12

The Uncertainty Principle

In this chapter, we will continue our investigation of the consequences of the commutation relations among the position and momentum operators. We will mostly consider a particle in $\mathbb{R}^1$, where we have

$$[X, P] = i\hbar I. \tag{12.1}$$

We have already seen that much of the analysis of the Hamiltonian $\hat{H}$ for the quantum harmonic oscillator (given by $c_1 P^2 + c_2 X^2$) can be carried out using only the commutation relation (12.1). There are two other main results that can be derived from these commutation relations: the Heisenberg uncertainty principle and the Stone–von Neumann theorem. The uncertainty principle states that the product of the uncertainty in X and the uncertainty in P cannot be smaller than $\hbar/2$. The Stone-von Neumann theorem, meanwhile, states that *any* two self-adjoint operators A and B satisfying $[A, B] = i\hbar I$ "look like" several copies of the standard position and momentum operators acting on $L^2(\mathbb{R})$. Both results are true only under certain technical domain conditions, which we will need to examine carefully. We discuss the uncertainty principle in this chapter and the Stone–von Neumann theorem in the next chapter.

The uncertainty principle states that for all ψ in $L^2(\mathbb{R})$ satisfying certain domain conditions, we have

$$(\Delta_\psi X)(\Delta_\psi P) \geq \frac{\hbar}{2},$$

where, for any observable A, we let $\Delta_\psi A$ denote the "uncertainty" in measurements of A in the state ψ (Definition 3.13). This means that one cannot

B.C. Hall, *Quantum Theory for Mathematicians*, Graduate Texts in Mathematics 267, DOI 10.1007/978-1-4614-7116-5_12,

make both the uncertainty in position and the uncertainty in momentum arbitrarily small in the same state ψ.

Although we can easily make $\Delta_\psi X$ as small as we want simply be taking ψ to be supported in a small interval, if we do that, $\Delta_\psi P$ will be large. Similarly, we can make $\Delta_\psi P$ as small as we like, by taking the momentum wave function $\tilde{\psi}(p)$ (Sect. 6.6) to be supported in a small interval, but then $\Delta_\psi X$ will get large. In the idealized limit in which the position wave function is concentrated at a single point, $\psi(x)$ would be a multiple of $\delta(x-a)$ for some a, in which case, the momentum wave function $\tilde{\psi}(p)$ would be a multiple of $e^{-ipa/\hbar}$. In that case, $|\tilde{\psi}(p)|^2$ is constant, meaning that the momentum wave function is completely spread out over the whole real line.

This uncertainty principle may be interpreted as saying that it is impossible to simultaneously measure the position and momentum of a quantum particle. After all, we have said (Axiom 4) that if we perform a measurement of an observable A with a discrete spectrum, then immediately after the measurement the state ψ of the system should be an eigenvector for A. If A has a continuous spectrum, this principle is replaced by the requirement that after the measurement, the uncertainty in A should very small. If we could measure both the position and the momentum of the particle simultaneously with arbitrary precision, then after the measurement, *both* ΔX and ΔP would have to be very small, violating the uncertainty principle.

Now, on the scale of everyday life, Planck's constant is very small. If, for example, we measure mass in units of grams, distance in units of centimeters, and time in units of seconds, then $\hbar$ has the numerical value of 1.054×10^{-27}. Thus, on "macroscopic" scales of energy and momentum, it is possible for the uncertainties in position and momentum both to be very small. But on the atomic scale, the uncertainty principle puts a substantial limitation on how localized the position and momentum of a particle can be.

In Sect. 12.1, we prove a version of the uncertainty principle for *any* two operators A and B satisfying $[A, B] = i\hbar I$, under a seemingly innocuous assumption on the domains of the operators involved. In Sect. 12.2, however, we see that the domain assumptions are not so innocuous after all. In that section, we encounter two operators satisfying $[A, B] = i\hbar I$ on a dense subspace of the Hilbert space, along with a vector ψ such that the uncertainty in A is finite and the uncertainty in B is zero. The existence of such a vector is surely contrary to the spirit of the uncertainty principle, even though it does not violate the version of the uncertainty principle proved in Sect. 12.1. (The vector ψ in Sect. 12.2 does not satisfy the domain assumptions of Theorem 12.4.) Finally, in Sect. 12.3, we show that for the usual position and momentum operators on $L^2(\mathbb{R})$, no such counterexamples occur: If $\Delta_\psi X$ and $\Delta_\psi P$ are both defined, then $(\Delta_\psi X)(\Delta_\psi P) \geq \hbar/2$.

12.1 Uncertainty Principle, First Version

In this section, it is essential that we make sure that all vectors are in the domains of the various operators we want to apply to these vectors. With this concern in mind, we make the following definition. (Compare Definition 9.36.)

Definition 12.1 *If A and B are unbounded operators on* $\mathbf{H}$, *define AB to be the operator with domain*

$$\mathrm{Dom}(AB) = \{\psi \in \mathrm{Dom}(B) \,|\, B\psi \in \mathrm{Dom}(A)\,\}$$

and given by $(AB)\psi = A(B\psi)$.

Even if $\mathrm{Dom}(A)$ and $\mathrm{Dom}(B)$ are dense in $\mathbf{H}$, it could happen that $\mathrm{Dom}(AB)$ is not dense in $\mathbf{H}$.

