Chapter 14

Probability, Expectation Value and Uncertainty

W̰e have seen that the physically observable properties of a quantum system are represented by Hermitean operators (also referred to as 'observables') such that the eigenvalues of the operator represents all the possible results that could be obtained if the associated physical observable were to be measured. The eigenstates of the operator are the states of the system for which the associated eigenvalue would be, with 100% certainty, the measured result, if the observable were measured. If the system were in any other state then the possible outcomes of the measurement cannot be predicted precisely – different possible results could be obtained, each one being an eigenvalue of the associated observable, but only the probabilities can be determined of these possible results. This physically observed state-of-affairs is reflected in the mathematical structure of quantum mechanics in that the eigenstates of the observable form a complete set of basis states for the state space of the system, and the components of the state of the system with respect to this set of basis states gives the probability amplitudes, and by squaring, the probabilities of the various outcomes being observed.

Given the probabilistic nature of the measurement outcomes, familiar tools used to analyze statistical data such as the mean value and standard deviation play a natural role in characterizing the results of such measurements. The expectation or mean value of an observable is a concept taken more or less directly from the classical theory of probability and statistics. Roughly speaking, it represents the (probability-weighted) average value of the results of many repetitions of the measurement of an observable, with each measurement carried out on one of very many identically prepared copies of the same system. The standard deviation of these results is then a measure of the spread of the results around the mean value and is known, in a quantum mechanical context, as the uncertainty.

14.1 Observables with Discrete Values

The probability interpretation of quantum mechanics plays a central, in fact a defining, role in quantum mechanics, but the precise meaning of this probability interpretation has as yet not been fully spelt out. However, for the purposes of defining the expectation value and the uncertainty it is necessary to look a little more closely at how this probability is *operationally* defined. The way this is done depends on whether the observable has a discrete or continuous set of eigenvalues, so each case is discussed separately. We begin here with the discrete case.

14.1.1 Probability

If A is an observable for a system with a discrete set of values $\{a_1, a_2, \ldots\}$, then this observable is represented by a Hermitean operator $\hat{A}$ that has these discrete values as its eigenvalues, and associated eigenstates $\{|a_n\rangle, n = 1, 2, 3, \ldots\}$ satisfying the eigenvalue equation $\hat{A}|a_n\rangle = a_n|a_n\rangle$.

These eigenstates form a complete, orthonormal set so that any state $|\psi\rangle$ of the system can be written

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

where, provided $\langle\psi|\psi\rangle = 1$, then

$$|\langle a_n|\psi\rangle|^2 = \text{ probability of obtaining the result } a_n \text{ on measuring } \hat{A}.$$

To see what this means in an operational sense, we can suppose that we prepare N identical copies of the system all in exactly the same fashion so that each copy is presumably in the same state $|\psi\rangle$. This set of identical copies is sometimes called an *ensemble*. If we then perform a measurement of $\hat{A}$ for each member of the ensemble, i.e. for each copy, we find that we get randomly varying results e.g.

Copy:	1	2	3	4	5	6	7	8	...	N
Result:	a_5	a_3	a_1	a_9	a_3	a_8	a_5	a_9	...	a_7

Now count up the number of times we get the result a_1 – call this N_1, and similarly for the number of times N_2 we get the result a_2 and so on. Then

$$\frac{N_n}{N} = \text{ fraction of times the result } a_n \text{ is obtained.} \tag{14.1}$$

What we are therefore saying is that if the experiment is performed on an increasingly large number of identical copies, i.e. as $N \to \infty$, then we find that

$$\lim_{N\to\infty} \frac{N_n}{N} = |\langle a_n|\psi\rangle|^2. \tag{14.2}$$

This is the so-called 'frequency' interpretation of probability in quantum mechanics, i.e. the probability predicted by quantum mechanics gives us the frequency with which an outcome will occur in the limit of a very large number of repetitions of an experiment.

