It is easily shown that $\hat{\wp}$ has only two (real) eigenvalues, ± 1. That is, if $\hat{\wp}\psi(\boldsymbol{r}) = \lambda\psi(\boldsymbol{r})$,

$$\begin{aligned}\hat{\wp}^2\psi(\boldsymbol{r}) &= \hat{\wp}\psi(-\boldsymbol{r}) = \psi(\boldsymbol{r}) \\ &= \lambda\hat{\wp}\psi(-\boldsymbol{r}) = \lambda^2\psi(\boldsymbol{r})\end{aligned} \tag{6.137}$$

so $\lambda = \pm 1$. Thus, the eigenfunctions of $\hat{\wp}$ are either even or odd.

The real eigenvalues suggest that $\hat{\wp}$ is Hermitian, but this can be proved. Using bra and ket notation we have

$$\langle\phi(\boldsymbol{r})|\left(\hat{\wp}\,|\psi(\boldsymbol{r})\rangle\right) = \pm\langle\phi(\boldsymbol{r})|\,\psi(\boldsymbol{r})\rangle \tag{6.138}$$

while

$$\left(\langle\phi(\boldsymbol{r})|\,\hat{\wp}^{\dagger}\right)|\psi(\boldsymbol{r})\rangle = \pm\langle\phi(\boldsymbol{r})|\,\psi(\boldsymbol{r})\rangle \tag{6.139}$$

which shows that $\hat{\wp} = \hat{\wp}^{\dagger}$.

If the parity operator commutes with the Hamiltonian, then the energy eigenfunctions have definite parity, that is, they are also eigenfunctions of $\hat{\wp}$. We already know that this occurs in one-dimension if the potential is even (see Section 2.9).

6.5 The Heisenberg Picture

We have seen that the time evolution operator converts a state vector at a given time, $|\Psi(t = t_0)\rangle = |\Psi\rangle$, into the state vector at the time t, $|\Psi(t)\rangle$. The state vector is often referred to as the state ket and it must be distinguished from the eigenvectors (eigenkets) which, according to Postulate IV, may serve as a basis set upon which to expand the state vector. To compute the time dependence of the expectation value of an operator $\hat{A}$, we must use time-dependent state vectors $|\Psi(t)\rangle$. Thus,

$$\left\langle\hat{A}(t)\right\rangle = \langle\Psi(t)|\,\hat{A}\,|\Psi(t)\rangle \tag{6.140}$$

Replacing $|\Psi(t)\rangle$ (and its complex conjugate $\langle\Psi(t)|$) using Equation 6.112 we have

$$\left\langle\hat{A}(t)\right\rangle = \langle\Psi(t_0)|\,\hat{U}^{\dagger}(t, t_0)\,\hat{A}\hat{U}(t, t_0)\,|\Psi(t_0)\rangle \tag{6.141}$$

Now, suppose that in Equation 6.141 we group the operators on the right-hand side. In essence, we have converted the time-independent operator $\hat{A}$ into a time-dependent operator $\hat{A}(t)$ according to the prescription

$$\hat{A}(t) = \hat{U}^\dagger(t, t_0)\,\hat{A}\hat{U}(t, t_0)$$
$$= e^{i\hat{H}(t-t_0)/\hbar}\hat{A}e^{-i\hat{H}(t-t_0)/\hbar} \tag{6.142}$$

where the absence of a noted time dependence associated with $\hat{A}$ implies its time *in*dependence. Thus, there are two ways of representing the time-dependent expectation value of a quantum mechanical observable, one using time-dependent state vectors and time-independent operators and the other using time-independent state vectors with time-dependent operators. So far in this book we have used time-dependent state vectors and time-independent operators. This formulation of quantum mechanics is known as the Schrödinger picture. The alternative formulation in which the state vectors remain fixed in time and the operators move is known as the Heisenberg picture. The Schrödinger picture is the most frequently used formulation of quantum physics, but the Heisenberg picture is equivalent.

