9

The Heisenberg Uncertainty Relations

9.1. Introduction

In classical mechanics a particle in a state (x_0, p_0) has associated with it well-defined values for any dynamical variable $\omega(x, p)$, namely, $\omega(x_0, p_0)$. In quantum theory, given a state $|\psi\rangle$, one can only give the probabilities $P(\omega)$ for the possible outcomes of a measurement of Ω. The probability distribution will be characterized by a mean or expectation value

$$\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle \tag{9.1.1}$$

and an uncertainty about this mean:

$$(\Delta\Omega) = [\langle\psi|(\Omega - \langle\Omega\rangle)^2|\psi\rangle]^{1/2} \tag{9.1.2}$$

There are, however, states for which $\Delta\Omega = 0$, and these are the eigenstates $|\omega\rangle$ of Ω.

If we consider two Hermitian operators Ω and Λ, they will generally have some uncertainties $\Delta\Omega$ and $\Delta\Lambda$ in an arbitrary state. In the next section we will derive the Heisenberg uncertainty relations, which will provide a lower bound on the product of uncertainties, $\Delta\Omega \cdot \Delta\Lambda$. Generally the lower bound will depend not only on the operators but also on the state. Of interest to us are those cases in which the lower bound is independent of the state. The derivation will make clear the conditions under which such a relation will exist.

9.2. Derivation of the Uncertainty Relations

Let Ω and Λ be two Hermitian operators, with a commutator

$$[\Omega, \Lambda] = i\Gamma \tag{9.2.1}$$

You may readily verify that Γ is also Hermitian. Let us start with the uncertainty product in a normalized state $|\psi\rangle$:

$$(\Delta\Omega)^2(\Delta\Lambda)^2 = \langle\psi|(\Omega-\langle\Omega\rangle)^2|\psi\rangle\langle\psi|(\Lambda-\langle\Lambda\rangle)^2|\psi\rangle \tag{9.2.2}$$

where $\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle$ and $\langle\Lambda\rangle = \langle\psi|\Lambda|\psi\rangle$. Let us next define the pair

$$\begin{aligned}\hat{\Omega} &= \Omega - \langle\Omega\rangle \\ \hat{\Lambda} &= \Lambda - \langle\Lambda\rangle\end{aligned} \tag{9.2.3}$$

which has the same commutator as Ω and Λ (verify this). In terms of $\hat{\Omega}$ and $\hat{\Lambda}$

$$\begin{aligned}(\Delta\Omega)^2(\Delta\Lambda)^2 &= \langle\psi|\hat{\Omega}^2|\psi\rangle\langle\psi|\hat{\Lambda}^2|\psi\rangle \\ &= \langle\hat{\Omega}\psi|\hat{\Omega}\psi\rangle\langle\hat{\Lambda}\psi|\hat{\Lambda}\psi\rangle\end{aligned} \tag{9.2.4}$$

since

$$\hat{\Omega}^2 = \hat{\Omega}\hat{\Omega} = \hat{\Omega}^\dagger\hat{\Omega}$$

and

$$\hat{\Lambda}^2 = \hat{\Lambda}^\dagger\hat{\Lambda} \tag{9.2.5}$$

If we apply the Schwartz inequality

$$|V_1|^2|V_2|^2 \geq |\langle V_1|V_2\rangle|^2 \tag{9.2.6}$$

(where the equality sign holds only if $|V_1\rangle = c|V_2\rangle$, where c is a constant) to the states $|\hat{\Omega}\psi\rangle$ and $|\hat{\Lambda}\psi\rangle$, we get from Eq. (9.2.4),

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\hat{\Omega}\psi|\hat{\Lambda}\psi\rangle|^2 \tag{9.2.7}$$

Let us now use the fact that

$$\langle\hat{\Omega}\psi|\hat{\Lambda}\psi\rangle = \langle\psi|\hat{\Omega}^\dagger\hat{\Lambda}|\psi\rangle = \langle\psi|\hat{\Omega}\hat{\Lambda}|\psi\rangle \tag{9.2.8}$$

to rewrite the above inequality as

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\psi|\hat{\Omega}\hat{\Lambda}|\psi\rangle|^2 \tag{9.2.9}$$

