of position, the momentum of a particle can have a continuous range of values, which raises certain mathematical issues that are discussed later. But we can consider the notion of momentum for our approximate position models in which the position can take only discrete values. We do this through the observation that the matrix representing the momentum will be a $N \times N$ matrix, where N is the dimension of the state space of the system. Thus, for the O_2^- ion, the momentum operator would be represented by a two by two matrix

$$\hat{p} \doteq \begin{pmatrix} \langle +a|\hat{p}|+a\rangle & \langle +a|\hat{p}|-a\rangle \\ \langle -a|\hat{p}|+a\rangle & \langle -a|\hat{p}|-a\rangle \end{pmatrix} \quad (13.19)$$

though, at this stage, it is not obvious what values can be assigned to the matrix elements appearing here. Nevertheless, we can see that, as \hat{p} must be a Hermitean operator, and as this is a 2×2 matrix, \hat{p} will have only 2 real eigenvalues: the momentum of the electron can be measured to have only two possible values, at least within the constraints of the model we are using.

13.5.3 Energy of a Particle (in one dimension)

According to classical physics, the energy of a particle is given by

$$E = \frac{p^2}{2m} + V(x) \quad (13.20)$$

where the first term on the RHS is the kinetic energy, and the second term $V(x)$ is the potential energy of the particle. In quantum mechanics, it can be shown, by a procedure known as canonical quantization, that the energy of a particle is represented by a Hermitean operator known as the Hamiltonian, written \hat{H} , which can be expressed as

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad (13.21)$$

where the classical quantities p and x have been replaced by the corresponding quantum operators. The term Hamiltonian is derived from the name of the mathematician Rowan Hamilton who made profoundly significant contributions to the theory of mechanics. Although the Hamiltonian can be identified here as being the total energy E , the term Hamiltonian is usually applied in mechanics if this total energy is expressed in terms of momentum and position variables, as here, as against say position and velocity.

That Eq. (13.21) is ‘quantum mechanical’ is not totally apparent. Dressing the variables up as operators by putting hats on them is not really saying that much. Perhaps most significantly there is no \hbar in this expression for \hat{H} , so it is not obvious how this expression can be ‘quantum mechanical’.

For instance, we have seen, at least for a particle in an infinite potential well (see Section 5.3), that the energies of a particle depend on \hbar . The quantum mechanics (and the \hbar) is to be found in the properties of the operators so created that distinguish them from the classical variables that they replace. Specifically, the two operators \hat{x} and \hat{p} do not commute, in fact, $[\hat{x}, \hat{p}] = i\hbar$ as shown later, Eq. (13.133), and it is this failure to commute by an amount proportional to \hbar that injects ‘quantum mechanics’ into the operator associated with the energy of a particle.

As the eigenvalues of the Hamiltonian are the possible energies of the particle, the eigenvalue is usually written E and the eigenvalue equation is

$$\hat{H}|E\rangle = E|E\rangle. \quad (13.22)$$

In the position representation, this equation becomes

$$\langle x|\hat{H}|E\rangle = E\langle x|E\rangle. \quad (13.23)$$

It is shown later that, from the expression Eq. (13.21) for \hat{H} , that this eigenvalue equation can be written as a differential equation for the wave function $\psi_E(x) = \langle x|E\rangle$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_E(x)}{dx^2} + V(x)\psi_E(x) = E\psi_E(x). \quad (13.24)$$

This is just the time independent Schrödinger equation.

Depending on the form of $V(\hat{x})$, this equation will have different possible solutions, and the Hamiltonian will have various possible eigenvalues. For instance, if $V(\hat{x}) = 0$ for $0 < x < L$ and is infinite otherwise, then we have the Hamiltonian of a particle in an infinitely deep potential well, or equivalently, a particle in a (one-dimensional) box with impenetrable walls. This problem was dealt with in Section 5.3 using the methods of wave mechanics, where it was found that the energy of the particle was limited to the values

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}, \quad n = 1, 2, \dots$$

Thus, in this case, the Hamiltonian has discrete eigenvalues E_n given by Eq. (13.5.3). If we write the associated energy eigenstates as $|E_n\rangle$, the eigenvalue equation is then

$$\hat{H}|E_n\rangle = E_n|E_n\rangle. \quad (13.25)$$

The wave function $\langle x|E_n\rangle$ associated with the energy eigenstate $|E_n\rangle$ was also derived in Section 5.3 and is given by

$$\begin{aligned} \psi_n(x) = \langle x|E_n\rangle &= \sqrt{\frac{2}{L}} \sin(n\pi x/L) & 0 < x < L \\ &= 0 & x < 0, \quad x > L. \end{aligned} \quad (13.26)$$

Another example is that for which $V(\hat{x}) = \frac{1}{2}k\hat{x}^2$, i.e. the simple harmonic oscillator potential. In this case, we find that the eigenvalues of \hat{H} are

$$E_n = (n + \frac{1}{2})\hbar\omega, \quad n = 0, 1, 2, \dots \quad (13.27)$$

where $\omega = \sqrt{k/m}$ is the natural frequency of the oscillator. The Hamiltonian is an observable of particular importance in quantum mechanics. As will be discussed in the next Chapter, it is the Hamiltonian which determines how a system evolves in time, i.e. the equation of motion of a quantum system is expressly written in terms of the Hamiltonian. In the position representation, this equation is just the time dependent Schrödinger equation.

The Energy Representation If the state of the particle is represented in component form with respect to the energy eigenstates as basis states, then this is said to be the *energy representation*. In contrast to the position and momentum representations, the components are often discrete. The energy representation is useful when the system under study can be found in states with different energies, e.g. an atom absorbing or emitting photons, and consequently making transitions to higher or lower energy states. The energy representation is also very important when it is the evolution in time of a system that is of interest.

13.5.4 The O_2^- Ion: An Example of a Two-State System

In order to illustrate the ideas developed in the preceding sections, we will see how it is possible, firstly, how to ‘construct’ the Hamiltonian of a simple system using simple arguments, then to look at the consequences of performing measurements of two observables for this system.

Constructing the Hamiltonian

The Hamiltonian of the ion in the position representation will be

$$\hat{H} \doteq \begin{pmatrix} \langle +a|\hat{H}|+a\rangle & \langle +a|\hat{H}|-a\rangle \\ \langle -a|\hat{H}|+a\rangle & \langle -a|\hat{H}|-a\rangle \end{pmatrix}. \quad (13.28)$$

Since there is perfect symmetry between the two oxygen atoms, we must conclude that the diagonal elements of this matrix must be equal i.e.

$$\langle +a|\hat{H}|+a\rangle = \langle -a|\hat{H}|-a\rangle = E_0. \quad (13.29)$$

We further know that the Hamiltonian must be Hermitean, so the off-diagonal elements are complex conjugates of each other. Hence we have

$$\hat{H} \doteq \begin{pmatrix} E_0 & V \\ V^* & E_0 \end{pmatrix} \quad (13.30)$$

or, equivalently

$$\hat{H} = E_0|+a\rangle\langle +a| + V|+a\rangle\langle -a| + V^*|-a\rangle\langle +a| + E_0|-a\rangle\langle -a|. \quad (13.31)$$

Rather remarkably, we have at hand the Hamiltonian for the system with the barest of physical information about the system.