In the Heisenberg picture it is the time dependence of the observables, operators, that describes the physical system. State vectors are of little consequence since they are evaluated at a fixed time. Of course, the possible results of a measurement, the eigenvalues, must be the same in both pictures, but the eigenvectors change with time in the Heisenberg picture. This may be shown by beginning with the eigenvalue equation for an operator $\hat{A}$ in the Schrödinger picture. The corresponding Heisenberg picture operator is $\hat{A}(t)$. Denoting the eigenkets of $\hat{A}$ in the Schrödinger picture by $|\alpha_i\rangle$, the eigenvalue equation in the Schrödinger picture at a fixed time, $t = 0$ for simplicity, is

$$\hat{A}\,|\alpha_i\rangle = \alpha_i\,|\alpha_i\rangle \tag{6.143}$$

Letting $\hat{U}(t, t_0 = 0) = \hat{U}$, we now operate on Equation 6.143 with $\hat{U}^\dagger$ and insert $\hat{U}\hat{U}^\dagger \equiv \hat{I}$ in front of the ket $|\alpha_i\rangle$ on the left-hand side to obtain

$$\hat{U}^\dagger\hat{A}\left(\hat{U}\hat{U}^\dagger\right)|\alpha_i\rangle = \alpha_i\hat{U}^\dagger\,|\alpha_i\rangle$$
$$\left(\hat{U}^\dagger\hat{A}\hat{U}\right)\left(\hat{U}^\dagger\,|\alpha_i\rangle\right) = \alpha_i\left(\hat{U}^\dagger\,|\alpha_i\rangle\right)$$
$$\hat{A}(t)\left(\hat{U}^\dagger\,|\alpha_i\rangle\right) = \alpha_i\left(\hat{U}^\dagger\,|\alpha_i\rangle\right) \tag{6.144}$$

The last equation is clearly the eigenvalue equation for the operator $\hat{A}(t)$ with eigenvectors $\hat{U}^\dagger\,|\alpha_i\rangle$. The eigenvalues α_i are the same as those in the Schrödinger picture which is consistent with Postulate I because the possible results of a measurement of the observable A cannot depend upon the representation (picture). The eigenvectors in Equation 6.144 are, however, time-dependent. Thus, while the eigenvectors of the operator $\hat{A}$ in the Schrödinger picture are the time-independent kets $|\alpha_i\rangle$, in the Heisenberg picture the eigenvectors are the time-*dependent* kets $\hat{U}\,|\alpha_i\rangle$. In the Schrödinger picture the state vectors move while those in the Heisenberg representation are stationary. Thus, we must make a distinction between the state vector and

Table 6.1 Contrast between the Schrödinger and Heisenberg pictures. The time dependences are denoted by “fixed” for time-independent and “moving” for time-dependent

Entity	Significance	Schrödinger	Heisenberg
operator	observable	$\hat{A}$ fixed	$\hat{A}(t)$ moving
state vector	system state	$\lvert\Psi(t)\rangle$ moving	$\lvert\Psi\rangle$ fixed
eigenvectors	basis vectors	$\lvert\alpha_i\rangle$ fixed	$\hat{U}^\dagger\lvert\alpha_i\rangle$ moving

the eigenvectors. The time dependences of these quantities in each of the pictures are summarized in Table 6.1.

In the Schrödinger picture the time evolution of the quantum mechanical system is dictated by the TDSE, Equation 6.88. This is the equation of motion of the time-dependent state vector $|\Psi\rangle$. In the Heisenberg picture we require an equation of motion for the time-dependent operators $\hat{A}(t)$. To obtain this equation of motion we simply take the total time derivative of Equation 6.142. For simplicity, we assume the usual case in which the operator $\hat{A}(t)$ has no explicit time dependence so that $\partial\hat{A}(t)/\partial t \equiv 0$. Also, because we assume that the Hamiltonian operator does not contain the time explicitly it is not necessary to make any distinction between the Schrödinger and Heisenberg versions of this operator because $\hat{U}\hat{H}\hat{U}^\dagger = \hat{H}$ which is true because $\hat{H}$ commutes with itself. We have

$$\begin{aligned}\frac{d\hat{A}(t)}{dt} &= \frac{i\hat{H}}{\hbar}\left[e^{i\hat{H}(t-t_0)/\hbar}\hat{A}e^{-i\hat{H}(t-t_0)/\hbar}\right] \\ &\qquad - \left[e^{i\hat{H}(t-t_0)/\hbar}\hat{A}e^{-i\hat{H}(t-t_0)/\hbar}\right]\frac{i\hat{H}}{\hbar} \\ &= \frac{i}{\hbar}\left(\hat{H}\hat{A}(t) - \hat{A}(t)\hat{H}\right) \\ &= \frac{i}{\hbar}\left[\hat{H}, \hat{A}(t)\right] \qquad (6.145)\end{aligned}$$

Equation 6.145 is the Heisenberg equation of motion from which we see immediately that if $\hat{A}(t)$ commutes with the Hamiltonian, then it is a constant of the motion because its time derivative vanishes. In this case $\hat{H}$ and $\hat{A}(t)$ can have simultaneous eigenvectors, the physical consequence of which is that these two observables, energy and A, may be measured simultaneously. That is, the measurement of one does not interfere with the measurement of the other. Moreover, if we take $\hat{A}(t) = \hat{H}$, it is seen immediately that the (total) time derivative of the Hamiltonian vanishes, thus confirming energy conservation.