Now, we know that the commutator has to enter the picture somewhere. This we arrange through the following identity:

$$\begin{aligned}\hat{\Omega}\hat{\Lambda} &= \frac{\hat{\Omega}\hat{\Lambda}+\hat{\Lambda}\hat{\Omega}}{2} + \frac{\hat{\Omega}\hat{\Lambda}-\hat{\Lambda}\hat{\Omega}}{2} \\ &= \tfrac{1}{2}[\hat{\Omega}, \hat{\Lambda}]_+ + \tfrac{1}{2}[\hat{\Omega}, \hat{\Lambda}]\end{aligned} \tag{9.2.10}$$

where $[\hat{\Omega}, \hat{\Lambda}]_+$ is called the *anticommutator*. Feeding Eq. (9.2.10) into the inequality (9.2.9), we get

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\psi|\tfrac{1}{2}[\hat{\Omega}, \hat{\Lambda}]_+ + \tfrac{1}{2}[\hat{\Omega}, \hat{\Lambda}]|\psi\rangle|^2 \tag{9.2.11}$$

We next use the fact that

(1) since $[\hat{\Omega}, \hat{\Lambda}] = i\Gamma$, where Γ is Hermitian, the expectation value of the commutator is pure imaginary;

(2) since $[\hat{\Omega}, \hat{\Lambda}]_+$ is Hermitian, the expectation value of the anticommutator is real.

Recalling that $|a+ib|^2 = a^2 + b^2$, we get

$$\begin{aligned}(\Delta\Omega)^2(\Delta\Lambda)^2 &\geq \tfrac{1}{4}|\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle + i\langle\psi|\Gamma|\psi\rangle|^2 \\ &\geq \tfrac{1}{4}\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle^2 + \tfrac{1}{4}\langle\psi|\Gamma|\psi\rangle^2\end{aligned} \tag{9.2.12}$$

This is the general uncertainty relation between any two Hermitian operators and is evidently state dependent. Consider now canonically conjugate operators, for which $\Gamma = \hbar$. In this case

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq \frac{1}{4}\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle^2 + \frac{\hbar^2}{4} \tag{9.2.13}$$

Since the first term is positive definite, we may assert that for *any* $|\psi\rangle$

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq \hbar^2/4$$

or

$$\Delta\Omega \cdot \Delta\Lambda \geq \hbar/2 \tag{9.2.14}$$

which is the celebrated uncertainty relation. Let us note that the above inequality becomes an equality only if

(1) $\hat{\Omega}|\psi\rangle = c\hat{\Lambda}|\psi\rangle$

and (9.2.15)

(2) $\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle = 0$

9.3. The Minimum Uncertainty Packet

In this section we will find the wave function $\psi(x)$ which saturates the lower bound of the uncertainty relation for X and P. According to Eq. (9.2.15) such a state is characterized by

$$(P - \langle P\rangle)|\psi\rangle = c(X - \langle X\rangle)|\psi\rangle \tag{9.3.1}$$

and

$$\langle\psi|(P-\langle P\rangle)(X-\langle X\rangle)+(X-\langle X\rangle)(P-\langle P\rangle)|\psi\rangle=0 \tag{9.3.2}$$

where $\langle P\rangle$ and $\langle X\rangle$ refer to the state $|\psi\rangle$, implicitly defined by these equations. In the X basis, Eq. (9.3.1) becomes

$$\left(-i\hbar\frac{d}{dx}-\langle P\rangle\right)\psi(x)=c(x-\langle X\rangle)\psi(x)$$

or

$$\frac{d\psi(x)}{\psi(x)}=\frac{i}{\hbar}\left[\langle P\rangle+c(x-\langle X\rangle)\right]dx \tag{9.3.3}$$

