Chapter 11

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 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.

11.1 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 insufficent 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 is macroscopic in size, and behaves according to the laws of classical physics. In Section 8.7, 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.

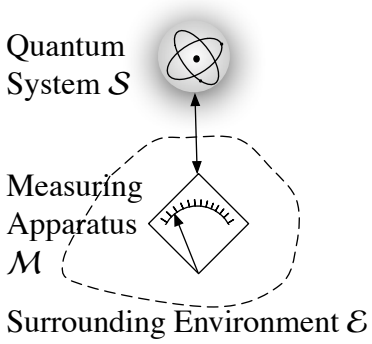

Figure 11.1: System $\mathcal{S}$ interacting with measuring apparatus $\mathcal{M}$ in the presence of the surrounding environment $\mathcal{E}$. The outcome of the measurement is registered on the dial on the measuring apparatus.

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*. 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.

11.2 Observables and Hermitean Operators

One crucial feature of any output of a measurement is that the result is usually, or at least can be, expressed as a *real* number. For instance, in the Stern-Gerlach experiment with the magnetic field oriented in the z direction, the outcomes of the measurement are that a spin-half particle will be observed to have a z component of spin with one or the other of the values $S_z = \pm\frac{1}{2}\hbar$. It is here that we make a very important connection. We have been

consistently saying that if an atom emerges in the $S_z = \frac{1}{2}\hbar$ beam, then we have assigned the spin state $|+\rangle$ to the atom, and similarly we associate the outcome $S_z = -\frac{1}{2}\hbar$ with the state $|-\rangle$. We therefore have a natural pairing off between measurement outcomes (two real numbers, $\pm\frac{1}{2}\hbar$) and the states $|\pm\rangle$. Moreover, as we have argued earlier in Section 8.2 these states are orthogonal in that if the atom is in state $|+\rangle$ for instance, there is zero probability of observing it in state $|-\rangle$, i.e. $\langle -|+\rangle = 0$: the two states are mutually exclusive. Finally, we note that we never see an atom emerge from the apparatus in other than the two beams associated with the two spins $\pm\frac{1}{2}\hbar$. Thus, if an atom is prepared in an arbitrary initial state $|S\rangle$, the probability amplitude of finding it in some other state $|S'\rangle$is

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

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 can be expressed as a linear combination of the states $|\pm\rangle$. Thus the states $|\pm\rangle$ constitute a complete set of 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 a Measurement of S_z
The eigenvalues of a Hermitean operator are all real.	Results of a measurement are real numbers.
Eigenvectors belonging to different eigenvalues are orthogonal.	States associated with different measurement outcomes are mutually exclusive.
The eigenstates form a complete set of basis states for the state space of the system.	The states associated with all the possible outcomes of a measurement form a complete set of basis states for the state space of the system.

It is therefore natural to associate with the quantity being measured here, that is 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.

$$\hat{S}_z|\pm\rangle = \pm\tfrac{1}{2}\hbar|\pm\rangle \tag{11.1}$$

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

$$\hat{S}_z \doteq \begin{pmatrix} \langle +|\hat{S}_z|+\rangle & \langle +|\hat{S}_z|-\rangle \\ \langle -|\hat{S}_z|+\rangle & \langle -|\hat{S}_z|-\rangle \end{pmatrix} \tag{11.2}$$

$$= \tfrac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{11.3}$$

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.

11.3 The Measurement Postulates

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.