There is another interpretation of this probability, more akin to 'betting odds' in the sense that in application, it is usually the case that the experiment is a 'one-off' affair, i.e. it is not possible to repeat the experiment many times over under identical conditions. It then makes more sense to try to understand this probability as a measure of the likelihood of a particular result being actually observed, in the same way that betting odds for a horse to win a race is a measure of the confidence there is in the horse actually winning. After all, a race is only run once, so while it is possible to imagine the race being run many times over under identical conditions, and that the odds would provide a measure of how many of these imagined races a particular horse would win, there appears to be some doubt of the practical value of this line of thinking. Nevertheless, the 'probability as frequency' interpretation of quantum probabilities is the interpretation that is still most commonly to be found in quantum mechanics.

14.1.2 Expectation Value

We can now use this result to arrive at an expression for the average or mean value of all these results. If the measurement is repeated N times, the average will be

$$\frac{N_1}{N}a_1 + \frac{N_2}{N}a_2 + \ldots = \sum_n \frac{N_n}{N}a_n. \tag{14.3}$$

Now take the limit of this result for $N \to \infty$, and call the result $\langle \hat{A} \rangle$:

$$\langle \hat{A} \rangle = \lim_{N \to \infty} \sum_n \frac{N_n}{N} a_n = \sum_n |\langle a_n | \psi \rangle|^2 a_n. \tag{14.4}$$

It is a simple matter to use the properties of the eigenstates of $\hat{A}$ to reduce this expression to a compact form:

$$\begin{aligned} \langle \hat{A} \rangle &= \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle a_n \\ &= \sum_n \langle \psi | \hat{A} | a_n \rangle \langle a_n | \psi \rangle \\ &= \langle \psi | \hat{A} \left\{ \sum_n | a_n \rangle \langle a_n | \right\} | \psi \rangle \\ &= \langle \psi | \hat{A} | \psi \rangle \end{aligned} \tag{14.5}$$

where the completeness relation for the eigenstates of $\hat{A}$ has been used.

This result can be readily generalized to calculate the expectation values of any function of the observable $\hat{A}$. Thus, in general, we have that

$$\langle f(\hat{A}) \rangle = \sum_n |\langle a_n | \psi \rangle|^2 f(a_n) = \langle \psi | f(\hat{A}) | \psi \rangle \tag{14.6}$$

a result that will find immediate use below when the uncertainty of an observable will be considered.

While the expectation value has been defined in terms of the outcomes of measurements of an observable, the same concept of an 'expectation value' is applied to non-Hermitean operators which do not represent observable properties of a system. Thus if $\hat{A}$ is not Hermitean and hence not an observable we cannot make use of the idea of a collection of results of experiments over which an average is taken to arrive at an expectation value. Nevertheless, we continue to make use of the notion of the expectation value $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$ even when $\hat{A}$ is not an observable.

14.1.3   Uncertainty

The uncertainty of the observable A is a measure of the spread of results around the mean $\langle \hat{A} \rangle$. It is defined in the usual way, that is the difference between each measured result and the mean is calculated, i.e. $a_n - \langle \hat{A} \rangle$, then the average taken of the *square* of all these differences. In the limit of $N \to \infty$ repetitions of the same experiment we arrive at an expression for the uncertainty $(\Delta A)^2$:

$$(\Delta A)^2 = \lim_{N \to \infty} \sum_n \frac{N_n}{N} (a_n - \langle \hat{A} \rangle)^2 = \sum_n |\langle a_n | \psi \rangle|^2 (a_n - \langle \hat{A} \rangle)^2. \tag{14.7}$$

As was the case for the expectation value, this can be written in a more compact form:

$$\begin{aligned} (\Delta A)^2 &= \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle (a_n - \langle \hat{A} \rangle)^2 \\ &= \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle (a_n^2 - 2 a_n \langle \hat{A} \rangle + \langle \hat{A} \rangle^2) \\ &= \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle a_n^2 - 2 \langle \hat{A} \rangle \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle a_n + \langle \hat{A} \rangle^2 \sum_n \langle \psi | a_n \rangle \langle a_n | \psi \rangle \end{aligned}$$