Now, whatever $\langle X\rangle$ may be, it is always possible to shift our origin (to $x=\langle X\rangle$) so that in the new frame of reference $\langle X\rangle=0$. In this frame, Eq. (9.3.3) has the solution

$$\psi(x)=\psi(0)\,e^{i\langle P\rangle x/\hbar}\,e^{icx^2/2\hbar} \tag{9.3.4}$$

Let us next consider the constraint, Eq. (9.3.2), which in this frame reads

$$\langle\psi|(P-\langle P\rangle)X+X(P-\langle P\rangle)|\psi\rangle=0$$

If we now exploit Eq. (9.3.1) and its adjoint, we find

$$\langle\psi|c^*X^2+cX^2|\psi\rangle=0$$
$$(c+c^*)\langle\psi|X^2|\psi\rangle=0$$

from which it follows that c is pure imaginary:

$$c=i|c| \tag{9.3.5}$$

Our solution, Eq. (9.3.4) now becomes

$$\psi(x)=\psi(0)\,e^{i\langle P\rangle x/\hbar}\,e^{-|c|x^2/2\hbar}$$

In terms of

$$\begin{gathered}\Delta^2=\hbar/|c|\\ \psi(x)=\psi(0)\,e^{i\langle P\rangle x/\hbar}\,e^{-x^2/2\Delta^2}\end{gathered} \tag{9.3.6}$$

where Δ^2, like $|c|$, is arbitrary. If the origin were not chosen to make $\langle X\rangle$ zero, we would have instead

$$\psi(x)=\psi(\langle X\rangle)\, e^{i\langle P\rangle(x-\langle X\rangle)/\hbar}\, e^{-(x-\langle X\rangle)^2/2\Delta^2} \tag{9.3.7}$$

Thus the *minimum uncertainty wave function* is a Gaussian of arbitrary width and center. This result, for the special case $\langle X\rangle=\langle P\rangle=0$, was used in the quest for the state that minimized the expectation value of the oscillator Hamiltonian.

9.4. Applications of the Uncertainty Principle

I now illustrate the use of the uncertainty principle by estimating the size of the ground-state energy and the spread in the ground-state wave function. It should be clear from this example that the success we had with the oscillator was rather atypical.

We choose as our system the hydrogen atom. The Hamiltonian for this system, assuming the proton is a spectator whose only role is to provide a Coulomb potential for the electron, may be written entirely in terms of the electron's variable as

$$H=\frac{P_x^2+P_y^2+P_z^2}{2m}-\frac{e^2}{(X^2+Y^2+Z^2)^{1/2}} \tag{9.4.1‡}$$

Let us begin by mimicking the analysis we employed for the oscillator. We evaluate $\langle H\rangle$ in a normalized state $|\psi\rangle$:

$$\begin{aligned}\langle H\rangle&=\frac{\langle P_x^2+P_y^2+P_z^2\rangle}{2m}-e^2\left\langle\frac{1}{(X^2+Y^2+Z^2)^{1/2}}\right\rangle\\&=\frac{\langle P_x^2\rangle+\langle P_y^2\rangle+\langle P_z^2\rangle}{2m}-e^2\left\langle\frac{1}{(X^2+Y^2+Z^2)^{1/2}}\right\rangle\end{aligned} \tag{9.4.2}$$

Since

$$\langle P_x^2\rangle=\langle\Delta P_x\rangle^2+\langle P_x\rangle^2 \quad \text{etc.}$$

the first step in minimizing $\langle H\rangle$ is to work only with states for which $\langle P_i\rangle=0$. For such states

$$\langle H\rangle=\frac{(\Delta P_x)^2+(\Delta P_y)^2+(\Delta P_z)^2}{2m}-e^2\left\langle\frac{1}{(X^2+Y^2+Z^2)^{1/2}}\right\rangle \tag{9.4.3}$$

‡ The operator $(X^2+Y^2+Z^2)^{-1/2}$ is just $1/r$ in the coordinate basis. We will occasionally denote it by $1/r$ even while referring to it in the abstract, to simplify the notation.