Recall (Definition 3.13) that the uncertainty of a symmetric operator A in a state ψ is defined to be

$$(\Delta_\psi A)^2 = \left\langle \left(A - \langle A\rangle_\psi\, I\right)^2 \right\rangle_\psi . \tag{12.2}$$

As written, this definition requires that ψ belong to the domain of $(A - \langle A\rangle_\psi\, I)^2$, which is the same as the domain of A^2. However, since we assume that A is symmetric, then $\langle A\rangle_\psi = \langle \psi, A\psi\rangle$ is real, so that $A - \langle A\rangle_\psi\, I$ is again symmetric. Thus, (12.2) can be rewritten as

$$(\Delta_\psi A)^2 = \left\langle (A - \langle A\rangle_\psi\, I)\psi, (A - \langle A\rangle_\psi\, I)\psi \right\rangle .$$

Having written the uncertainty in this way, it is natural to extend the definition of uncertainty to vectors that belong only to $\mathrm{Dom}(A)$, as follows.

Definition 12.2 *If A is a symmetric operator on* $\mathbf{H}$, *then for all unit vectors ψ in* $\mathrm{Dom}(A)$, *the* ***uncertainty*** *$\Delta_\psi A$ of A in the state ψ is given by*

$$(\Delta_\psi A)^2 = \left\langle (A - \langle A\rangle_\psi\, I)\psi, (A - \langle A\rangle_\psi\, I)\psi \right\rangle . \tag{12.3}$$

By expanding out the right-hand side of (12.3), we see that the uncertainty may also be computed as

$$(\Delta_\psi A)^2 = \langle A\psi, A\psi\rangle - (\langle \psi, A\psi\rangle)^2.$$

[Compare (3.24).] Of course, if ψ happens to be in the domain of A^2, then Definition 12.2 agrees with (12.2).

Proposition 12.3 *If A is a symmetric operator on* $\mathbf{H}$, *then for all unit vectors $\psi \in \mathrm{Dom}(A)$, we have $\Delta_\psi A = 0$ if and only if ψ is an eigenvector for A.*

Proof. If $\Delta_\psi A = 0$, then from (12.3), we see that $(A - \langle A \rangle_\psi I)\psi = 0$, meaning that ψ is an eigenvector for A with eigenvalue $\langle A \rangle_\psi$. Conversely, if $A\psi = \lambda\psi$ for some λ, then $\langle \psi, A\psi \rangle = \lambda \langle \psi, \psi \rangle = \lambda$. Thus, $(A - \langle A \rangle_\psi I)\psi = 0$, which, by (12.3), means that $\Delta_\psi A = 0$. ■

As discussed in the introduction to this chapter, we expect that immediately after a measurement of an observable A, the state of the system will have very small uncertainty for A. Indeed, if A has discrete spectrum, we expect that the state of the system will be an eigenvector for A. Even in the case of a continuous spectrum, we expect that the uncertainty in A can be made as small as one wishes, by making more and more precise measurements. Suppose now that one wishes to observe simultaneously two (or more) different observables, represented by operators A and B. In the case of a discrete spectrum, the system after the measurement should be *simultaneously* an eigenvector for A and an eigenvector for B. In the case where A and B commute, this idea is reasonable. There is a version of the spectral theorem for commuting self-adjoint operators; in the case of discrete spectrum, it says that two commuting self-adjoint operators have an orthonormal basis of simultaneous eigenvectors with real eigenvalues. (In the case of unbounded operators, there are, as usual, technical domain conditions in defining what it means for two self-adjoint operators to commute.)

In the case where A and B do not commute, they do not need to have any simultaneous eigenvectors. Certainly, A and B cannot have an orthonormal basis of simultaneous eigenvectors, or they *would* in fact commute. The lack of simultaneous eigenvectors suggests, then, that it is simply not possible to make a simultaneous measurement of two self-adjoint operators unless they commute. In standard physics terminology, the quantities A and B are said to be "incommensurable," meaning not capable of being measured at the same time. (See Exercise 2 for a classification of the simultaneous eigenvectors of a representative pair of noncommuting operators.)

In the case of a continuous spectrum, the notion of an eigenvector is replaced by the notion of a state with very small uncertainty for the relevant operator. In light of our discussion of simultaneous eigenvectors, we may expect that for noncommuting operators, it may be difficult to find states where the uncertainties of both operators are small. This expectation is realized in the following version of the uncertainty principle.

Theorem 12.4 *Suppose A and B are symmetric operators and ψ is a unit vector belonging to* $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$. *Then*

$$(\Delta_\psi A)^2 (\Delta_\psi B)^2 \geq \frac{1}{4} \left| \langle [A, B] \rangle_\psi \right|^2 . \tag{12.4}$$

Note that if $\psi \in \mathrm{Dom}(AB)$ then in particular, $\psi \in \mathrm{Dom}(B)$, and if $\psi \in \mathrm{Dom}(BA)$ then $\psi \in \mathrm{Dom}(A)$. Thus, the assumptions on ψ are sufficient to guarantee that $\Delta_\psi A$ and $\Delta_\psi B$ make sense as in Definition 12.2.