Using $f(\hat{A})|a_n\rangle = f(a_n)|a_n\rangle$ then gives

$$(\Delta A)^2 = \sum_n \langle\psi|\hat{A}^2|a_n\rangle\langle a_n|\psi\rangle - 2\langle\hat{A}\rangle \sum_n \langle\psi|\hat{A}|a_n\rangle\langle a_n|\psi\rangle + \langle\hat{A}\rangle^2\langle\psi|\left\{\sum_n |a_n\rangle\langle a_n|\right\}|\psi\rangle$$

$$= \langle\psi|\hat{A}^2\left\{\sum_n |a_n\rangle\langle a_n|\right\}|\psi\rangle - 2\langle\hat{A}\rangle\langle\psi|\hat{A}\left\{\sum_n |a_n\rangle\langle a_n|\right\}|\psi\rangle + \langle\hat{A}\rangle^2\langle\psi|\psi\rangle$$

Assuming that the state $|\psi\rangle$ is normalized to unity, and making further use of the completeness relation for the basis states $|a_n\rangle$ this becomes

$$(\Delta A)^2 = \langle\psi|\hat{A}^2|\psi\rangle - 2\langle\hat{A}\rangle^2 + \langle\hat{A}\rangle^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2. \tag{14.8}$$

We can get another useful expression for the uncertainty if we proceed in a slightly different fashion:

$$(\Delta\hat{A})^2 = \sum_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle(a_n - \langle\hat{A}\rangle)^2$$

$$= \sum_n \langle\psi|a_n\rangle(a_n - \langle\hat{A}\rangle)^2\langle a_n|\psi\rangle$$

Now using $f(\hat{A})|a_n\rangle = f(a_n)|a_n\rangle$ then gives

$$(\Delta\hat{A})^2 = \sum_n \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|a_n\rangle\langle a_n|\psi\rangle$$

$$= \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2\left\{\sum_n |a_n\rangle\langle a_n|\right\}|\psi\rangle$$

$$= \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle$$

$$= \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle. \tag{14.9}$$

Thus we have, for the uncertainty $\Delta\hat{A}$, the two results

$$(\Delta\hat{A})^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2. \tag{14.10}$$

Just as was the case for the expectation value, we can also make use of this expression to formally calculate the uncertainty of some operator $\hat{A}$ even if it is not an observable, though the fact that the results cannot be interpreted as the standard deviation of a set of actually observed results means that the physical interpretation of the uncertainty so obtained is not particularly clear.

Ex 14.1 For the O_2^- ion (see p 98) calculate the expectation value and standard deviation of the position of the electron if the ion is prepared in the state $|\psi\rangle = \alpha|+a\rangle + \beta|-a\rangle$.

In this case, the position operator is given by

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

so that

$$\hat{x}|\psi\rangle = a\alpha|+a\rangle - a\beta|-a\rangle$$

and hence the expectation value of the position of the electron is

$$\langle\psi|\hat{x}|\psi\rangle = \langle\hat{x}\rangle = a(|\alpha|^2 - |\beta|^2)$$

which can be recognized as being just

$\langle \hat{x} \rangle = (+a) \times$ probability $|\alpha|^2$ of measuring electron position to be $+a$

$+ (-a) \times$ probability $|\beta|^2$ of measuring electron position to be $-a$.

In particular, if the probability of the electron being found on either oxygen atom is equal, that is $|\alpha|^2 = |\beta|^2 = \frac{1}{2}$, then the expectation value of the position of the electron is $\langle \hat{x} \rangle = 0$.