In the following we shall assume $V = -A$ and that A is a real number so that the Hamiltonian matrix becomes

$$\hat{H} \doteq \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} \quad (13.32)$$

The physical content of the results are not changed by doing this, and the results are a little easier to write down. First we can determine the eigenvalues of \hat{H} by the usual method. If we write $\hat{H}|E\rangle = E|E\rangle$, and put $|E\rangle = \alpha|+a\rangle + \beta|-a\rangle$, this becomes, in matrix form

$$\begin{pmatrix} E_0 - E & -A \\ -A & E_0 - E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0. \quad (13.33)$$

The characteristic equation yielding the eigenvalues is then

$$\begin{vmatrix} E_0 - E & -A \\ -A & E_0 - E \end{vmatrix} = 0. \quad (13.34)$$

Expanding the determinant this becomes

$$(E_0 - E)^2 - A^2 = 0 \quad (13.35)$$

with solutions

$$E_1 = E_0 + A \quad E_2 = E_0 - A. \quad (13.36)$$

Substituting each of these two values back into the original eigenvalue equation then gives the equations for the eigenstates. We find that

$$|E_1\rangle = \frac{1}{\sqrt{2}}(|+a\rangle - |-a\rangle) \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (13.37)$$

$$|E_2\rangle = \frac{1}{\sqrt{2}}(|+a\rangle + |-a\rangle) \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (13.38)$$

where each eigenvector has been normalized to unity. Thus we have constructed the eigenstates and eigenvalues of the Hamiltonian of this system. We can therefore write the Hamiltonian as

$$\hat{H} = E_1|E_1\rangle\langle E_1| + E_2|E_2\rangle\langle E_2| \quad (13.39)$$

which is just the spectral decomposition of the Hamiltonian.

We have available two useful sets of basis states: the basis states for the position representation $\{|+a\rangle, |-a\rangle\}$ and the basis states for the energy representation, $\{|E_1\rangle, |E_2\rangle\}$. Any state of the system can be expressed as linear combinations of either of these sets of basis states.

Measurements of Energy and Position

Suppose we prepare the O_2^- ion in the state

$$\begin{aligned} |\psi\rangle &= \frac{1}{5}[3|+a\rangle + 4|-a\rangle] \\ &\doteq \frac{1}{5} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \end{aligned} \quad (13.40)$$

and we measure the energy of the ion. We can get two possible results of this measurement: E_1 or E_2 . We will get the result E_1 with probability $|\langle E_1|\psi\rangle|^2$, i.e.

$$\langle E_1|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \end{pmatrix} \cdot \frac{1}{5} \begin{pmatrix} 3 \\ 4 \end{pmatrix} = -\frac{1}{5\sqrt{2}} \quad (13.41)$$

so that

$$|\langle E_1|\psi\rangle|^2 = 0.02 \quad (13.42)$$

and similarly

$$\langle E_2|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix} \cdot \frac{1}{5} \begin{pmatrix} 3 \\ 4 \end{pmatrix} = \frac{7}{5\sqrt{2}} \quad (13.43)$$

so that

$$|\langle E_2|\psi\rangle|^2 = 0.98. \quad (13.44)$$

It is important to note that if we get the result E_1 , then according to the von Neumann postulate, the system ends up in the state $|E_1\rangle$, whereas if we got the result E_2 , then the new state is $|E_2\rangle$.

Of course we could have measured the position of the electron, with the two possible outcomes $\pm a$. In fact, the result $+a$ will occur with probability

$$|\langle +a|\psi\rangle|^2 = 0.36 \quad (13.45)$$

and the result $-a$ with probability

$$|\langle -a|\psi\rangle|^2 = 0.64. \quad (13.46)$$

Once again, if the outcome is $+a$ then the state of the system after the measurement is $|+a\rangle$, and if the result $-a$ is obtained, then the state after the measurement is $|-a\rangle$.

Finally, we can consider what happens if we were to do a sequence of measurements, first of energy, then position, and then energy again. Suppose the system is initially in the state $|\psi\rangle$, as above, and the measurement of energy gives the result E_1 . The system is now in the state $|E_1\rangle$. If we now perform a measurement of the position of the electron, we can get either of the two results $\pm a$ with equal probability:

$$|\langle \pm a|E_1\rangle|^2 = 0.5. \quad (13.47)$$

Suppose we get the result $+a$, so the system is now in the state $|+a\rangle$ and we remeasure the energy. We find that now it is not guaranteed that we will regain the result E_1 obtained in the first measurement. In fact, we find that there is an equal chance of getting either E_1 or E_2 :

$$|\langle E_1|+a\rangle|^2 = |\langle E_2|+a\rangle|^2 = 0.5. \quad (13.48)$$

Thus we must conclude that the intervening measurement of the position of the electron has scrambled the energy of the system. In fact, if we suppose that we get the result E_2 for this second energy measurement, thereby placing the system in the state $|E_2\rangle$ and we measure the position of the electron again, we find that we will get either result $\pm a$ with equal probability again! The measurement of energy and electron position for this system clearly interfere with one another. It is not possible to have a precisely defined value for *both* the energy of the system and the position of the electron: they are incompatible observables. We can apply the test discussed in Section 13.4.1 for incompatibility of \hat{x} and \hat{H} here by evaluating the commutator $[\hat{x}, \hat{H}]$ using their representative matrices:

$$\begin{aligned} [\hat{x}, \hat{H}] &= \hat{x}\hat{H} - \hat{H}\hat{x} \\ &= a \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} - a \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= -2aA \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \neq 0. \end{aligned} \quad (13.49)$$

13.5.5 Observables for a Single Mode EM Field

A somewhat different example from those presented above is that of the field inside a single mode cavity (see pp 113, 131). In this case, the basis states of the electromagnetic field are the number states $\{|n\rangle, n = 0, 1, 2, \dots\}$ where the state $|n\rangle$ is the state of the field in which there are n photons present.

Number Operator From the annihilation operator \hat{a} (Eq. (11.57)) and creation operator \hat{a}^\dagger (Eq. (11.72)) for this field, defined such that

$$\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle, & \hat{a}|0\rangle &= 0 \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned}$$

we can construct a Hermitean operator \hat{N} defined by

$$\hat{N} = \hat{a}^\dagger \hat{a} \quad (13.50)$$

which can be readily shown to be such that

$$\hat{N}|n\rangle = n|n\rangle. \quad (13.51)$$

This operator is an observable of the system of photons. Its eigenvalues are the integers $n = 0, 1, 2, \dots$ which correspond to the possible results obtained when the number of photons in the cavity are measured, and $|n\rangle$ are the corresponding eigenstates, the number states, representing the state in which there are exactly n photons in the cavity. This observable has the spectral decomposition

$$\hat{N} = \sum_{n=0}^{\infty} n|n\rangle\langle n|. \quad (13.52)$$

Hamiltonian If the cavity is designed to support a field of frequency ω , then each photon would have the energy $\hbar\omega$, so that the energy of the field when in the state $|n\rangle$ would be $n\hbar\omega$. From this information we can construct the Hamiltonian for the cavity field. It will be

$$\hat{H} = \hbar\omega\hat{N}. \quad (13.53)$$

A more rigorous analysis based on ‘quantizing’ the electromagnetic field yields an expression $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$ for the Hamiltonian. The additional term $\frac{1}{2}\hbar\omega$ is known as the zero point energy of the field. Its presence is required by the uncertainty principle, though it apparently plays no role in the dynamical behaviour of the cavity field as it merely represents a shift in the zero of energy of the field.