Proof. Define operators A' and B' by $A' := A - \langle\psi, A\psi\rangle I$ and $B' := B - \langle\psi, B\psi\rangle I$. (We use the same domains for A' and B' as for A and B, and it is easily verified that A' and B' are still symmetric on those domains.) Then by the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}\langle A'\psi, A'\psi\rangle \langle B'\psi, B'\psi\rangle &\geq |\langle A'\psi, B'\psi\rangle|^2 &(12.5)\\ &\geq |\mathrm{Im}\,\langle A'\psi, B'\psi\rangle|^2 &(12.6)\\ &= \frac{1}{4}\,|\langle A'\psi, B'\psi\rangle - \langle B'\psi, A'\psi\rangle|^2 . &(12.7)\end{aligned}$$

The assumptions on ψ guarantee that $B\psi \in \mathrm{Dom}(A)$ and hence also that $B'\psi \in \mathrm{Dom}(A')$, and similarly with A' and B' reversed. Since A' and B' are symmetric, we may rewrite (12.7) as

$$\begin{aligned}\langle A'\psi, A'\psi\rangle \langle B'\psi, B'\psi\rangle &\geq \frac{1}{4}\,|\langle\psi, A'B'\psi\rangle - \langle\psi, B'A'\psi\rangle|^2\\ &= \frac{1}{4}\,|\langle\psi, [A', B']\psi\rangle|^2 .\end{aligned}$$

Now, since the identity operator commutes with everything, the commutator of A' and B' is the same as the commutator of A and B. Furthermore, $\langle A'\psi, A'\psi\rangle$ is nothing but $(\Delta_\psi A)^2$ and similarly for B. Thus, we obtain

$$(\Delta_\psi A)^2(\Delta_\psi B)^2 \geq \frac{1}{4}\,|\langle\psi, [A, B]\psi\rangle|^2 ,$$

which is what we wanted to prove. ∎

We now specialize Theorem 12.4 to the case in which the commutator is $i\hbar I$ and take the square root of both sides.

Corollary 12.5 *Suppose A and B are symmetric operators satisfying*

$$[A, B] = i\hbar I$$

on $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$. *Then if* $\psi \in \mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$ *is a unit vector, we have*

$$(\Delta_\psi A)(\Delta_\psi B) \geq \frac{\hbar}{2}. \tag{12.8}$$

In particular, for all unit vectors $\psi \in L^2(\mathbb{R})$ *in* $\mathrm{Dom}(XP) \cap \mathrm{Dom}(PX)$, *we have*

$$(\Delta_\psi X)(\Delta_\psi P) \geq \frac{\hbar}{2}. \tag{12.9}$$

Note that the factor of $\hbar$ appearing on the right-hand side of (12.8) is really just $|\langle\psi, [A, B]\psi\rangle|$. Since, however, ψ is a unit vector and $[A, B] = i\hbar I$, ψ drops out of the right-hand side of our inequality. We see then that both sides of (12.9) make sense whenever $\Delta_\psi X$ and $\Delta_\psi P$ make sense, namely, whenever ψ belongs to $\mathrm{Dom}(X)$ and to $\mathrm{Dom}(P)$. (Recall Definition 12.2.)

On the other hand, the *proof* that we have given for (12.9) requires ψ to be in both $\mathrm{Dom}(XP)$ and $\mathrm{Dom}(PX)$. Nevertheless, it is natural to ask whether (12.9) holds for all ψ in $\mathrm{Dom}(X) \cap \mathrm{Dom}(P)$. We may similarly ask whether (12.8) holds for all ψ in $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$. As we will see in Sects. 12.2 and 12.3, the answer to the first question is yes and the answer to the second question is no.

Meanwhile, it is of interest to investigate "minimum uncertainty states," that is, states ψ for which the inequality (12.4) is an equality.

Proposition 12.6 *If A and B are symmetric and ψ is a unit vector in* $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$, *equality holds in (12.4) if and only if one of the following holds: (1) ψ is an eigenvector for A, (2) ψ is an eigenvector for B, or (3) ψ is an eigenvector for an operator of the form*

$$A - i\gamma B$$

for some nonzero real number γ.

In the case $A = X$ and $B = P$, we will consider examples where equality holds in Sect. 12.4.

Proof. To get equality in (12.4), we must have equality in both (12.5) and (12.6). Equality in (12.5) occurs if and only if $A'\psi = 0$ or $B'\psi = 0$ or $A'\psi = cB'\psi$ for some nonzero constant c. If $A'\psi$ is zero, ψ is an eigenvector for A with eigenvalue $\langle A \rangle_\psi$. In that case, equality holds in (12.6) as well. Conversely, if ψ is an eigenvector for A with some eigenvalue λ, then $\langle A \rangle_\psi = \lambda$ and $A'\psi = 0$. Similarly, $B'\psi = 0$ if and only if ψ is an eigenvector for B.