11.3.1 Measurement of Observables with Discrete Values

Suppose we have an observable Q of a system that is found to have the values q_1, q_2, ... through an exhaustive series of measurements. If we furthermore represent by $|q_1\rangle$, $|q_2\rangle$, ... those states of the system for which we are guaranteed to get the results q_1, q_2, ... respectively on measuring Q, we can then claim the following:

1. The states $\{|q_n\rangle; n = 1, 2, 3, \ldots\}$ 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

$$|\psi\rangle = \sum_n c_n |q_n\rangle \tag{11.4}$$

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

$$\sum_n |q_n\rangle\langle q_n| = \hat{1} \tag{11.5}$$

2. 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 $|q_1\rangle, |q_2\rangle, \ldots$ 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

$$\sum_n |\langle q_n|\psi\rangle|^2 \neq 0. \tag{11.6}$$

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

3. The observable Q is represented by a Hermitean operator $\hat{Q}$ whose eigenvalues are the possible results $q_1, q_2, \ldots$ of a measurement of Q, and the associated eigenstates are the states $|q_1\rangle, |q_2\rangle, \ldots$, 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

$$\hat{Q} = \sum_n q_n|q_n\rangle\langle q_n|. \tag{11.7}$$

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 assoociated 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.

While every observable of a system is represented by a Hermitean operator, and in principle every Hermitean operator represents a possible observable of a system, it is not always clear what observable property of a system an arbitrary Hermitean operator might correspond to. In any case,

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:

4. 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 **??**. Thus, if we write

$$\hat{P}_n = |q_n\rangle\langle q_n| \tag{11.8}$$

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

$$\frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} = \frac{\hat{P}_n|\psi\rangle}{\sqrt{|\langle q_n|\psi\rangle|^2}} \tag{11.9}$$

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

This last property is known as the von Neumann measurement postulate, or, as it is most succinctly expressed in terms of projection operators, it is also referred to as the von Neumann projection postulate. The postulate is named after John von Neumann, one of the most famous mathematical physicists of the 20$^{\text{th}}$ century who was responsible, amongst other achievements, for putting quantum theory on a sound mathematical footing.

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. We will not be considering this theory here.

11.3.2 Measurement of 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 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.

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 lead to requiring that any state $|\psi\rangle$ of the particle mut be expressible as

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \, dx \tag{11.10}$$

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

$$\langle x|x'\rangle = \delta(x - x'). \tag{11.11}$$

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 contect 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 the point in the middle of the n^{th} 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 $\{x_n; n = 0, \pm 1, \pm 2 \ldots\}$, 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 $\{x_n; n = 0, \pm 1, \pm 2 \ldots\}$ and associated eigenvectors $\{|x_n\rangle; n = 0, \pm 1, \pm 2, \ldots\}$ such that

$$\hat{x}_{\delta x}|x_n\rangle = x_n|x_n\rangle. \tag{11.12}$$

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

$$|\psi\rangle = \sum_n |x_n\rangle\langle x_n|\psi\rangle \tag{11.13}$$

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

$$\hat{x}_{\delta x} = \sum_n x_n |x_n\rangle\langle x_n|. \tag{11.14}$$

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

$$\frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}} \tag{11.15}$$

where $\hat{P}_n$ is the projection operator

$$\hat{P}_n = |x_n\rangle\langle x_n|. \tag{11.16}$$

To relate all this back to the continuous case, it is then necessary to take the limit, in some sense, of $\delta x \to 0$. This limiting process has already been discussed in Section 8.6.2, in an equivalent but slightly different model of the continuous limit. The essential points will be repeated here.

Returning to Eq. (11.13), we can define a new, unnormalized state vector $\overline{|x_n\rangle}$ by

$$\overline{|x_n\rangle} = \frac{|x_n\rangle}{\sqrt{\delta x}} \tag{11.17}$$

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

$$\hat{x}_{\delta x}\overline{|x_n\rangle} = x_n\overline{|x_n\rangle} \tag{11.18}$$

as the factor $1/\sqrt{\delta x}$ merely renormalizes the length of the vectors. Thus these states $\overline{|x_n\rangle}$ 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. (11.13) becomes

$$|\psi\rangle = \sum_n \overline{|x_n\rangle}\,\overline{\langle x_n|}\psi\rangle\delta x. \tag{11.19}$$