13.6 Observables with Continuous Values

In the case of measurements being made of an observable with a continuous range of possible values such as position or momentum, or in some cases, energy, the above postulates need to be modified somewhat. The modifications arise first, from the fact that the eigenvalues are continuous, but also because the state space of the system will be of infinite dimension.

To see why there is an issue here in the first place, we need to see where any of the statements made in the case of an observable with discrete values comes unstuck. This can best be seen if we consider a particular example, that of the position of a particle.

13.6.1 Measurement of Particle Position

If we are to suppose that a particle at a definite position x is to be assigned a state vector $|x\rangle$, and if further we are to suppose that the possible positions are continuous over the range $(-\infty, +\infty)$ and that the associated states are complete, then we are led to requiring that any state $|\psi\rangle$ of the particle must be expressible as

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle dx \quad (13.54)$$

with the states $|x\rangle$ δ -function normalised, i.e.

$$\langle x|x'\rangle = \delta(x - x'). \quad (13.55)$$

The difficulty with this is that the state $|x\rangle$ has infinite norm: it cannot be normalized to unity and hence cannot represent a possible physical state of the system. This makes it problematical to introduce the idea of an observable – the position of the particle – that can have definite values x associated with unphysical states $|x\rangle$. There is a further argument about the viability of this idea, at least in the context of measuring the position of a particle, which is to say that if the position were to be precisely defined at a particular value, this would mean, by the uncertainty principle $\Delta x\Delta p \geq \frac{1}{2}\hbar$ that the momentum of the particle would have infinite uncertainty, i.e. it could have any value from $-\infty$ to ∞ . It is a not very difficult exercise to show that to localize a particle to a region of infinitesimal size would require an infinite amount of work to be done, so the notion of preparing a particle in a state $|x\rangle$ does not even make physical sense.

The resolution of this impasse involves recognizing that the measurement of the position of a particle is, in practice, only ever done to within the accuracy, δx say, of the measuring apparatus. In other words, rather than measuring the precise position of a particle, what is measured is its position as lying somewhere in a range $(x - \frac{1}{2}\delta x, x + \frac{1}{2}\delta x)$. We can accommodate this situation within the theory by defining a new set of states that takes this into account. This could be done in a number of ways, but the simplest is to suppose we divide the continuous range of values of x into intervals of length δx , so that the n^{th} segment is the interval $((n-1)\delta x, n\delta x)$ and let x_n be a point within the n^{th} interval. This could be any point within this interval but it is simplest to take it to be the midpoint of the interval, i.e. $x_n = (n - \frac{1}{2})\delta x$. We then say that the particle is in the state $|x_n\rangle$ if the measuring apparatus indicates that the position of the particle is in the n^{th} segment.

In this manner we have replaced the continuous case by the discrete case, and we can now proceed along the lines of what was presented in the preceding Section. Thus we can introduce an observable $x_{\delta x}$ that can be measured to have the values $\{x_n; n = 0, \pm 1, \pm 2, \dots\}$, with $|x_n\rangle$ being the state of the particle for which $x_{\delta x}$ has the value x_n . We can then construct a Hermitean operator $\hat{x}_{\delta x}$ with eigenvalues $\{x_n; n = 0, \pm 1, \pm 2, \dots\}$ and associated eigenvectors $\{|x_n\rangle; n = 0, \pm 1, \pm 2, \dots\}$ such that

$$\hat{x}_{\delta x}|x_n\rangle = x_n|x_n\rangle. \quad (13.56)$$

The states $\{|x_n; n = 0, \pm 1, \pm 2, \dots\}$ will form a complete set of orthonormal basis states for the particle, so that any state of the particle can be written

$$|\psi\rangle = \sum_n |x_n\rangle \langle x_n|\psi\rangle \quad (13.57)$$

with $\langle x_n|x_m\rangle = \delta_{nm}$. The observable $\hat{x}_{\delta x}$ would then be given by

$$\hat{x}_{\delta x} = \sum_n x_n |x_n\rangle \langle x_n|. \quad (13.58)$$

Finally, if a measurement of $x_{\delta x}$ is made and the result x_n is observed, then the immediate post-measurement state of the particle will be

$$\frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} \quad (13.59)$$

where \hat{P}_n is the projection operator

$$\hat{P}_n = |x_n\rangle \langle x_n|. \quad (13.60)$$

To relate all this back to the continuous case, it is then necessary to take the limit, in some sense, of $\delta x \rightarrow 0$. This limiting process has already been discussed in Section 10.2.2, in an equivalent but slightly different model of the continuous limit. The essential points will be repeated here.

Returning to Eq. (13.57), we can define a new, unnormalized state vector $|\widetilde{x}_n\rangle$ by

$$|\widetilde{x}_n\rangle = \frac{|x_n\rangle}{\sqrt{\delta x}} \quad (13.61)$$

The states $|\widetilde{x}_n\rangle$ continue to be eigenstates of $\hat{x}_{\delta x}$, i.e.

$$\hat{x}_{\delta x}|\widetilde{x}_n\rangle = x_n|\widetilde{x}_n\rangle \quad (13.62)$$

as the factor $1/\sqrt{\delta x}$ merely renormalizes the length of the vectors. Thus these states $|\widetilde{x}_n\rangle$ continue to represent the same physical state of affairs as the normalized state, namely that when in this state, the particle is in the interval $(x_n - \frac{1}{2}\delta x, x_n + \frac{1}{2}\delta x)$.

In terms of these unnormalized states, Eq. (13.57) becomes

$$|\psi\rangle = \sum_n \widetilde{|x_n\rangle} \langle x_n|\psi\rangle \delta x. \quad (13.63)$$

If we let $\delta x \rightarrow 0$, then, in this limit the sum in Eq. (13.63) will define an integral with respect to x :

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle \langle x|\psi\rangle dx \quad (13.64)$$

where we have introduced the symbol $|x\rangle$ to represent the $\delta x \rightarrow 0$ limit of $\widetilde{|x_n\rangle}$ i.e.

$$|x\rangle = \lim_{\delta x \rightarrow 0} \frac{\widetilde{|x_n\rangle}}{\sqrt{\delta x}}. \quad (13.65)$$

This then is the idealized state of the particle for which its position is specified to within a vanishingly small interval around x as δx approaches zero. From Eq. (13.64) we can extract the completeness relation for these states

$$\int_{-\infty}^{\infty} |x\rangle \langle x| dx = \hat{1}. \quad (13.66)$$

This is done at a cost, of course. By the same arguments as presented in Section 10.2.2, the new states $|x\rangle$ are δ -function normalized, i.e.

$$\langle x|x'\rangle = \delta(x - x') \quad (13.67)$$

and, in particular, are of infinite norm, that is, they cannot be normalized to unity and so do not represent physical states of the particle.

Having introduced these idealized states, we can investigate some of their further properties and uses. The first and probably the most important is that it gives us the means to write down the probability of finding a particle in any small region in space. Thus, provided the state $|\psi\rangle$ is normalized to unity, Eq. (13.64) leads to

$$\langle \psi|\psi\rangle = 1 = \int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2 dx \quad (13.68)$$

which can be interpreted as saying that the total probability of finding the particle somewhere in space is unity. More particularly, we also conclude that $|\langle x|\psi\rangle|^2 dx$ is the probability of finding the position of the particle to be in the range $(x, x + dx)$.