Meanwhile, suppose $A'\psi$ and $B'\psi$ are nonzero and $A'\psi = cB'\psi$, so that equality holds in (12.5). Then equality holds (12.6) if and only if $c = i\gamma$ for some nonzero $\gamma \in \mathbb{R}$. Thus, when $A'\psi$ and $B'\psi$ are nonzero, we get equality in (12.4) if and only if

$$A'\psi = i\gamma B'\psi \tag{12.10}$$

for some nonzero real number γ. Recalling the definition of A' and B', (12.10) says that

$$(A - \langle \psi, A\psi \rangle I)\psi = i\gamma(B - \langle \psi, B\psi \rangle I)\psi \tag{12.11}$$

or

$$(A - i\gamma B)\psi = \lambda\psi, \tag{12.12}$$

where $\lambda = \langle \psi, A\psi \rangle - i\gamma \langle \psi, B\psi \rangle$.

Thus, if (12.11) holds, ψ is an eigenvector of $A - i\gamma B$. Conversely, if ψ is an eigenvector for $A - i\gamma B$ with some eigenvalue $\lambda = c + id$ in $\mathbb{C}$, then

$$(c + id) \|\psi\|^2 = \langle \psi, (A - i\gamma B)\psi \rangle = \langle \psi, A\psi \rangle - i\gamma \langle \psi, B\psi \rangle. \tag{12.13}$$

Since A and B are assumed to be symmetric and ψ is a unit vector, we may equate real and imaginary parts in (12.13) to obtain

$$c = \langle \psi, A\psi \rangle; \quad d = -\gamma \langle \psi, B\psi \rangle.$$

From this we can see that (12.11) and (12.10) hold, and thus equality holds in (12.4). ■

12.2 A Counterexample

In this section, we consider the Hilbert space $L^2[-1,1]$. As our "position" operator, we use the usual formula,

$$A\psi(x) = x\psi(x).$$

Note that A is a *bounded* operator, because we restrict x to the bounded interval $[-1,1]$. As such, A is defined (and self-adjoint) on the whole Hilbert space $L^2(\mathbb{R})$. As our "momentum" operator, we again use the usual formula,

$$B = -i\hbar\frac{d}{dx}.$$

As the domain of B we will take the space of continuously differentiable functions ψ on $[-1,1]$ satisfying the *periodic boundary condition*,

$$\psi(-1) = \psi(1). \tag{12.14}$$

To verify that B is symmetric, note that for any C^1 functions ϕ and ψ, we have

$$\int_{-1}^{1} \overline{\phi(x)}\frac{d\psi}{dx}\ dx = \overline{\phi(1)}\psi(1) - \overline{\phi(-1)}\psi(-1) - \int_{-1}^{1} \overline{\frac{d\phi}{dx}}\psi(x)\ dx.$$

If both ϕ and ψ satisfy the periodic boundary condition (12.14), the boundary terms cancel out to zero. This shows that the operator d/dx is skew-symmetric on $\mathrm{Dom}(B)$, from which it follows that $-i\hbar d/dx$ is symmetric on $\mathrm{Dom}(B)$. Actually, since the functions

$$\psi_n(x) := \frac{1}{\sqrt{2}}e^{\pi inx}, \quad n \in \mathbb{Z}, \tag{12.15}$$

constitute an orthonormal basis of eigenvectors for B with real eigenvalues, B is essentially self-adjoint, by Example 9.25.

Now, for all $\psi \in \mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$ we have, by direct calculation,

$$AB\psi - BA\psi = i\hbar\psi, \tag{12.16}$$

just as for the usual position and momentum operators. Furthermore, $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$ is dense in $\mathbf{H}$, since it contains all continuously differentiable functions ψ such that $\psi(0) = \psi(1) = 0$. Consider, now, the function $\psi_n(x)$ in (12.15), for some integer n. Clearly, ψ_n is in the domain of B, since $B\psi_n$ is just a multiple of ψ_n. Since ψ_n is an eigenvector for B, the uncertainty of B in the state ψ_n is zero! Meanwhile, since A is bounded, the uncertainty of A is well defined and finite. Thus, $\Delta_{\psi_n}A$ and $\Delta_{\psi_n}B$ are both unambiguously defined and

$$(\Delta_{\psi_n}A)(\Delta_{\psi_n}B) = 0. \tag{12.17}$$

How can (12.17) hold? Is it not, in light of (12.16), a violation of (12.8) in Corollary 12.5? The answer is no, for the reason that ψ_n does not satisfy the domain assumptions in that corollary. Specifically, $A\psi_n$ is not in the domain of B, since $A\psi_n$ is does not satisfy the periodic boundary condition in the definition of $\mathrm{Dom}(B)$. Thus, ψ_n does not belong to $\mathrm{Dom}(BA)$.

Although it does not contradict Corollary 12.5, (12.17) certainly violates the spirit of the uncertainty principle. In the next section, we will show that no such strange counterexamples occur for the usual position and momentum operators.

12.3 Uncertainty Principle, Second Version

In this section, we will see that if A and B are taken to be the usual position and momentum operators X and P, the uncertainty principle holds whenever $\Delta_\psi X$ and $\Delta_\psi P$ are defined. We continue to use Definition 12.2 for the definition of the uncertainty in any operator, in which case, for $\Delta_\psi X$ and $\Delta_\psi P$ to be defined, we require only that ψ belong to $\mathrm{Dom}(X)$ and $\mathrm{Dom}(P)$.

We are now ready to formulate the strong version of the uncertainty principle.