If we let $\delta x \to 0$, the discrete points $x_n = (n - \frac{1}{2})\Delta x$ will eventually form a continuum. In particular, any point x in this continuum will be the limit of a sequence of discrete points x_n for which $\delta x \to 0$ and $n \to \infty$ such that $x_n = (n - \frac{1}{2})\delta x$ remains equal to x. Further, in this limit the sum in Eq. (11.19) will define an integral with respect to x:

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle\, dx \tag{11.20}$$

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

$$|x\rangle = \lim_{\delta x\to 0} \frac{|x_n\rangle}{\sqrt{\delta x}}. \tag{11.21}$$

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. (11.20) we can extract the completeness relation for these states

$$\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = \hat{1}. \tag{11.22}$$

This is done at a cost, of course. By the same arguments as presented in Section 8.6.2, the new states $|x\rangle$ are δ-function normalized, i.e. $\langle x|x'\rangle = \delta(x - x')$, 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. (11.20) leads to

$$\langle\psi|\psi\rangle = 1 = \int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2\, dx \tag{11.23}$$

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. (11.14) and rewrite it in terms of the unnormalized states we have

$$\hat{x}_{\delta x} = \sum_n x_n \overline{|x_n\rangle}\, \overline{\langle x_n|}\delta x \tag{11.24}$$

so that in a similar way to the derivation of Eq. (11.20) this gives, in the limit of $\delta x \to 0$, the new operator $\hat{x}$, i.e.

$$\hat{x} = \int_{-\infty}^{\infty} x|x\rangle\langle x|\, dx. \tag{11.25}$$

This then leads to the $\delta x \to 0$ limit of the eigenvalue equation for $\hat{x}_{\delta x}$, Eq. (11.18) i.e.

$$\hat{x}|x\rangle = x|x\rangle \tag{11.26}$$

a result that also follows from Eq. (11.25) 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. (11.15) 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

$$\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |\langle x'|\psi\rangle|^2 dx' = \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} \langle\psi|x'\rangle\langle x'|\psi\rangle dx'$$
$$= \langle\psi|\left[\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle\langle x'|dx'\right]|\psi\rangle = \langle\psi|\hat{P}(x,\delta x)|\psi\rangle \quad (11.27)$$

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

$$\hat{P}(x,\delta x) = \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle\langle x'|dx'. \quad (11.28)$$

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

$$\left[\hat{P}(x,\delta x)\right]^2 = \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx' \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx''|x'\rangle\langle x'|x''\rangle\langle x''|$$
$$= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx' \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx''|x'\rangle\delta(x'-x'')\langle x''|$$
$$= \int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} dx'|x'\rangle\langle x'|$$
$$= \hat{P}(x,\delta x). \quad (11.29)$$

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 immmediately after measurement be given by

$$\frac{\hat{P}(x,\delta x)|\psi\rangle}{\sqrt{\langle\psi|\hat{P}(x,\delta x)|\psi\rangle}} = \frac{\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |x'\rangle\langle x'|\psi\rangle dx'}{\sqrt{\int_{x-\frac{1}{2}\delta x}^{x+\frac{1}{2}\delta x} |\langle x'|\psi\rangle|^2 dx'}} \quad (11.30)$$

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 quan tity with a continuous range of possible values. The way in which this is done is presented in the following Section.

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 $\Delta q \to 0$, 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

$$|\psi\rangle = \int_{\theta_1}^{\theta_2} c(q)|q\rangle \tag{11.31}$$

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

$$|\psi\rangle = \int_{\theta_1}^{\theta_2} |q\rangle\langle q|\psi\rangle \, dq. \tag{11.32}$$