The uncertainty in the position of the electron is given by

$$(\Delta \hat{x})^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2.$$

We already have $\langle \hat{x} \rangle$, and to calculate $\langle \hat{x}^2 \rangle$ it is sufficient to make use of the expression above for $\hat{x}|\psi\rangle$ to give

$$\hat{x}^2|\psi\rangle = \hat{x}[a\alpha| + a\rangle - a\beta| - a\rangle]$$
$$= a^2[\alpha| + a\rangle + \beta| - a\rangle]$$
$$= a^2|\psi\rangle$$

so that $\langle \psi|\hat{x}^2|\psi\rangle = \langle \hat{x}^2 \rangle = a^2$. Consequently, we find that

$$(\Delta \hat{x})^2 = a^2 - a^2(|\alpha|^2 - |\beta|^2)^2$$
$$= a^2\left[1 - (|\alpha|^2 - |\beta|^2)^2\right]$$
$$= a^2(1 - |\alpha|^2 + |\beta|^2)(1 + |\alpha|^2 - |\beta|^2)$$

Using $\langle \psi|\psi\rangle = |\alpha|^2 + |\beta|^2 = 1$ this becomes

$$(\Delta \hat{x})^2 = 4a^2|\alpha|^2|\beta|^2$$

from which we find that

$$\Delta \hat{x} = 2a|\alpha\beta|.$$

This result is particularly illuminating in the case of $|\alpha|^2 = |\beta|^2 = \frac{1}{2}$ where we find that $\Delta \hat{x} = a$. This is the symmetrical situation in which the mean position of the electron is $\langle \hat{x} \rangle = 0$, and the uncertainty is exactly equal to the displacement of the two oxygen atoms on either side of this mean.

Ex 14.2 As an example of an instance in which it is useful to deal with the expectation values of non-Hermitean operators, we can turn to the system consisting of identical photons in a single mode cavity (see pp 113, 131, 174). If the cavity field is prepared in the number state $|n\rangle$, an eigenstate of the number operator $\hat{N}$ defined in Eq. (13.50), then we immediately have $\langle \hat{N} \rangle = n$ and $\Delta \hat{N} = 0$.

However, if we consider a state such as $|\psi\rangle = (|n\rangle + |n + 1\rangle)/\sqrt{2}$ we find that

$$\langle \hat{N} \rangle = \tfrac{1}{2}(\langle n| + \langle n + 1|)\hat{N}(|n\rangle + |n + 1\rangle)$$
$$= \tfrac{1}{2}(\langle n| + \langle n + 1|)(n|n\rangle + (n + 1)|n + 1\rangle)$$
$$= n + \tfrac{1}{2}.$$

while

$$(\Delta \hat{N})^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$$
$$= \tfrac{1}{2}(\langle n| + \langle n + 1|)\hat{N}\,\hat{N}(|n\rangle + |n + 1\rangle) - (n + \tfrac{1}{2})^2$$
$$= \tfrac{1}{2}(n\langle n| + (n + 1)\langle n + 1|)(n|n\rangle + (n + 1)|n + 1\rangle) - (n + \tfrac{1}{2})^2$$
$$= \tfrac{1}{2}(n^2 + (n + 1)^2) - (n + \tfrac{1}{2})^2$$
$$= \tfrac{1}{4}.$$

Not unexpectedly,we find that the uncertainty in the photon number is now non-zero.

We can also evaluate the expectation value of the annihilation operator $\hat{a}$, Eq. (11.57) for the system in each of the above states. Thus, for the number state $|n\rangle$ we have

$$\langle \hat{a} \rangle = \langle n|\hat{a}|n\rangle = \sqrt{n}\langle n|n-1\rangle = 0$$

while for the state $|\psi\rangle = (|n\rangle + |n+1\rangle)/\sqrt{2}$ we find that

$$\langle \hat{a} \rangle = \tfrac{1}{2}\sqrt{n+1}.$$

It is an interesting exercise to try to give some kind of meaning to these expectation values for $\hat{a}$, particularly since the expectation value of a non-Hermitean operator does not, in general, represent the average of a collection of results obtained when measuring some observable. The meaning is provided via the demonstration in Section 13.5.5 that $\hat{a}$ is directly related to the electric field strength inside the cavity. From that demonstration, it can be seen that the imaginary part of $\langle \hat{a} \rangle$ is to be understood as being proportional to the average strength of the electric (or magnetic) field inside the cavity, i.e. $\text{Im}\langle \hat{a}\rangle \propto \langle \hat{E} \rangle$ where $\hat{E}$ is the electric field operator. We can then interpret the expressions obtained above for the expectation value of the field as saying little more than that for the field in the number state $|n\rangle$, the electric field has an average value of zero. However, this is not to say that the field is not overall zero. Thus, we can calculate the uncertainty in the field strength $\Delta\hat{E}$. This entails calculating