Theorem 12.7 *Suppose ψ is a unit vector in $L^2(\mathbb{R})$ belonging to $\mathrm{Dom}(X) \cap \mathrm{Dom}(P)$. Then*

$$(\Delta_\psi X)(\Delta_\psi P) \geq \frac{\hbar}{2}, \tag{12.18}$$

where $\Delta_\psi X$ and $\Delta_\psi P$ are given by Definition 12.2.

Proof. According to Stone's theorem and Example 10.16, the operator P is $\hbar$ times the infinitesimal generator of the group $U(\cdot)$ of translations. That is to say, for all $\psi \in \mathrm{Dom}(P)$, we have

$$(P\psi)(x) = -i\hbar \lim_{a\to 0} \frac{\psi(x+a) - \psi(x)}{a},$$

where the limit is in the L^2 norm sense. Thus,

$$\begin{aligned}\langle X\psi, P\psi\rangle &= \lim_{a\to 0}\left\langle X\psi, -i\hbar\left(\frac{\psi(x+a)-\psi(x)}{a}\right)\right\rangle \\ &= \lim_{a\to 0}\left(\frac{1}{a}\langle x\psi(x), -i\hbar\psi(x+a)\rangle + \frac{i\hbar}{a}\langle X\psi,\psi\rangle\right) \\ &= \lim_{a\to 0}\left(\frac{1}{a}\langle i\hbar(y-a)\psi(y-a),\psi(y)\rangle + \frac{i\hbar}{a}\langle X\psi,\psi\rangle\right),\end{aligned}$$

where in the last step we have made the change of variable $y = x + a$.

If we rename the variable of integration back to x, we get

$$\begin{aligned}&\langle X\psi, P\psi\rangle \\ &= \lim_{a\to 0}\left(\left\langle i\hbar X\left(\frac{\psi(x-a)-\psi(x)}{a}\right),\psi(x)\right\rangle + i\hbar\langle\psi(x-a),\psi(x)\rangle\right) \\ &= \lim_{a\to 0}\left(\left\langle i\hbar\left(\frac{\psi(x-a)-\psi(x)}{a}\right), X\psi(x)\right\rangle + i\hbar\langle\psi(x-a),\psi(x)\rangle\right) \\ &= \langle P\psi, X\psi\rangle + i\hbar\langle\psi,\psi\rangle\,. \qquad (12.19)\end{aligned}$$

In the second equality, we have used that X is symmetric and that (check) if $\psi\in\mathrm{Dom}(X)$, then $\psi(x-a)\in\mathrm{Dom}(X)$ for each fixed a. In the last equality, we get a minus sign from having $\psi(x-a)-\psi(x)$ rather than $\psi(x+a)-\psi(x)$, and we use that translation is strongly continuous.

It should be noted that (12.19) is precisely what we would get by formally moving X to the right-hand side of the inner product, using the commutation relation $XP - PX = i\hbar I$, and then moving P to the left-hand side of the inner product. But to make *that* calculation rigorous, we would need to assume that ψ is in the domain of XP and the domain of PX. In (12.19), on the other hand, we have obtained the desired conclusion assuming only that ψ is in the domain of X and in the domain of P.

Having obtained (12.19), we can easily verify that for any real constants α and β, we have

$$\langle (X-\alpha I)\psi, (P-\beta I)\psi\rangle = \langle (P-\beta I)\psi, (X-\alpha I)\psi\rangle + i\hbar\langle\psi,\psi\rangle\,. \qquad (12.20)$$

Solving (12.20) for $\langle\psi,\psi\rangle$ gives

$$\begin{aligned}\langle\psi,\psi\rangle &= \frac{1}{i\hbar}\left(\langle (X-\alpha I)\psi, (P-\beta I)\psi\rangle - \langle (P-\beta I)\psi, (X-\alpha I)\psi\rangle\right) \\ &= \frac{2}{\hbar}\,\mathrm{Im}\,\langle (X-\alpha I)\psi, (P-\beta I)\psi\rangle \\ &\le \frac{2}{\hbar}\,\|(X-\alpha I)\psi\|\,\|(P-\beta I)\psi\|\,, \qquad (12.21)\end{aligned}$$

by the Cauchy–Schwarz inequality. If ψ is a unit vector and we take $\alpha = \langle X\rangle_\psi$, and $\beta = \langle P\rangle_\psi$, then $\|(X-\alpha I)\psi\|^2 = (\Delta_\psi X)^2$ and $\|(P-\beta I)\psi\|^2 = (\Delta_\psi P)^2$. Thus, we get

$$1 \leq \frac{2}{\hbar}(\Delta_\psi X)(\Delta_\psi P),$$

which is equivalent to what we want to prove. ■

We know from Sect. 12.2 that the strong form of the uncertainty principle does not hold if X and P are replaced by two arbitrary operators satisfying $AB - BA = i\hbar I$ on $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$, even if $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$ is dense in $\mathbf{H}$. Nevertheless, if we look carefully at the proof of Theorem 12.7, we can see what assumptions we would need on A and B to make the proof go through in a more general setting.