If we now turn to Eq. (13.58) and rewrite it in terms of the unnormalized states we have

$$\hat{x}_{\delta x} = \sum_n x_n \widetilde{|x_n\rangle} \langle x_n| \delta x \quad (13.69)$$

so that in a similar way to the derivation of Eq. (13.64) this gives, in the limit of $\delta x \rightarrow 0$, the new operator \hat{x} , i.e.

$$\hat{x} = \int_{-\infty}^{\infty} x |x\rangle \langle x| dx. \quad (13.70)$$

This then leads to the $\delta x \rightarrow 0$ limit of the eigenvalue equation for $\hat{x}_{\delta x}$, Eq. (13.62) i.e.

$$\hat{x}|x\rangle = x|x\rangle \quad (13.71)$$

a result that also follows from Eq. (13.70) on using the δ -function normalization condition. This operator \hat{x} therefore has as eigenstates the complete set of δ -function normalized states $\{|x\rangle; -\infty <$

$x < \infty$ with associated eigenvalues x and can be looked on as being the observable corresponding to an idealized, precise measurement of the position of a particle.

While these states $|x\rangle$ can be considered idealized limits of the normalizable states $|x_n\rangle$ it must always be borne in mind that these are not physically realizable states – they are not normalizable, and hence are not vectors in the state space of the system. They are best looked on as a convenient fiction with which to describe idealized situations, and under most circumstances these states can be used in much the same way as discrete eigenstates. Indeed it is one of the benefits of the Dirac notation that a common mathematical language can be used to cover both the discrete and continuous cases. But situations can and do arise in which the cavalier use of these states can lead to incorrect or paradoxical results. We will not be considering such cases here.

The final point to be considered is the projection postulate. We could, of course, idealize this by saying that if a result x is obtained on measuring \hat{x} , then the state of the system after the measurement is $|x\rangle$. But given that the best we can do in practice is to measure the position of the particle to within the accuracy of the measuring apparatus, we cannot really go beyond the discrete case prescription given in Eq. (13.59) except to express it in terms of the idealized basis states $|x\rangle$. So, if the particle is in some state $|\psi\rangle$, we can recognize that the probability of getting a result x with an accuracy of δx will be given by

$$\begin{aligned} \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |\langle x'|\psi\rangle|^2 dx' &= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} \langle \psi|x'\rangle \langle x'|\psi\rangle dx' \\ &= \langle \psi | \left[\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle \langle x'| dx' \right] | \psi \rangle = \langle \psi | \hat{P}(x, \delta x) | \psi \rangle \quad (13.72) \end{aligned}$$

where we have introduced an operator $\hat{P}(x, \delta x)$ defined by

$$\hat{P}(x, \delta x) = \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle \langle x'| dx'. \quad (13.73)$$

We can readily show that this operator is in fact a projection operator since

$$\begin{aligned} [\hat{P}(x, \delta x)]^2 &= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx' \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx'' |x'\rangle \langle x'| x'' \rangle \langle x''| \\ &= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx' \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx'' |x'\rangle \delta(x' - x'') \langle x''| \\ &= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx' |x'\rangle \langle x'| \\ &= \hat{P}(x, \delta x). \quad (13.74) \end{aligned}$$

This suggests, by comparison with the corresponding postulate in the case of discrete eigenvalues, that if the particle is initially in the state $|\psi\rangle$, then the state of the particle immediately after measurement be given by

$$\frac{\hat{P}(x, \delta x)|\psi\rangle}{\sqrt{\langle \psi | \hat{P}(x, \delta x) | \psi \rangle}} = \frac{\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle \langle x'|\psi\rangle dx'}{\sqrt{\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |\langle x'|\psi\rangle|^2 dx'}} \quad (13.75)$$

It is this state that is taken to be the state of the particle immediately after the measurement has been performed, with the result x being obtained to within an accuracy δx .

Further development of these ideas is best done in the language of generalized measurements where the projection operator is replaced by an operator that more realistically represents the outcome of the measurement process. We will not be pursuing this any further here.

At this point, we can take the ideas developed for the particular case of the measurement of position and generalize them to apply to the measurement of any observable quantity with a continuous range of possible values. The way in which this is done is presented in the following Section.

13.6.2 General Postulates for Continuous Valued Observables

Suppose we have an observable Q of a system that is found, for instance through an exhaustive series of measurements, to have a continuous range of values $\theta_1 < q < \theta_2$. In practice, it is not the observable Q that is measured, but rather a discretized version in which Q is measured to an accuracy δq determined by the measuring device. If we represent by $|q\rangle$ the idealized state of the system in the limit $\delta q \rightarrow 0$, for which the observable definitely has the value q , then we claim the following:

1. The states $\{|q\rangle; \theta_1 < q < \theta_2\}$ form a complete set of δ -function normalized basis states for the state space of the system.

That the states form a complete set of basis states means that any state $|\psi\rangle$ of the system can be expressed as

$$|\psi\rangle = \int_{\theta_1}^{\theta_2} c(q)|q\rangle \quad (13.76)$$

while δ -function normalized means that $\langle q|q'\rangle = \delta(q - q')$ from which follows $c(q) = \langle q|\psi\rangle$ so that

$$|\psi\rangle = \int_{\theta_1}^{\theta_2} |q\rangle\langle q|\psi\rangle dq. \quad (13.77)$$

The completeness condition can then be written as

$$\int_{\theta_1}^{\theta_2} |q\rangle\langle q| dq = \hat{1} \quad (13.78)$$

2. For the system in state $|\psi\rangle$, the probability of obtaining the result q lying in the range $(q, q + dq)$ on measuring Q is $|\langle q|\psi\rangle|^2 dq$ provided $\langle \psi|\psi\rangle = 1$.

Completeness means that for any state $|\psi\rangle$ it must be the case that

$$\int_{\theta_1}^{\theta_2} |\langle q|\psi\rangle|^2 dq \neq 0 \quad (13.79)$$

i.e. there must be a non-zero probability to get some result on measuring Q .

3. The observable Q is represented by a Hermitean operator \hat{Q} whose eigenvalues are the possible results $\{q; \theta_1 < q < \theta_2\}$, of a measurement of Q , and the associated eigenstates are the states $\{|q\rangle; \theta_1 < q < \theta_2\}$, i.e. $\hat{Q}|q\rangle = q|q\rangle$. The name ‘observable’ is often applied to the operator \hat{Q} itself.

The spectral decomposition of the observable \hat{Q} is then

$$\hat{Q} = \int_{\theta_1}^{\theta_2} q|q\rangle\langle q| dq. \quad (13.80)$$

As in the discrete case, the eigenvectors of an observable constitute a set of basis states for the state space of the associated quantum system.