$$\Delta\hat{E} = \sqrt{\langle n|\hat{E}^2|n\rangle - \langle n|\hat{E}|n\rangle^2} = \sqrt{\langle n|\hat{E}^2|n\rangle}.$$

Using the expression

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

we see that

$$\langle n|\hat{E}^2|n\rangle = \frac{\hbar\omega}{2\mathcal{V}\epsilon_0}\langle n|\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}|n\rangle$$

where the other contributions, $\langle n|\hat{a}\hat{a}|n\rangle = \langle n|\hat{a}^\dagger\hat{a}^\dagger|n\rangle = 0$. It then follows from the properties of the creation and annihilation operators that

$$\langle n|\hat{E}^2|n\rangle = \frac{\hbar\omega}{2\mathcal{V}\epsilon_0}(2n+1)$$

and hence

$$\Delta\hat{E} = \sqrt{\frac{\hbar\omega}{2\mathcal{V}\epsilon_0}}\,\sqrt{(2n+1)}.$$

So, while the field has an expectation value of zero, it has non-zero fluctuations about this mean. In fact, if the cavity contains no photons ($n = 0$), we see that even then there is a random electric field present:

$$\Delta\hat{E} = \sqrt{\frac{\hbar\omega}{2\mathcal{V}\epsilon_0}}.$$

This non-vanishing electric random electric field is known as the vacuum field fluctuations, and its presence shows that even the quantum vacuum is alive with energy!

14.2   Observables with Continuous Values

Much of what has been said in the preceding Section carries through with relatively minor changes in the case in which the observable under consideration has a continuous eigenvalue spectrum. However, rather than discussing the general case, we will consider only the particular instance of the measurement of the position represented by the position operator $\hat{x}$ of a particle.

14.2.1   Probability

Recall from Section 13.6.1, p 175, that in order to measure the position – an observable with a continuous range of possible values – it was necessary to suppose that the measuring apparatus had a finite resolution δx in which case we divide the continuous range of values of x into intervals of length δx, so that the nth segment is the interval $((n-1)\delta x, n\delta x)$. If we let x_n be the point in the middle of the nth 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 nth segment. The observable being measured is now represented by the Hermitean operator $\hat{x}_{\delta x}$ with discrete 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 $\hat{x}_{\delta x}|x_n\rangle = x_n|x_n\rangle$.

We can now imagine setting up, as in the discrete case discussed above, an ensemble of N identical systems all prepared in the state $|\psi\rangle$, and the position of the particle measured with a resolution δx. We then take note of the number of times N_n in which the particle was observed to lie in the nth interval and from this data construct a histogram of the frequency N_n/N of the results for each interval. An example of such a set of results is illustrated in Fig. 14.1.
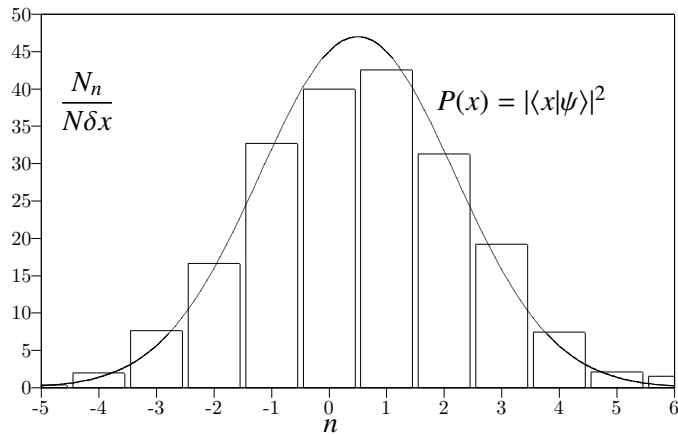