We cannot exploit the uncertainty relations

$$\Delta P_x \Delta X \geq \hbar/2, \quad \text{etc.}$$

yet since $\langle H\rangle$ is not a function of ΔX and ΔP. The problem is that $\langle (X^2+Y^2+Z^2)^{-1/2}\rangle$ is not simply related to ΔX, ΔY, and ΔZ. Now the handwaving begins. We argue that (see Exercise 9.4.2),

$$\left\langle \frac{1}{(X^2+Y^2+Z^2)^{1/2}} \right\rangle \simeq \frac{1}{\langle (X^2+Y^2+Z^2)^{1/2}\rangle} \tag{9.4.4}$$

where the $\simeq$ symbol means that the two sides of Eq. (9.4.4) are not strictly equal, but of the same order of magnitude. So we write

$$\langle H\rangle \simeq \frac{(\Delta P_x)^2+(\Delta P_y)^2+(\Delta P_z)^2}{2m} - \frac{e^2}{\langle (X^2+Y^2+Z^2)^{1/2}\rangle}$$

Once again, we argue that

$$\langle (X^2+Y^2+Z^2)^{1/2}\rangle \simeq (\langle X^2\rangle + \langle Y^2\rangle + \langle Z^2\rangle)^{1/2}$$

and get‡

$$\langle H\rangle \simeq \frac{(\Delta P_x)^2+(\Delta P_y)^2+(\Delta P_z)^2}{2m} - \frac{e^2}{(\langle X^2\rangle + \langle Y^2\rangle + \langle Z^2\rangle)^{1/2}}$$

From the relations

$$\langle X^2\rangle = (\Delta X)^2 + \langle X\rangle^2 \quad \text{etc.}$$

it follows that we may confine ourselves to states for which $\langle X\rangle = \langle Y\rangle = \langle Z\rangle = 0$ in looking for the state with the lowest mean energy. For such states

$$\langle H\rangle \simeq \frac{\Delta P_x^2+\Delta P_y^2+\Delta P_z^2}{2m} - \frac{e^2}{[(\Delta X)^2+(\Delta Y)^2+(\Delta Z)^2]^{1/2}}$$

For a problem such as this, with spherical symmetry, it is intuitively clear that the configuration of least energy will have

$$(\Delta X)^2 = (\Delta Y)^2 = (\Delta Z)^2$$

‡ We are basically arguing that the mean of the functions (of X, Y, and Z) and the functions of the mean ($\langle X\rangle$, $\langle Y\rangle$, and $\langle Z\rangle$) are of the same order of magnitude. They are in fact equal if there are no fluctuations around the mean and approximately equal if the fluctuations are small (recall the discussion toward the end of Chapter 6).

and

$$(\Delta P_x)^2 = (\Delta P_y)^2 = (\Delta P_z)^2$$

so that

$$\langle H \rangle \simeq \frac{3(\Delta P_x)^2}{2m} - \frac{e^2}{3^{1/2}\,\Delta X} \tag{9.4.5}$$

Now we use

$$\Delta P_x \Delta X \geq \hbar/2$$

to get

$$\langle H \rangle \gtrsim \frac{3\hbar^2}{8m(\Delta X)^2} - \frac{e^2}{3^{1/2}\,\Delta X}$$

We now differentiate the right-hand side with respect to ΔX to find its minimum:

$$\frac{-6\hbar^2}{8m(\Delta X)^3} + \frac{e^2}{3^{1/2}(\Delta X)^2} = 0$$

or

$$\Delta X = \frac{3(3^{1/2})\hbar^2}{4me^2} \simeq 1.3\,\frac{\hbar^2}{me^2} \tag{9.4.6}$$