The completeness condition can then be written as

$$\int_{\theta_1}^{\theta_2} |q\rangle\langle q| \, dq = \hat{1} \tag{11.33}$$

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

$$\int_{\theta_1}^{\theta_2} |\langle q|\psi\rangle|^2 dq \neq 0 \tag{11.34}$$

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

$$\hat{Q} = \int_{\theta_1}^{\theta_2} q|q\rangle\langle q|\, dq. \tag{11.35}$$

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 q is obtained, then the system will end up in the state

$$\frac{\hat{P}(q, \Delta q)|\psi\rangle}{\sqrt{\langle\psi|\hat{P}(q, \Delta q)|\psi\rangle}} \tag{11.36}$$

where

$$\hat{P}(q, \Delta q) = \int_{q-\frac{1}{2}\Delta q}^{q+\frac{1}{2}\Delta q} |q'\rangle\langle q'|dq'. \tag{11.37}$$

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.

11.3.3 State Vector Collapse

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 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, the picture that is more recently emerging 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 that could have proceeded gently over a long period of time. This emphasizes the notion that quantum states are as much states of knowledge as they are physical states. Einstein-Rosen-Podolsky type experiments also show that this updating of the observers knowledge may or may not be associated with any physical disruption to the system itself.

11.4 Examples of 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.

11.4.1 Position of a particle (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

$$\hat{x}|x\rangle = x|x\rangle, \qquad -\infty < x < \infty. \tag{11.38}$$

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

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \tag{11.39}$$

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

$$\langle x|x'\rangle = \delta(x - x'). \tag{11.40}$$

The operator itself can be expressed as

$$\hat{x} = \int_{-\infty}^{\infty} x|x\rangle\langle x|\, dx. \tag{11.41}$$

In many of the examples that have been used in earlier Chapters, the idea was used of a molecular ion such as the O_2^- ion in which the position of the electron was assumed to have only discrete values, namely at the positions of the atoms in the molecule. Thus, in the case of the O_2^- ion, there were only two possible positions for the electron in this model, on the oxygen atom at $x = a$ or on the oxygen atom at $x = -a$. In this case, the position operator $\hat{x}$ has only two eigenvalues, $x = \pm a$, and two corresponding eigenstates $|\pm a\rangle$ so that the spectral decomposition of this observable is then

$$\hat{x} = a|+a\rangle\langle+a| - a|-a\rangle\langle-a|. \tag{11.42}$$

In this case, the position operator is best regarded as an 'approximate' position operator.

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 10 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:

$$\langle x|\hat{x}|x'\rangle = x\delta(x - x'). \tag{11.43}$$

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.

11.4.2 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:

$$\hat{p}|p\rangle = p|p\rangle, \qquad -\infty < p < \infty. \tag{11.44}$$

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

$$|\psi\rangle = \int_{-\infty}^{+\infty} |p\rangle\langle p|\psi\rangle \, dp \tag{11.45}$$

where the basis states are delta-function normalized:

$$\langle p|p'\rangle = \delta(p - p'). \tag{11.46}$$

The operator itself can be expressed as

$$\hat{p} = \int_{-\infty}^{\infty} p|p\rangle\langle p|\, dp. \tag{11.47}$$

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 later in Chapter **??**.

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.

11.4.3 Energy of a Particle

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

$$E = \frac{p^2}{2m} + V(x) \tag{11.48}$$

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{11.49}$$

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 significant contributions to the theory of mechanics, in particular introducing the quantity we have simply called the total energy E, but usually written H, and called the Hamiltonian, if the total energy is expressed in terms of momentum and

position variables, as here. Through his work, a connection between the mathematical description of classical optics and the motion of particles could be established, a connection that Schrödinger exploited in deriving his wave equation.

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 $\hbar$. However there is no $\hbar$ in this expression for $\hat{H}$, so it is not obvious how this expression can be 'quantum mechanical'. The quantum mechanics comes about through the properties of the position and momentum operators, specifically, these two operators do not commute. In fact, we find that

$$\hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x}, \hat{p}] = i\hbar \tag{11.50}$$

and it is this failure to commute that injects 'quantum mechanics' into the operator associated with the energy of a particle.