Theorem 12.8 *Suppose A and B are self-adjoint operators on $\mathbf{H}$. Suppose that for all $a \in \mathbb{R}$ and $\psi \in \mathrm{Dom}(A)$, we have that $e^{iaB}\psi$ belongs to $\mathrm{Dom}(A)$ and that*

$$Ae^{iaB}\psi = e^{iaB}A\psi - \hbar a e^{iaB}\psi. \tag{12.22}$$

Then for all unit vectors ψ in $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$, we have

$$(\Delta_\psi A)(\Delta_\psi B) \geq \frac{\hbar}{2},$$

where $\Delta_\psi A$ and $\Delta_\psi B$ are defined by Definition 12.2.

The relation

$$e^{iaB}A = Ae^{iaB} + \hbar a e^{iaB}, \quad a \in \mathbb{R}, \tag{12.23}$$

which holds on $\mathrm{Dom}(A)$, is a "semi-exponentiated" form of the canonical commutation relations. As shown in Exercise 6, there is a *formal* argument (ignoring domain issues) that the commutation relations $[A, B] = i\hbar I$ ought to imply the relations (12.22). Nevertheless, as Exercise 7 shows, this formal argument does not always give the correct conclusion. In Sect. 14.2, we will encounter a "fully exponentiated" form of the canonical commutation relations, in which both A and B are exponentiated.

Proof. See Exercise 5. ■

Corollary 12.9 *For any $j = 1, \ldots n$ and any unit vector $\psi \in L^2(\mathbb{R}^n)$ with $\psi \in \mathrm{Dom}(X_j) \cap \mathrm{Dom}(P_j)$, we have*

$$(\Delta_\psi X_j)(\Delta_\psi P_j) \geq \frac{\hbar}{2}.$$

Proof. In the case that $A = X_j$ and $B = P_j$, we have $(e^{iaB/\hbar}\psi)(\mathbf{x}) = \psi(\mathbf{x} + a\mathbf{e}_j)$, by Exercise 2 in Chap. 10. Thus, in this case, (12.22) says that

$$(x_j + a)\psi(\mathbf{x} + a\mathbf{e}_j) = x_j\psi(\mathbf{x} + a\mathbf{e}_j) + a\psi(\mathbf{x} + a\mathbf{e}_j),$$

which is true. ■

12.4 Minimum Uncertainty States

In this section, we look at the states that give equality in the uncertainty principle. Such states are known as minimum uncertainty states or *coherent states*. As in the general setting of Proposition 12.6, the condition for a equality is an eigenvector condition. That is to say, even though in Theorem 12.7, we allow ψ's that are not $\mathrm{Dom}(XP) \cap \mathrm{Dom}(PX)$, we do not get any new minimum uncertainty states by this weakening of our domain assumptions.

Proposition 12.10 *A unit vector* $\psi \in \mathrm{Dom}(X) \cap \mathrm{Dom}(P)$ *satisfies*

$$(\Delta_\psi X)(\Delta_\psi P) = \frac{\hbar}{2}$$

if and only if ψ *satisfies*

$$(X + i\delta P)\psi = \lambda\psi \tag{12.24}$$

for some nonzero real number δ *and some complex number* λ.

For convenience, we have made the substitution $\delta = -\gamma$ in (12.24) relative to Proposition 12.6.

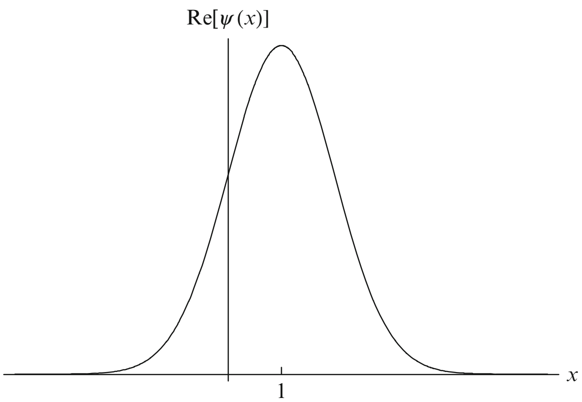

FIGURE 12.1. Minimum uncertainty state with $\langle X \rangle = 1$, $\langle P \rangle = 0$, and $\Delta X = 1/2$.

Proof. All the relations in the proof of Theorem 12.7 are equalities, except for the inequality in the last line of (12.21). Equality will hold in that line if and only if one of $(X - \alpha I)\psi$ and $(P - \beta I)\psi$ is zero or $(P - \beta I)\psi$ is a pure-imaginary multiple of $(X - \alpha I)\psi$. Now, if ψ is a unit vector in $L^2(\mathbb{R})$, then neither ψ nor the Fourier transform of ψ can be supported at a single point; thus, neither $(X - \alpha I)\psi$ nor $(P - \beta I)\psi$ can be zero. We are left, then, with the condition that

$$(X - \alpha I)\psi = i\gamma(P - \beta I)\psi, \tag{12.25}$$

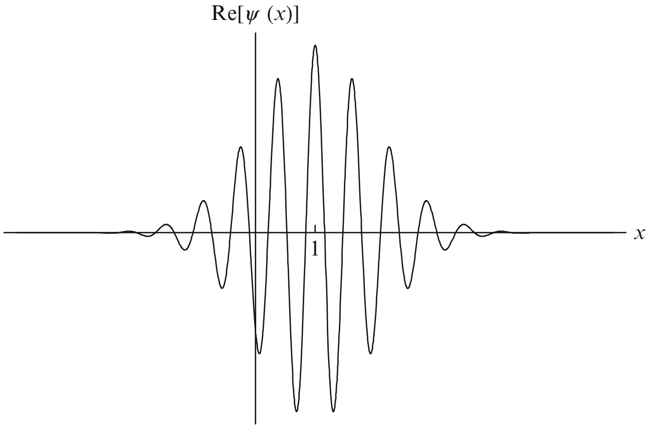

FIGURE 12.2. Minimum uncertainty state with $\langle X\rangle = 1$, $\langle P\rangle = 10$, and $\Delta X = 1/2$.