A more subtle difficulty is now encountered if we turn to the von Neumann postulate concerning the state of the system after a measurement is made. If we were to transfer the discrete state postulate directly to the continuous case, we would be looking at proposing that obtaining the result q in a measurement of \hat{Q} would mean that the state after the measurement is $|q\rangle$. This is a state that is not permitted as it cannot be normalized to unity. Thus we need to take account of the way a measurement is carried out in practice when considering the state of the system after the measurement. Following on from the particular case of position measurement presented above, we will suppose that Q is measured with a device of accuracy δq . This leads to the following general statement of the von Neumann measurement postulate for continuous eigenvalues:

4. If on performing a measurement of Q with an accuracy δq , the result is obtained in the range $(q - \frac{1}{2}\delta q, q + \frac{1}{2}\delta q)$, then the system will end up in the state

$$\frac{\hat{P}(q, \delta q)|\psi\rangle}{\sqrt{\langle\psi|\hat{P}(q, \delta q)|\psi\rangle}} \quad (13.81)$$

where

$$\hat{P}(q, \delta q) = \int_{q-\frac{1}{2}\delta q}^{q+\frac{1}{2}\delta q} |q'\rangle\langle q'| dq'. \quad (13.82)$$

Even though there exists this precise statement of the projection postulate for continuous eigenvalues, it is nevertheless a convenient fiction to assume that the measurement of an observable Q with a continuous set of eigenvalues will yield one of the results q with the system ending up in the state $|q\rangle$ immediately afterwards. While this is, strictly speaking, not really correct, it can be used as a convenient shorthand for the more precise statement given above.

As mentioned earlier, further development of these ideas is best done in the language of generalized measurements.

13.7 Examples of Continuous Valued Observables

13.7.1 Position and momentum of a particle (in one dimension)

These two observables are those which are most commonly encountered in wave mechanics. In the case of position, we are already able to say a considerable amount about the properties of this observable. Some further development is required in order to be able to deal with momentum.

Position observable (in one dimension)

In one dimension, the position x of a particle can range over the values $-\infty < x < \infty$. Thus the Hermitean operator \hat{x} corresponding to this observable will have eigenstates $|x\rangle$ and associated eigenvalues x such that

$$\hat{x}|x\rangle = x|x\rangle, \quad -\infty < x < \infty. \quad (13.83)$$

As the eigenvalues cover a continuous range of values, the completeness relation will be expressed as an integral:

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \quad (13.84)$$

where $\langle x|\psi\rangle = \psi(x)$ is the wave function associated with the particle. Since there is a continuously infinite number of basis states $|x\rangle$, these states are delta-function normalized:

$$\langle x|x'\rangle = \delta(x - x'). \quad (13.85)$$

The operator itself can be expressed as

$$\hat{x} = \int_{-\infty}^{\infty} x|x\rangle\langle x| dx. \quad (13.86)$$

The Position Representation The wave function is, of course, just the components of the state vector $|\psi\rangle$ with respect to the position eigenstates as basis vectors. Hence, the wave function is often referred to as being the state of the system in the *position representation*. The probability amplitude $\langle x|\psi\rangle$ is just the wave function, written $\psi(x)$ and is such that $|\psi(x)|^2 dx$ is the probability of the particle being observed to have a momentum in the range x to $x + dx$.

The one big difference here as compared to the discussion in Chapter 12 is that the basis vectors here are continuous, rather than discrete, so that the representation of the state vector is not a simple column vector with discrete entries, but rather a function of the continuous variable x . Likewise, the operator \hat{x} will not be represented by a matrix with discrete entries labelled, for instance, by pairs of integers, but rather it will be a function of two continuous variables:

$$\langle x|\hat{x}|x'\rangle = x\delta(x - x'). \quad (13.87)$$

The position representation is used in quantum mechanical problems where it is the position of the particle in space that is of primary interest. For instance, when trying to determine the chemical properties of atoms and molecules, it is important to know how the electrons in each atom tend to distribute themselves in space in the various kinds of orbitals as this will play an important role in determining the kinds of chemical bonds that will form. For this reason, the position representation, or the wave function, is the preferred choice of representation. When working in the position representation, the wave function for the particle is found by solving the Schrödinger equation for the particle.

Momentum of a particle (in one dimension)

As for position, the momentum p is an observable which can have any value in the range $-\infty < p < \infty$ (this is non-relativistic momentum). Thus the Hermitean operator \hat{p} will have eigenstates $|p\rangle$ and associated eigenvalues p :

$$\hat{p}|p\rangle = p|p\rangle, \quad -\infty < p < \infty. \quad (13.88)$$

As the eigenvalues cover a continuous range of values, the completeness relation will also be expressed as an integral:

$$|\psi\rangle = \int_{-\infty}^{+\infty} |p\rangle\langle p|\psi\rangle dp \quad (13.89)$$

where the basis states are delta-function normalized:

$$\langle p|p'\rangle = \delta(p - p'). \quad (13.90)$$

The operator itself can be expressed as

$$\hat{p} = \int_{-\infty}^{+\infty} p|p\rangle\langle p| dp. \quad (13.91)$$

Momentum Representation If the state vector is represented in component form with respect to the momentum eigenstates as basis vectors, then this is said to be the *momentum representation*. The probability amplitude $\langle p|\psi\rangle$ is sometimes referred to as the momentum wave function, written $\tilde{\psi}(p)$ and is such that $|\tilde{\psi}(p)|^2 dp$ is the probability of the particle being observed to have a momentum in the range p to $p + dp$. It turns out that the momentum wave function and the position wave function are Fourier transform pairs, a result that is shown below.

The momentum representation is preferred in problems in which it is not so much where a particle might be in space that is of interest, but rather how fast it is going and in what direction. Thus, the momentum representation is often to be found when dealing with scattering problems in which a particle of well defined momentum is directed towards a scattering centre, e.g. an atomic nucleus, and the direction in which the particle is scattered, and the momentum and/or energy of the scattered particle are measured, though even here, the position representation is used more often than not as it provides a mental image of the scattering process as waves scattering off an obstacle. Finally, we can also add that there is an equation for the momentum representation wave function which is equivalent to the Schrödinger equation.

Properties of the Momentum Operator

The momentum operator can be introduced into quantum mechanics by a general approach based on the space displacement operator. But at this stage it is nevertheless possible to draw some conclusions about the properties of the momentum operator based on the de Broglie hypothesis concerning the wave function of a particle of precisely known momentum p and energy E .

The momentum operator in the position representation From the de Broglie relation and Einstein's formula, the wave function $\Psi(x, t)$ to be associated with a particle of momentum p and energy E will have a wave number k and angular frequency ω given by $p = \hbar k$ and $E = \hbar\omega$. We can then guess what this wave function would look like:

$$\Psi(x, t) = \langle x|\Psi(t)\rangle = Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)} + Ce^{i(kx+\omega t)} + De^{-i(kx+\omega t)}. \quad (13.92)$$

The expectation is that the wave will travel in the same direction as the particle, i.e. if $p > 0$, then the wave should travel in the direction of positive x . Thus we must reject those terms with the argument $(kx + \omega t)$ and so we are left with

$$\langle x|\Psi(t)\rangle = Ae^{i(px/\hbar-\omega t)} + Be^{-i(px/\hbar-\omega t)} \quad (13.93)$$

where we have substituted for k in terms of p . The claim then is that the state $|\Psi(t)\rangle$ is a state for which the particle definitely has momentum p , and hence it must be an eigenstate of the momentum operator \hat{p} , i.e.