Depending on the form of $V(\hat{x})$, the Hamiltonian can 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

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}, \qquad n = 1, 2, \ldots.$$

Thus, in this case, the Hamiltonian has eigenvalues E_n given by Eq. (11.4.3). If we write the associated energy eigenstates as $|E_n\rangle$, the eigenvalue equation is then

$$\hat{H}|E_n\rangle = E_n|E_n\rangle. \tag{11.51}$$

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

$$\begin{aligned} \psi_n(x) = \langle x|E_n\rangle &= \sqrt{\frac{2}{L}}\sin(n\pi x/L) \quad 0 < x < L \\ &= 0 \qquad\qquad\qquad\qquad x < 0, \quad x > L. \end{aligned} \tag{11.52}$$

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

$$E_n = (n + \tfrac{1}{2})\hbar\omega, \qquad n = 0, 1, 2, \ldots \tag{11.53}$$

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.

11.4.4 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 95, 122). In this case, the basis states of the electromagnetic field are the number states $\{|n\rangle, n = 0, 1, 2, \ldots\}$ 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. (9.56)) and creation operator $\hat{a}^\dagger$ (Eq. (9.71)) for this field, defined such that

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

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

$$\hat{N} = \hat{a}^\dagger \hat{a} \tag{11.54}$$

which can be readily shown to be such that

$$\hat{N}|n\rangle = n|n\rangle. \tag{11.55}$$

This operator is an observable of the system of photons. Its eigenvalues are the integers $n = 0, 1, 2, \ldots$ 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

$$\hat{N} = \sum_{n=0}^{\infty} n|n\rangle\langle n|. \tag{11.56}$$

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

$$\hat{H} = \hbar\omega\hat{N}. \tag{11.57}$$

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.

Electric Field A physical meaning can be given to the annihilation and creation operators defined above in terms of observables of the field inside the cavity. The essential point to note is that the Hamiltonian of the cavity field is given in Eq. (11.57) by $\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a}$ which can be compared with the classical expression for the energy of the single mode EM field inside the cavity, that is $H = \frac{1}{2}\epsilon_0\mathcal{E}^*\mathcal{E}\mathcal{V}$ where $\mathcal{V}$ is the volume of the cavity, and where the classical field is assumed to be a uniform standing wave of complex amplitude $\mathcal{E}e^{-i\omega t}$. The electric field E is then simply the real part of $\mathcal{E}$. We therefore want to establish a correspondence between these two expressions, i.e.

$$\hbar\omega\hat{a}^\dagger\hat{a} \longleftrightarrow \tfrac{1}{2}\epsilon_0\mathcal{E}^*\mathcal{E}\mathcal{V}$$

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 reorganising the various terms so that the correspondence looks like

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

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. By convention it is taken to be i. The most obvious next step is to identify an *electric field* operator $\hat{\mathcal{E}}$ by

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

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

$$\hat{E} = \tfrac{1}{2}[\hat{\mathcal{E}} + \hat{\mathcal{E}}^\dagger] = i\sqrt{\frac{\hbar\omega}{2\mathcal{V}\epsilon_0}}\,[\hat{a} - \hat{a}^\dagger]$$

to complete the picture. In this way we have identified a new observable for the field inside the cavity, the electric field operator. In contrast to the number operator, this observable can be shown to have a continuous range of eigenvalues, $-\infty < E < \infty$.

11.5 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. The system we will consider is the O_2^- ion, discussed in Section 8.4.