Figure 14.1: Histogram of the frequencies of detections in each interval $((n-1)\delta x, n\delta x), n = 0, \pm 1, \pm 2, \ldots$ for the measurement of the position of a particle for N identical copies all prepared in the state $|\psi\rangle$ and using apparatus with resolution δx. Also plotted is the probability distribution $|\langle x|\psi\rangle|^2$ expected in the limit of $N \to \infty$ and $\delta x \to 0$.

As was discussed earlier, the claim is now made that for N large, the frequency with which the particle is observed to lie in the nth interval $((n-1)\delta x, n\delta x)$, that is N_n/N, should approximate to the probability predicted by quantum mechanics, i.e.

$$\frac{N_n}{N} \approx |\langle x|\psi\rangle|^2 \delta x \qquad (14.11)$$

or, in other words

$$\frac{N_n}{N\delta x} \approx |\langle x|\psi\rangle|^2. \qquad (14.12)$$

Thus, a histogram of the frequency N_n/N normalized per unit δx should approximate to the idealized result $|\langle x|\psi\rangle|^2$ expected in the limit of $N \to \infty$. This is also illustrated in Fig. 14.1. In the limit of the resolution $\delta x \to 0$, the tops of the histograms would approach the smooth curve in Fig. 14.1. All this amounts to saying that

$$\lim_{\delta x \to 0} \left(\lim_{N \to \infty} \frac{N_n}{N\delta x} \right) = |\langle x|\psi\rangle|^2. \qquad (14.13)$$

The generalization of this result to other observables with continuous eigenvalues is essentially along the same lines as presented above for the position observable.

14.2.2   Expectation Values

We can now calculate the expectation value of an observable with continuous eigenvalues by making use of the limiting procedure introduced above. Rather than confining our attention to the particular case of particle position, we will work through the derivation of the expression for the expectation value of an arbitrary observable with a continuous eigenvalue spectrum. Thus, suppose we are measuring an observable $\hat{A}$ with a continuous range of eigenvalues $\alpha_1 < a < \alpha_2$. We do this, as indicated in the preceding Section by supposing that the range of possible values is divided up into small segments of length δa. Suppose the measurement is repeated N times on N identical copies of the same system, all prepared in the same state $|\psi\rangle$. In general, the same result will not be obtained every time, so suppose that on N_n occasions, a result a_n was obtained which lay in the nth interval $((n-1)\delta a, n\delta a)$. The average of all these results will then be

$$\frac{N_1}{N}a_1 + \frac{N_2}{N}a_2 + \dots . \tag{14.14}$$

If we now take the limit of this result for $N \to \infty$, then we can replace the ratios N_n/N by $|\langle a_n|\psi\rangle|^2 \delta a$ to give

$$|\langle a_1|\psi\rangle|^2 a_1 \delta a + |\langle a_2|\psi\rangle|^2 a_2 \delta a + |\langle a_3|\psi\rangle|^2 a_3 \delta a + \dots = \sum_n |\langle a_n|\psi\rangle|^2 a_n \delta a. \tag{14.15}$$

Finally, if we let $\delta a \to 0$ the sum becomes an integral. Calling the result $\langle \hat{A} \rangle$, we get:

$$\langle \hat{A} \rangle = \int_{\alpha_1}^{\alpha_2} |\langle a|\psi\rangle|^2 a\,da. \tag{14.16}$$

It is a simple matter to use the properties of the eigenstates of $\hat{A}$ to reduce this expression to a compact form:

$$\begin{aligned}
\langle \hat{A} \rangle &= \int_{\alpha_1}^{\alpha_2} \langle \psi|a\rangle a \langle a|\psi\rangle da \\
&= \int_{\alpha_1}^{\alpha_2} \langle \psi|\hat{A}|a\rangle \langle a|\psi\rangle da \\
&= \langle \psi|\hat{A}\left\{ \int_{\alpha_1}^{\alpha_2} |a\rangle\langle a|da \right\}|\psi\rangle \\
&= \langle \psi|\hat{A}|\psi\rangle
\end{aligned} \tag{14.17}$$

where the completeness relation for the eigenstates of $\hat{A}$ has been used. This is the same compact expression that was obtained in the discrete case earlier.