where γ is a nonzero real number, $\alpha = \langle A\rangle_\psi$ and $\beta = \langle B\rangle_\psi$. As in the proof of Proposition 12.6, (12.25) is equivalent to the assertion that ψ is an eigenvector for the operator $X - i\gamma P$. Letting $\delta = -\gamma$ gives the desired result. ■

Proposition 12.11 *If the parameter δ in (12.24) is negative, there are no nonzero solutions to (12.24). If the parameter δ is positive, there exists a unique (up to multiplication by a constant) solution $\psi_{\delta,\lambda}$ to (12.24) for every complex number λ. The function $\psi_{\delta,\lambda}$ has the following additional properties*

$$\begin{aligned}\langle X\rangle &= \operatorname{Re}\lambda \\ \langle P\rangle &= \frac{1}{\delta}\operatorname{Im}\lambda \\ \frac{\Delta X}{\Delta P} &= \delta.\end{aligned}$$

Explicitly, we have

$$\begin{aligned}\psi_{\delta,\lambda}(x) &= c_1 \exp\left\{-\frac{(x-\lambda)^2}{2\delta\hbar}\right\} \\ &= c_2 \exp\left\{-\frac{(x-\langle X\rangle)^2}{2\delta\hbar}\right\}\exp\left\{\frac{i\langle P\rangle x}{\hbar}\right\},\end{aligned}$$

where all expectation values are taken in the state $\psi_{\delta,\lambda}$.

Note that among states with $(\Delta X)(\Delta P) = \hbar/2$, we can arrange for $\Delta X/\Delta P$ to be any positive real number, and once we have chosen $\Delta X/\Delta P$, we can then arrange for $\langle X\rangle$ and $\langle P\rangle$ to be any two real numbers. On the

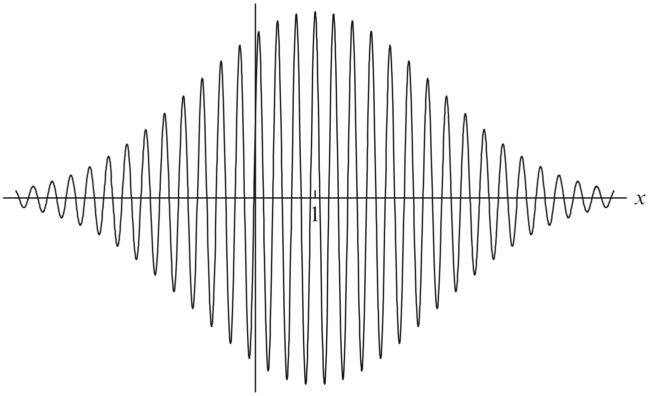

FIGURE 12.3. Minimum uncertainty state with $\langle X\rangle = 1$, $\langle P\rangle = 20$, and $\Delta X = 1$.

other hand, once $\Delta X/\Delta P$ and $\langle X\rangle$ and $\langle P\rangle$ have been specified, there is a unique quantum state with $(\Delta X)(\Delta P) = \hbar/2$. In Figs. 12.1–12.3, we have plotted the real part of $\psi_{\delta,\lambda}$ for several different values of the parameters, in a system of units for which $\hbar = 1$.

Proof. The equation $(X + i\delta P)\psi = \lambda\psi$ amounts to

$$x\psi + \delta\hbar\frac{d\psi}{dx} = \lambda\psi(x), \tag{12.26}$$

where ψ is assumed to be in the domain of P, so that the distributional derivative of ψ is an L^2 function. If ψ were smooth, then the unique solution to (12.26) would be the function $\psi_{\delta,\lambda}$ given in the proposition, which is square-integrable if and only if $\delta > 0$. Even (12.26) is only assumed to hold in the distribution sense, the argument in the proof of Proposition 9.29 (with $e^{-x/\hbar}\psi(x)$ replaced by $\exp[(x-\lambda)^2/(2\delta\hbar)]\psi(x)$) shows that there are no additional solutions. The formulas for $\langle X\rangle$, $\langle P\rangle$, and $\Delta X/\Delta P$ can be computed either by tracing through the arguments in the proof of Theorem 12.7 or by direct calculation with the formula for $\psi_{\delta,\lambda}$. ■

12.5 Exercises

1. Let α be a positive real number. Show that the following "additive" version of the uncertainty principle holds for all unit vectors $\psi \in \mathrm{Dom}(X) \cap \mathrm{Dom}(P)$:

$$\alpha\Delta_\psi X + \frac{1}{\alpha}\Delta_\psi P \geq \sqrt{2\hbar}.$$

2. In this exercise, we classify the simultaneous eigenvectors of the *non-commuting* operators $\hat{J}_1$ and $\hat{J}_2$. Let $\hat{J}_1$, $\hat{J}_2$, and $\hat{J}_3$ denote the angular

momentum operators on $L^2(\mathbb{R}^3)$ as defined in Sect. 3.10. Suppose ψ is in the domain of any product $\hat{J}_j\hat{J}_k$ of two angular momentum operators. (For example, ψ could be a Schwartz function.) Suppose also that ψ is an eigenvector for $\hat{J}_1$ and for $\hat{J}_2$ with eigenvalues α and β, respectively.