Finally,

$$\langle H \rangle \gtrsim \frac{-2me^4}{9\hbar^2} \tag{9.4.7}$$

What prevents us from concluding (as we did in the case of the oscillator), that the ground-state energy is $-2me^4/9\hbar^2$ or that the ground-state wave function is a Gaussian [of width $3(3^{1/2})\hbar^2/4me^2$] is the fact that Eq. (9.4.7) is an approximate inequality. However, the exact ground-state energy

$$E_g = -me^4/2\hbar^2 \tag{9.4.8}$$

differs from our estimate, Eq. (9.4.7), only by a factor $\simeq 2$. Likewise, the true ground-state wave function is not a Gaussian but an exponential $\psi(x, y, z) = c\exp[-(x^2+y^2+z^2)^{1/2}/a_0]$, where

$$a_0 = \hbar^2/me^2$$

is called the *Bohr radius*. However, the ΔX associated with this wave function is

$$\Delta X = \hbar^2/me^2 \tag{9.4.9}$$

which also is within a factor of 2 of the estimated ΔX in (9.4.6).

In conclusion, the uncertainty principle gives us a lot of information about the ground state, but not always as much as in the case of the oscillator.

*Exercise 9.4.1.** Consider the oscillator in the state $|n=1\rangle$ and verify that

$$\left\langle \frac{1}{X^2} \right\rangle \simeq \frac{1}{\langle X^2 \rangle} \simeq \frac{m\omega}{\hbar}$$

Exercise 9.4.2. (1) By referring to the table of integrals in Appendix A.2, verify that

$$\psi = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a_0}, \qquad r = (x^2+y^2+z^2)^{1/2}$$

is a normalized wave function (of the ground state of hydrogen). Note that in three dimensions the normalization condition is

$$\begin{aligned}\langle \psi | \psi \rangle &= \int \psi^*(r, \theta, \phi)\psi(r, \theta, \phi) r^2 \, dr \, d(\cos\theta) \, d\phi \\ &= 4\pi \int \psi^*(r)\psi(r) r^2 \, dr = 1\end{aligned}$$

for a function of just r.

(2) Calculate $(\Delta X)^2$ in this state [argue that $(\Delta X)^2 = \frac{1}{3}\langle r^2 \rangle$] and regain the result quoted in Eq. (9.4.9).

(3) Show that $\langle 1/r \rangle \simeq 1/\langle r \rangle \simeq me^2/\hbar^2$ in this state.

Exercise 9.4.3. Ignore the fact that the hydrogen atom is a three-dimensional system and pretend that

$$H = \frac{P^2}{2m} - \frac{e^2}{(R^2)^{1/2}} \qquad (P^2 = P_x^2 + P_y^2 + P_z^2,\ R^2 = X^2 + Y^2 + Z^2)$$

corresponds to a one-dimensional problem. Assuming

$$\Delta P \cdot \Delta R \geq \hbar/2$$

estimate the ground-state energy.

*Exercise 9.4.4.** Compute $\Delta T \cdot \Delta X$, where $T = P^2/2m$. Why is this relation not so famous?

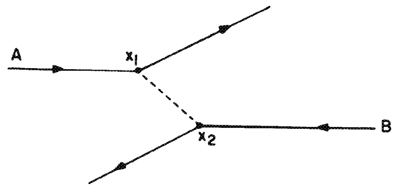

Figure 9.1. At the point x_1, skater A throws the snowball towards skater B, who catches it at the point x_2.

9.5. The Energy–Time Uncertainty Relation

There exists an uncertainty relation

$$\Delta E \cdot \Delta t \geq \hbar/2 \tag{9.5.1}$$

which does not follow from Eq. (9.2.12), since time t is not a dynamical variable but a parameter. The content of this equation is quite different from the others involving just dynamical variables. The rough meaning of this inequality is that the energy of a system that has been in existence only for a finite time Δt has a spread (or uncertainty) of at least ΔE, where ΔE and Δt are related by (9.5.1). To see how this comes about, recall that eigenstates of energy have a time dependence $e^{-iEt/\hbar}$, i.e., a definite energy is associated with a definite frequency, $\omega = E/\hbar$. Now, only a wave train that is infinitely long in time (that is to say, a system that has been in existence for infinite time) has a well-defined frequency. Thus a system that has been in existence only for a finite time, even if its time dependence goes as $e^{-iEt/\hbar}$ during this period, is not associated with a pure frequency $\omega = E/\hbar$ or definite energy E.