In the particular case in which the observable is the position of a particle, then the expectation value of position will be given by

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} |\langle x|\psi\rangle|^2 x\,dx = \int_{-\infty}^{+\infty} |\psi(x)|^2 x\,dx \tag{14.18}$$

Also, as in the discrete case, this result can be readily generalized to calculate the expectation values of any function of the observable $\hat{A}$. Thus, in general, we have that

$$\langle f(\hat{A}) \rangle = \int_{\alpha_1}^{\alpha_2} |\langle a|\psi\rangle|^2 f(a)\,da = \langle \psi|f(\hat{A})|\psi\rangle \tag{14.19}$$

a result that will find immediate use below when the uncertainty of an observable with continuous eigenvalues will be considered.

Once again, as in the discrete case, if $\hat{A}$ is not Hermitean and hence not an observable we cannot make use of the idea of a collection of results of experiments over which an average is taken to arrive at an expectation value. Nevertheless, we continue to make use of the notion of the expectation value as defined by $\langle \hat{A} \rangle = \langle \psi|\hat{A}|\psi\rangle$ even when $\hat{A}$ is not an observable.

14.2.3   Uncertainty

We saw in the preceding subsection how the expectation value of an observabel with a continuous range of possible values can be obtained by first 'discretizing' the data, then making use of the ideas developed in the discrete case to set up the expectation value, and finally taking appropriate limits. The standard deviation or uncertainty in the outcomes of a collection of measurements of a continuously valued observable can be calculated in essentially the same fashion – after all it is nothing but another kind of expectation value, and not surprisingly, the same formal expression is obtained for the uncertainty. Thus, if $\hat{A}$ is an observable with a continuous range of possible eigenvalues $\alpha_1 < a < \alpha_2$, then the uncertainty $\Delta\hat{A}$ is given by $\langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle$

$$(\Delta A)^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 \tag{14.20}$$

where

$$\langle\hat{A}^2\rangle = \int_{\alpha_1}^{\alpha_2} a^2|\langle a|\psi\rangle|^2 \, da \qquad \text{and} \qquad \langle\hat{A}\rangle = \int_{\alpha_1}^{\alpha_2} a|\langle a|\psi\rangle|^2 \, da \tag{14.21}$$

In particular, the uncertainty in the position of a particle would be given by Δx where

$$(\Delta x)^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 = \int_{-\infty}^{+\infty} x^2|\psi(x)|^2 \, dx - \left(\int_{-\infty}^{+\infty} x|\psi(x)|^2 \, dx\right)^2. \tag{14.22}$$

Ex 14.3 In the case of a particle trapped in the region $0 < x < L$ by infinitely high potential barriers – i.e. the particle is trapped in an infinitely deep potential well – the wave function for the energy eigenstates are given by

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}}\sin(n\pi x/L) & 0 < x < L \\ 0 & x < 0 \quad x > L \end{cases}$$

The integrals are straightforward (see Eq. (5.37)) and yield

$$\Delta x = \frac{L}{2n\pi}\sqrt{\frac{n^2\pi^2 - 6}{3}}$$

which approaches, for $n \to \infty$

$$\Delta x \to \frac{L}{2\sqrt{3}}$$

which is the result that would be expected for a particle that was equally likely to be found anywhere within the potential well.

14.3   The Heisenberg Uncertainty Relation

14.4   Compatible and Incompatible Observables

In all the discussion so far regarding measurement of observables of a system, we have confined our attention to considering one observable only at a time. However, it is clear that physical systems will in general possess a number of observable properties.

14.4.1   Degeneracy