(a) Using the commutation relations in Exercise 10 in Chap. 3, show that ψ is an eigenvector for $\hat{J}_3$ with eigenvalue 0.
(b) Show that the eigenvalues α and β for $\hat{J}_1$ and $\hat{J}_2$ must be zero.
(c) What type of function $\psi \in L^2(\mathbb{R}^3)$ satisfies $\hat{J}_j\psi = 0$ for $j = 1, 2, 3$?

3. Given any unit vector $\psi \in \mathrm{Dom}(X) \cap \mathrm{Dom}(P)$, consider another vector ϕ given by
$$\phi(x) = e^{ibx/\hbar}\psi(x - a).$$
Show that ϕ is a unit vector belonging to $\mathrm{Dom}(X) \cap \mathrm{Dom}(P)$ and that
$$\begin{aligned} \langle X\rangle_\phi &= \langle X\rangle_\psi + a \\ \Delta_\phi X &= \Delta_\psi X \end{aligned}$$
and
$$\begin{aligned} \langle P\rangle_\phi &= \langle P\rangle_\psi + b \\ \Delta_\phi P &= \Delta_\psi P. \end{aligned}$$

4. We have seen that a unit vector $\psi \in \mathrm{Dom}(X)\cap\mathrm{Dom}(P)$ is a minimum uncertainty state [i.e., $(\Delta_\psi X)(\Delta_\psi P) = \hbar/2$] if and only if there exists some $\delta > 0$ such that ψ is an eigenvector of the operator $X + i\delta P$. In that case, ψ is also an eigenvector for any operator of the form $c(X + i\delta P)$, with c being a nonzero constant. Consider, then, some fixed $\delta > 0$ and define an operator a by the formula
$$a = \frac{\frac{1}{\delta}(X + i\delta P)}{\sqrt{2\hbar/\delta}}.$$
Then a is just the annihilation operator, as defined in Chap. 11, for a harmonic oscillator with $m\omega = 1/\delta$. Thus, a and its adjoint a^* satisfy the relation $[a, a^*] = I$, and we have the "chain" of eigenvectors $\psi_n \in L^2(\mathbb{R})$ satisfying the properties listed in Theorem 11.2.

(a) For any $\lambda \in \mathbb{C}$, find constants c_n so that the vector
$$\phi_\lambda := \sum_{n=0}^{\infty} c_n\psi_n$$
is an eigenvector for a with eigenvalue λ. Show that the resulting series converges in $\mathbf{H}$.

(b) Let ϕ_λ denote the eigenvector obtained in Part (a), normalized so that $c_0 = 1$. Show that

$$\phi_\lambda = e^{\lambda a^*}\phi_0,$$

where the exponential is defined by

$$e^{\lambda a^*}\phi_0 = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}(a^*)^n \phi_0.$$

with convergence in $L^2(\mathbb{R})$.

5. Prove Theorem 12.8, following the outline of the proof of Theorem 12.7. Recall from Sect. 10.2 that $B/\hbar$ is the infinitesimal generator of the one-parameter unitary group $U(a) := e^{iaB/\hbar}$.

6. If X and Y are bounded operators, we may define $\mathrm{ad}_X(Y) = [X, Y]$, where $[X, Y] = XY - YX$. Thus, say, $(\mathrm{ad}_X)^3(Y) = [X, [X, [X, Y]]]$. It is not hard to show that for any bounded operators Y and X, we have

$$\begin{aligned} e^X Y e^{-X} &= e^{\mathrm{ad}_X}(Y) \\ &= Y + [X, Y] + \frac{[X, [X, Y]]}{2!} + \frac{[X, [X, [X, Y]]]}{3!} + \cdots . \end{aligned} \tag{12.27}$$

(See Proposition 2.25 and Exercise 2.19 of [21].)

Suppose A and B are unbounded self-adjoint operators satisfying $[A, B] = i\hbar I$ on $\mathrm{Dom}(AB) \cap \mathrm{Dom}(BA)$. Show that *if* we could apply (12.27) with $X = iaB/\hbar$ and $Y = A$ (even though X and Y are unbounded), then A and B would satisfy (12.22).

7. Let A be the operator in Sect. 12.2, and let B be the unique self-adjoint extension of the operator B in that section. Show that the operators $X = iaB/\hbar$ and $Y = A$ *do not* satisfy (12.27).

Note: This result shows the hazards involved formally applying results for bounded operators to unbounded operators.

Hint: Show that the unitary operators $U(a) := \exp(iaB/\hbar)$ consist of "translation with wrap around," first on the eigenvectors of B and then on the whole Hilbert space.