11.5.1 The Position Operator

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 we have the completeness relation for these basis states:

$$|+a\rangle\langle+a| + |-a\rangle\langle-a| = \hat{1}. \tag{11.58}$$

The position operator $\hat{x}$ of the electron is such that

$$\hat{x}|\pm a\rangle = \pm a|\pm a\rangle \tag{11.59}$$

which leads to

$$\hat{x} = a|+a\rangle\langle+a| - a|-a\rangle\langle-a|. \tag{11.60}$$

The position operator can be written in the position representation as a matrix:

$$\hat{x} \doteq \begin{pmatrix} \langle+a|\hat{x}|+a\rangle & \langle+a|\hat{x}|-a\rangle \\ \langle-a|\hat{x}|+a\rangle & \langle-a|\hat{x}|-a\rangle \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}. \tag{11.61}$$

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 will use this to construct the possible form of the Hamiltonian for this system.

11.5.2 Contructing the Hamiltonian

The Hamiltonian of the ion in the position representation will be

$$\hat{H} \doteq \begin{pmatrix} \langle+a|\hat{H}|+a\rangle & \langle+a|\hat{H}|-a\rangle \\ \langle-a|\hat{H}|+a\rangle & \langle-a|\hat{H}|-a\rangle \end{pmatrix}. \tag{11.62}$$

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.

$$\langle+a|\hat{H}|+a\rangle = \langle-a|\hat{H}|-a\rangle = E_0. \tag{11.63}$$

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

$$\hat{H} \doteq \begin{pmatrix} E_0 & V \\ V^* & E_0 \end{pmatrix} \tag{11.64}$$

or, equivalently

$$\hat{H} = E_0|+a\rangle\langle+a| + V|+a\rangle\langle-a| + V^*|-a\rangle\langle+a| + E_0|-a\rangle\langle-a|. \tag{11.65}$$

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. 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

$$\begin{pmatrix} E_0 - E & -A \\ -A & E_0 - E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0. \tag{11.66}$$

The characteristic equation yielding the eigenvalues is then

$$\begin{vmatrix} E_0 - E & -A \\ -A & E_0 - E \end{vmatrix} = 0. \tag{11.67}$$

Expanding the determinant this becomes

$$(E_0 - E)^2 - A^2 = 0 \tag{11.68}$$

with solutions

$$E_1 = E_0 + A \qquad E_2 = E_0 - A. \tag{11.69}$$

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

$$|E_1\rangle = \frac{1}{\sqrt{2}}(|+a\rangle - |-a\rangle) \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{11.70}$$

$$|E_2\rangle = \frac{1}{\sqrt{2}}(|+a\rangle + |-a\rangle) \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{11.71}$$

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

$$\hat{H} = E_1|E_1\rangle\langle E_1| + E_2|E_2\rangle\langle E_2| \tag{11.72}$$

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.

11.5.3 Measurements of Energy and Position

Suppose we prepare the O_2^- ion in the state

$$\begin{aligned} |\psi\rangle =& \frac{1}{5}[3|+a\rangle + 4|-a\rangle] \\ \doteq& \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix} \end{aligned} \tag{11.73}$$

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.

$$\langle E_1|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \end{pmatrix} \cdot \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix} = -\frac{1}{5\sqrt{2}} \tag{11.74}$$

so that

$$|\langle E_1|\psi\rangle|^2 = 0.02 \tag{11.75}$$

and similarly

$$\langle E_2|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix} \cdot \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix} = \frac{7}{5\sqrt{2}} \tag{11.76}$$

so that

$$|\langle E_2|\psi\rangle|^2 = 0.98. \tag{11.77}$$

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, withthe two possible outcomes $\pm a$. In fact, the result $+a$ will occur with probability

$$|\langle +a|\psi\rangle|^2 = 0.36 \tag{11.78}$$

and the result $-a$ with probability

$$|\langle -a|\psi\rangle|^2 = 0.64. \tag{11.79}$$

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:

$$|\langle \pm a|E_1\rangle|^2 = 0.5. \tag{11.80}$$

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:

$$|\langle E_1|+a\rangle|^2 = |\langle E_2|+a\rangle|^2 = 0.5. \tag{11.81}$$

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 said to be incompatible observables. This is a topic we will discuss in more detail in a later Chapter.