$$\hat{p}|\Psi(t)\rangle = p|\Psi(t)\rangle \quad (13.94)$$

which becomes, in the position representation

$$\begin{aligned} \langle x|\hat{p}|\Psi(t)\rangle &= p\langle x|\Psi(t)\rangle \\ &= p\left(Ae^{i(px/\hbar-\omega t)} + Be^{-i(px/\hbar-\omega t)}\right). \end{aligned} \quad (13.95)$$

The only simple way of obtaining the factor p is by taking the derivative of the wave function with respect to x , though this does not immediately give us what we want, i.e.

$$\langle x|\hat{p}|\Psi(t)\rangle = -i\hbar \frac{\partial}{\partial x} \left(Ae^{i(px/\hbar-\omega t)} - Be^{-i(px/\hbar-\omega t)} \right) \neq p\langle x|\Psi(t)\rangle \quad (13.96)$$

which tells us that the state $|\Psi(t)\rangle$ is not an eigenstate of \hat{p} , at least if we proceed along the lines of introducing the derivative with respect to x . However, all is not lost. If we choose one or the other of the two terms in the expression for $\langle x|\Psi(t)\rangle$ e.g.

$$\langle x|\Psi(t)\rangle = Ae^{i(px/\hbar-\omega t)} \quad (13.97)$$

we find that

$$\langle x|\hat{p}|\Psi(t)\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\Psi(t)\rangle = p\langle x|\Psi(t)\rangle \quad (13.98)$$

as required. This suggests that we have arrived at a candidate for the wave function for a particle of definite momentum p . But we could have chosen the other term with coefficient B . However, this other choice amounts to reversing our choice of the direction of positive x and positive t — its exponent can be written $i(p(-x)/\hbar - \omega(-t))$. This is itself a convention, so we can in fact use either possibility as the required momentum wave function without affecting the physics. To be in keeping with the convention that is usually adopted, the choice Eq. (13.97) is made here.

Thus, by this process of elimination, we have arrived at an expression for the wave function of a particle with definite momentum p . Moreover, we have extracted an expression for the momentum operator \hat{p} in that, if $|p\rangle$ is an eigenstate of \hat{p} , then, in the position representation

$$\langle x|\hat{p}|p\rangle = -i\hbar\frac{d}{dx}\langle x|p\rangle. \quad (13.99)$$

This is a result that can be readily generalized to apply to any state of the particle. By making use of the fact that the momentum eigenstate form a complete set of basis states, we can write any state $|\psi\rangle$ as

$$|\psi\rangle = \int_{-\infty}^{+\infty} |p\rangle\langle p|\psi\rangle dp \quad (13.100)$$

so that

$$\begin{aligned} \langle x|\hat{p}|\psi\rangle &= \int_{-\infty}^{+\infty} \langle x|\hat{p}|p\rangle\langle p|\psi\rangle dp \\ &= -i\hbar\frac{d}{dx} \int_{-\infty}^{+\infty} \langle x|p\rangle\langle p|\psi\rangle dp \\ &= -i\hbar\frac{d}{dx}\langle x|\psi\rangle \end{aligned}$$

or

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x). \quad (13.101)$$

From this result it is straightforward to show that

$$\langle x|\hat{p}^n|\psi\rangle = (-i\hbar)^n\frac{d^n}{dx^n}\psi(x). \quad (13.102)$$

For instance,

$$\langle x|\hat{p}^2|\psi\rangle = \langle x|\hat{p}|\phi\rangle \quad (13.103)$$

where $|\phi\rangle = \hat{p}|\psi\rangle$. Thus

$$\langle x|\hat{p}^2|\psi\rangle = -i\hbar\frac{d}{dx}\phi(x). \quad (13.104)$$

But

$$\phi(x) = \langle x|\phi\rangle = \langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x). \quad (13.105)$$

Using this and Eq. (13.104), we get

$$\langle x|\hat{p}^2|\psi\rangle = -i\hbar\frac{d}{dx}\left(-i\hbar\frac{d}{dx}\right)\psi(x) = -\hbar^2\frac{d^2}{dx^2}\psi(x) \quad (13.106)$$

In general we see that, when working in the position representation, the substitution

$$\hat{p} \longrightarrow -i\hbar\frac{d}{dx} \quad (13.107)$$

can consistently be made. This is an exceedingly important result that plays a central role in wave mechanics, in particular in setting up the Schrödinger equation for the wave function.

One final result can be established using this correspondence. Consider the action of the operator

$$\hat{D}(a) = e^{i\hat{p}a/\hbar} \quad (13.108)$$

on an arbitrary state $|\psi\rangle$ i.e.

$$|\phi\rangle = \hat{D}(a)|\psi\rangle \quad (13.109)$$

which becomes, in the position representation

$$\langle x|\phi\rangle = \phi(x) = \langle x|\hat{D}(a)|\psi\rangle. \quad (13.110)$$

Expanding the exponential and making the replacement Eq. (13.107) we have

$$\hat{D}(a) = \hat{1} + i\hat{p}a/\hbar + (ia/\hbar)^2 \frac{1}{2!} \hat{p}^2 + (ia/\hbar)^3 \frac{1}{3!} \hat{p}^3 + \dots \longrightarrow 1 + a \frac{d}{dx} + \frac{a^2}{2!} \frac{d^2}{dx^2} + \frac{a^3}{3!} \frac{d^3}{dx^3} + \dots \quad (13.111)$$

we get

$$\begin{aligned} \phi(x) &= \left(1 + a \frac{d}{dx} + \frac{a^2}{2!} \frac{d^2}{dx^2} + \frac{a^3}{3!} \frac{d^3}{dx^3} + \dots \right) \psi(x) \\ &= \psi(x) + a\psi'(x) + \frac{a^2}{2!} \psi''(x) + \frac{a^3}{3!} \psi'''(x) + \dots \\ &= \psi(x+a) \end{aligned} \quad (13.112)$$

where the series appearing above is recognized as the Maclaurin series expansion about $x = a$. Thus we see that the state $|\phi\rangle$ obtained by the action of the operator $\hat{D}(a)$ on $|\psi\rangle$ is to displace the wave function a distance a along the x axis. This result illustrates the deep connection between momentum and displacement in space, a relationship that is turned on its head in Chapter 16 where momentum is defined in terms of the displacement operator.

The normalized momentum eigenfunction Returning to the differential equation Eq. (13.99), we can readily obtain the solution

$$\langle x|p\rangle = Ae^{ipx/\hbar} \quad (13.113)$$

where A is a coefficient to be determined by requiring that the states $|p\rangle$ be delta function normalized. Note that our wave function Eq. (13.97) gives the time development of the eigenfunction $\langle x|p\rangle$, Eq. (13.113).