Consider the following example. At time $t=0$, we turn on light of frequency ω on an ensemble of hydrogen atoms all in their ground state. Since the light is supposed to consist of photons of energy $\hbar\omega$, we expect transitions to take place only to a level (if it exists) $\hbar\omega$ above the ground state. It will however be seen that initially the atoms make transitions to several levels not obeying this constraint. However, as t increases, the deviation ΔE from the expected final-state energy will decrease according to $\Delta E \simeq \hbar/t$. Only as $t \to \infty$ do we have a rigid law of conservation of energy in the classical sense. We interpret this result by saying that the light source is not associated with a definite frequency (i.e., does not emit photons of definite energy) if it has been in operation only for a finite time, even if the dial is set at a definite frequency ω during this time. [The output of the source is not just $e^{-i\omega t}$ but rather $\theta(t)\, e^{-i\omega t}$, whose transform is not a delta function peaked at ω.] Similarly when the excited atoms get deexcited and drop to the ground state, they do not emit photons of a definite energy $E = E_e - E_g$ (the subscripts e and g stand for "excited" and "ground") but rather with a spread $\Delta E \simeq \hbar/\Delta t$, Δt being the duration for which they were in the excited state. [The time dependence of the atomic wave function is not $e^{-iE_e t/\hbar}$ but rather $\theta(t)\theta(T-t)\, e^{-iE_e t/\hbar}$ assuming it abruptly got excited to this state at $t=0$ and abruptly got deexcited at $t=T$.] We shall return to this point when we discuss the interaction of atoms with radiation in a later chapter.

Another way to describe this uncertainty relation is to say that violations in the classical energy conservation law by ΔE are possible over times $\Delta t \sim \hbar/\Delta E$. The following example should clarify the meaning of this statement.

Example 9.5.1. (Range of the Nuclear Force.) Imagine two ice skaters each equipped with several snowballs, and skating toward each other on trajectories that are parallel but separated by some perpendicular distance (Fig. 9.1). When skater A reaches some point x_1

let him throw a snowball toward B. He (A) will then recoil away from B and start moving along a new straight line. Let B now catch the snowball. He too will recoil as a result, as shown in the figure. If this whole process were seen by someone who could not see the snow balls, he would conclude that there is a repulsive force between A and B. If A (or B) can throw the ball at most 10 ft, the observer would conclude that the *range of the force* is 10 ft, meaning A and B will not affect each other if the perpendicular distance between them exceeds 10 ft.

This is roughly how elementary particles interact with each other: if they throw photons at each other the force is called the electromagnetic force and the ability to throw and catch photons is called "electric charge." If the projectiles are pions the force is called the nuclear force. We would like to estimate the range of the nuclear force using the uncertainty principle. Now, unlike the two skaters endowed with snowballs, the protons and neutrons (i.e., nucleons) in the nucleus do not have a ready supply of pions, which have a mass μ and energy μc^2. A nucleon can, however, produce a pion from nowhere (violating the classical law of energy conservation by $\simeq \mu c^2$) provided it is caught by the other nucleon within a time Δt such that $\Delta t \simeq \hbar/\Delta E = \hbar/\mu c^2$. Even if the pion travels toward the receiver at the speed of light, it can only cover a distance $r = c\ \Delta t = \hbar/\mu c$, which is called the *Compton wavelength* of the pion and is a measure of the range of nuclear force. The value of r is approximately 1 Fermi $= 10^{-13}$ cm.

The picture of nuclear force given here is rather simpleminded and should be taken with a grain of salt. For example, neither is the pion the only particle that can be "exchanged" between nucleons nor is the number of exchanges limited to one per encounter. (The pion is, however, the lightest object that can be exchanged and hence responsible for the nuclear force of the longest range.) Also our analogy with snowballs does not explain any attractive interaction between particles. □