The normalization condition is that

$$\langle p|p'\rangle = \delta(p-p') \quad (13.114)$$

which can be written, on using the completeness relation for the position eigenstates

$$\begin{aligned} \delta(p-p') &= \int_{-\infty}^{+\infty} \langle p|x\rangle \langle x|p'\rangle dx \\ &= |A|^2 \int_{-\infty}^{+\infty} e^{-i(p-p')x/\hbar} dp \\ &= |A|^2 2\pi\hbar \delta(p-p') \end{aligned} \quad (13.115)$$

where we have used the representation of the Dirac delta function given in Section 10.2.3. Thus we conclude

$$|A|^2 = \frac{1}{2\pi\hbar}. \quad (13.116)$$

It then follows that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}. \quad (13.117)$$

This result can be used to relate the wave function for a particle in the momentum and position representations. Using the completeness of the momentum states we can write for any state $|\psi\rangle$ of the particle

$$|\psi\rangle = \int_{-\infty}^{+\infty} |p\rangle\langle p|\psi\rangle dp \quad (13.118)$$

which becomes, in the position representation

$$\langle x|\psi\rangle = \int_{-\infty}^{+\infty} \langle x|p\rangle\langle p|\psi\rangle dp \quad (13.119)$$

or, in terms of the wave functions:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{ipx/\hbar} \tilde{\psi}(p) dp \quad (13.120)$$

which immediately shows that the momentum and position representation wave functions are Fourier transform pairs. It is a straightforward procedure to then show that

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-ipx/\hbar} \psi(x) dx \quad (13.121)$$

either by simply inverting the Fourier transform, or by expanding the state vector $|\psi\rangle$ in terms of the position eigenstates.

That the position and momentum wave functions are related in this way has a very important consequence that follows from a fundamental property of Fourier transform pairs. Roughly speaking, there is an inverse relationship between the width of a function and its Fourier transformed companion. This is most easily seen if suppose, somewhat unrealistically, that $\psi(x)$ is of the form

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{a}} & |x| \leq \frac{1}{2}a \\ 0 & |x| > \frac{1}{2}a \end{cases} \quad (13.122)$$

The full width of $\psi(x)$ is a . The momentum wave function is

$$\tilde{\psi}(p) = \sqrt{\frac{2\hbar}{\pi}} \frac{\sin(pa/\hbar)}{p}. \quad (13.123)$$

An estimate of the width of $\tilde{\psi}(p)$ is given by determining the positions of the first zeroes of $\tilde{\psi}(p)$ on either side of the central maximum at $p = 0$, that is at $p = \pm\pi\hbar/a$. The separation of these two zeroes, $2\pi\hbar/a$, is an overestimate of the width of the peak so we take this width to be half this separation, thus giving an estimate of $\pi\hbar/a$. Given that the square of the wave functions i.e. $|\psi(x)|^2$ and $|\tilde{\psi}(p)|^2$ give the probability distribution for position and momentum respectively, it is clearly the case that the wider the spread in the possible values of the position of the particle, i.e. the larger a is made, there is a narrowing of the spread in the range of values of momentum, and vice versa. This inverse relationship is just the Heisenberg uncertainty relation reappearing, and is more fully quantified in terms of the uncertainties in position and momentum defined in Chapter 14.

Position momentum commutation relation The final calculation in here is to determine the commutator $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$ of the two operators \hat{x} and \hat{p} . This can be done most readily in the position representation. Thus we will consider

$$\langle x|[\hat{x}, \hat{p}]|\psi\rangle = \langle x|(\hat{x}\hat{p} - \hat{p}\hat{x})|\psi\rangle \quad (13.124)$$

where $|\psi\rangle$ is an arbitrary state of the particle. This becomes, on using the fact that the state $\langle x|$ is an eigenstate of \hat{x} with eigenvalue x

$$\langle x|[\hat{x}, \hat{p}]|\psi\rangle = x\langle x|\hat{p}|\psi\rangle - \langle x|\hat{p}|\xi\rangle \quad (13.125)$$

where $|\xi\rangle = \hat{x}|\psi\rangle$. Expressed in terms of the differential operator, this becomes

$$\langle x|[\hat{x}, \hat{p}]|\psi\rangle = -i\hbar \left(x \frac{d}{dx} \psi(x) - \frac{d}{dx} \xi(x) \right). \quad (13.126)$$

But

$$\xi(x) = \langle x|\xi\rangle = \langle x|\hat{x}|\psi\rangle = x\langle x|\psi\rangle = x\psi(x) \quad (13.127)$$

so that

$$\frac{d}{dx} \xi(x) = x \frac{d}{dx} \psi(x) + \psi(x). \quad (13.128)$$

Combining this altogether then gives

$$\langle x|[\hat{x}, \hat{p}]|\psi\rangle = i\hbar\psi(x) = i\hbar\langle x|\psi\rangle. \quad (13.129)$$

The completeness of the position eigenstates can be used to write this as

$$\int_{-\infty}^{+\infty} |x\rangle\langle x|[\hat{x}, \hat{p}]|\psi\rangle = i\hbar \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle \quad (13.130)$$

or

$$[\hat{x}, \hat{p}]|\psi\rangle = i\hbar\hat{1}|\psi\rangle. \quad (13.131)$$

Since the state $|\psi\rangle$ is arbitrary, we can conclude that

$$[\hat{x}, \hat{p}] = i\hbar\hat{1} \quad (13.132)$$

though the unit operator on the right hand side is usually understood, so the relation is written

$$[\hat{x}, \hat{p}] = i\hbar. \quad (13.133)$$

This is perhaps the most important result in non-relativistic quantum mechanics as it embodies much of what makes quantum mechanics ‘different’ from classical mechanics. For instance, if the position and momentum operators were classical quantities, then the commutator would vanish, or to put it another way, it is that fact that $\hbar \neq 0$ that gives us quantum mechanics. It turns out that, amongst other things, the fact that the commutator does not vanish implies that it is not possible to have precise information on the position and the momentum of a particle, i.e. position and momentum are *incompatible* observables.

13.7.2 Field operators for a single mode cavity

A physical meaning can be given to the annihilation and creation operators defined above in terms of observables of the field inside the cavity. This done here in a non-rigorous way, relying on a trick by which we relate the classical and quantum ways of specifying the energy of the field. We have earlier arrived at an expression for the quantum Hamiltonian of the cavity field as given in Eq. (13.53), i.e. $\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a}$, which as we have already pointed out, is missing the zero-point

contribution $\frac{1}{2}\hbar\omega$ that is found in a full quantum theory of the electromagnetic field. However, assuming we had never heard of this quantum theory, then we could proceed by comparing the quantum expression we have derived with the classical expression for the energy of the single mode EM field inside the cavity.

A little more detail about the single mode field is required before the classical Hamiltonian can be obtained. This field will be assumed to be a plane polarized standing wave confined between two mirrors of area \mathcal{A} , separated by a distance L in the z direction. Variation of the field in the x and y directions will also be ignored, so the total energy of the field will be given by

$$H = \frac{1}{2} \int_{\mathcal{V}} (\epsilon_0 E^2(z, t) + B^2(z, t)/\mu_0) dx dy dz \quad (13.134)$$

where the classical electric field is $E(z, t) = \text{Re}[\mathcal{E}(t)] \sin(\omega z/c)$, i.e. of complex amplitude $\mathcal{E}(t) = \mathcal{E}e^{-i\omega t}$, the magnetic field is $B(z, t) = c^{-1}\text{Im}[\mathcal{E}(t)] \cos(\omega z/c)$, and where $\mathcal{V} = \mathcal{A}L$ is the volume of the cavity.

The integral can be readily carried out to give

$$H = \frac{1}{4}\epsilon_0 \mathcal{E}^* \mathcal{E} \mathcal{V} \quad (13.135)$$

We want to establish a correspondence between the two expressions for the Hamiltonian, i.e.

$$\hbar\omega \hat{a}^\dagger \hat{a} \longleftrightarrow \frac{1}{4}\epsilon_0 \mathcal{E}^* \mathcal{E} \mathcal{V}$$

in order to give some sort of physical interpretation of \hat{a} , apart from its interpretation as a photon annihilation operator. We can do this by reorganizing the various terms so that the correspondence looks like

$$\left(2e^{-i\phi} \sqrt{\frac{\hbar\omega}{\mathcal{V}\epsilon_0}} \hat{a}^\dagger \right) \left(2e^{i\phi} \sqrt{\frac{\hbar\omega}{\mathcal{V}\epsilon_0}} \hat{a} \right) \longleftrightarrow \mathcal{E}^* \mathcal{E}$$

where $\exp(i\phi)$ is an arbitrary phase factor, i.e. it could be chosen to have any value and the correspondence would still hold. A common choice is to take this phase factor to be i . The most obvious next step is to identify an operator $\hat{\mathcal{E}}$ closely related to the classical quantity \mathcal{E} by

$$\hat{\mathcal{E}} = 2i \sqrt{\frac{\hbar\omega}{\mathcal{V}\epsilon_0}} \hat{a}$$

so that we get the correspondence $\hat{\mathcal{E}}^\dagger \hat{\mathcal{E}} \longleftrightarrow \mathcal{E}^* \mathcal{E}$.

We can note that the operator $\hat{\mathcal{E}}$ is still not Hermitean, but recall that the classical electric field was obtained from the real part of \mathcal{E} , so that we can define a Hermitean electric field operator by

$$\hat{E}(z) = \frac{1}{2}[\hat{\mathcal{E}} + \hat{\mathcal{E}}^\dagger] \sin(\omega z/c) = i \sqrt{\frac{\hbar\omega}{\mathcal{V}\epsilon_0}} [\hat{a} - \hat{a}^\dagger] \sin(\omega z/c)$$

to complete the picture. In this way we have identified a new observable for the field inside the cavity, the electric field operator. This operator is, in fact, an example of a quantum field operator. Of course, the derivation presented here is far from rigorous. That this operator is indeed the electric field operator can be shown to follow from the full analysis as given by the quantum theory of the electromagnetic field.

In the same way, an expression for the magnetic field operator can be determined from the expression for the classical magnetic field, with the result:

$$\hat{B}(z) = \sqrt{\frac{\mu_0 \hbar \omega}{\mathcal{V}}} (\hat{a} + \hat{a}^\dagger) \cos(\omega z/c). \quad (13.136)$$

The above are two new observables for the system so it is natural to ask what is their eigenvalue spectrum. We can get at this in an indirect fashion by examining the properties of the two Hermitian operators $i(\hat{a} - \hat{a}^\dagger)$ and $\hat{a} + \hat{a}^\dagger$. For later purposes, it is convenient to rescale these two operators and define

$$\hat{X} = \sqrt{\frac{\hbar}{2\omega}}(\hat{a} + \hat{a}^\dagger) \quad \text{and} \quad \hat{P} = -i\sqrt{\frac{\hbar\omega}{2}}(\hat{a} - \hat{a}^\dagger). \quad (13.137)$$

As the choice of notation implies, the aim is to show that these new operators are, mathematically at least, closely related to the position and momentum operators \hat{x} and \hat{p} for a single particle. The distinctive quantum feature of these latter operators is their commutation relation, so the aim is to evaluate the commutator of \hat{X} and \hat{P} . To do so, we need to know the value of the commutator $[\hat{a}, \hat{a}^\dagger]$. We can determine this by evaluating $[\hat{a}, \hat{a}^\dagger]|n\rangle$ where $|n\rangle$ is an arbitrary number state. Using the properties of the annihilation and creation operators \hat{a} and \hat{a}^\dagger given by

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

we see that

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger]|n\rangle &= \hat{a}\hat{a}^\dagger|n\rangle - \hat{a}^\dagger\hat{a}|n\rangle \\ &= \hat{a}\sqrt{n+1}|n+1\rangle - \hat{a}^\dagger\sqrt{n}|n-1\rangle \\ &= (n+1)|n\rangle - n|n\rangle \\ &= |n\rangle \end{aligned}$$

from which we conclude

$$[\hat{a}, \hat{a}^\dagger] = \hat{1}. \quad (13.138)$$

If we now make use of this result when evaluating $[\hat{X}, \hat{P}]$ we find

$$[\hat{X}, \hat{P}] = -i\frac{1}{2}\hbar[\hat{a} + \hat{a}^\dagger, \hat{a} - \hat{a}^\dagger] = i\hbar \quad (13.139)$$

where use has been made of the properties of the commutator as given in Eq. (11.24).

In other words, the operators \hat{X} and \hat{P} obey exactly the same commutation relation as position and momentum for a single particle, \hat{x} and \hat{p} respectively. This is of course a mathematical correspondence i.e. there is no massive particle ‘behind the scenes’ here, but the mathematical correspondence is one that is found to arise in the formulation of the quantum theory of the electromagnetic field. But what it means to us here is that the two observables \hat{X} and \hat{P} will, to all intents and purposes have the same properties as \hat{x} and \hat{p} . In particular, the eigenvalues of \hat{X} and \hat{P} will be continuous, ranging from $-\infty$ to $+\infty$. Since we can write the electric field operator as

$$\hat{E}(z) = -\sqrt{\frac{2}{\mathcal{V}\epsilon_0}}\hat{P}\sin(\omega z/c) \quad (13.140)$$

we conclude that the electric field operator will also have a continuous range of eigenvalues from $-\infty$ to $+\infty$. This is in contrast to the number operator or the Hamiltonian which both have a discrete range of values. A similar conclusion applies for the magnetic field, which can be written in terms of \hat{X} :

$$\hat{B}(z) = \omega\sqrt{\frac{2\mu_0}{\mathcal{V}}}\hat{X}\cos(\omega z/c). \quad (13.141)$$

What remains is to check the form of the Hamiltonian of the field as found directly from the expressions for the electric and magnetic field operators. This can be calculated via the quantum version of the classical expression for the field energy, Eq. (13.134), i.e.

$$\hat{H} = \frac{1}{2} \int_{\mathcal{V}} [\epsilon_0\hat{E}^2(z) + \hat{B}^2(z)/\mu_0] dx dy dz. \quad (13.142)$$

Substituting for the field operators and carrying out the spatial integrals gives

$$= \frac{1}{4} \hbar \omega \left[-(\hat{a} - \hat{a}^\dagger)^2 + (\hat{a} + \hat{a}^\dagger)^2 \right] \quad (13.143)$$

$$= \frac{1}{2} \hbar \omega \left[\hat{a} \hat{a}^\dagger + \hat{a}^\dagger \hat{a} \right]. \quad (13.144)$$

Using the commutation rule $[\hat{a}, \hat{a}^\dagger] = \hat{1}$ we can write this as

$$\hat{H} = \hbar \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right). \quad (13.145)$$

Thus, we recover the original expression for the Hamiltonian, but now with the additional zero-point energy contribution $\frac{1}{2} \hbar \omega$. That we do not recover the assumed starting point for the Hamiltonian is an indicator that the above derivation is not entirely rigorous. Nevertheless, it does achieve a useful purpose in that we have available expressions for the electric and magnetic field operators, and the Hamiltonian, for the a single mode electromagnetic field.