From the Heisenberg equation of motion, Equation 6.145, we can immediately derive the Ehrenfest theorem, Equation 6.121 (we again assume that the operator $\hat{A}(t)$ does not contain any explicit time dependence). Since the Heisenberg state vectors are fixed in time we simply take the expectation value of Equation 6.145 with the Heisenberg state vector $|\Psi\rangle$ and its complex conjugate. The left-hand side of Equation 6.145, $\langle d\hat{A}(t)/dt\rangle$, is simply

$$\left\langle \frac{d\hat{A}(t)}{dt} \right\rangle = \frac{d\langle \hat{A}(t) \rangle}{dt} \tag{6.146}$$

Next we determine the right-hand side, the expectation value of the commutator in the Schrödinger picture:

$$\begin{aligned}
\frac{i}{\hbar}\left\langle\left[\hat{H}, \hat{A}(t)\right]\right\rangle &= \frac{i}{\hbar}\langle\Psi|\left[\hat{H}, \hat{A}(t)\right]|\Psi\rangle \\
&= \frac{i}{\hbar}\langle\Psi|\left[\hat{H}, \hat{U}^\dagger\hat{A}\hat{U}\right]|\Psi\rangle \\
&= \frac{i}{\hbar}\langle\Psi|\left[\hat{H}\hat{U}^\dagger\hat{A}\hat{U} - \hat{U}^\dagger\hat{A}\hat{U}\hat{H}\right]|\Psi\rangle \\
&= \frac{i}{\hbar}\langle\Psi|\left[\hat{U}^\dagger\hat{U}\hat{H}\hat{U}^\dagger\hat{A}\hat{U} - \hat{U}^\dagger\hat{A}\hat{U}\hat{H}\hat{U}^\dagger\hat{U}\right]|\Psi\rangle \\
&= \frac{i}{\hbar}\left(\langle\Psi|\hat{U}^\dagger\right)\left[\hat{U}\hat{H}\hat{U}^\dagger\hat{A} - \hat{A}\hat{U}\hat{H}\hat{U}^\dagger\right]\left(\hat{U}|\Psi\rangle\right) \\
&= \frac{i}{\hbar}\langle\Psi(t)|\left[\hat{H}\hat{A} - \hat{A}\hat{H}\right]|\Psi(t)\rangle \\
&= \frac{i}{\hbar}\langle\Psi(t)|\left[\hat{H}, \hat{A}\right]|\Psi(t)\rangle
\end{aligned} \tag{6.147}$$

which, when equated to the result from Equation 6.146, is Equation 6.121, the Ehrenfest theorem.

As stated above, most problems in quantum physics are attacked using the Schrödinger picture. Why then even bother with the Heisenberg picture? Of course, there is the aesthetic beauty attendant to proving that the two pictures are equivalent. Another reason is that the Heisenberg picture makes the connection between classical and quantum physics clearer than does the Schrödinger picture. After all, wave functions and state vectors have no classical analog. On the other hand, the observables in classical physics are usually time-dependent quantities so the Heisenberg equation of motion for an observable (Hermitian operator) is indeed analogous. Moreover, there is a close connection between this equation and Hamilton's equations of classical motion as well as a relationship between the Poisson brackets of classical physics and the commutator of quantum physics. We will not pursue these correspondences further in this book, but clearly Bohr's correspondence principle is at work here. Let us examine the time evolution of the position and momentum operators for a particle of mass m under the influence of an arbitrary one-dimensional potential $U(x)$. The Hamiltonian in the Heisenberg picture is

$$\hat{H} = \frac{\hat{p}_x(t)^2}{2m} + U\{\hat{x}(t)\} \tag{6.148}$$

where we have placed a hat over x to emphasize its operator status. To use the Heisenberg picture we must compute the commutators $\left[\hat{H}, \hat{x}(t)\right]$ and $\left[\hat{H}, \hat{p}_x(t)\right]$ and insert them into Equation 6.145. An important point in this calculation is to note that the commutators in the Heisenberg picture have exactly the same form as in the Schrödinger picture (see Problem 7). We may therefore use the relations listed as Equations 6.42 and 6.43 for this computation. Thus

$$\left[\hat{x}(t), \frac{\hat{p}_x(t)^2}{2m}\right] = \frac{i\hbar}{2m}\frac{\partial\left\{\hat{p}_x(t)^2\right\}}{\partial x} \\ = i\hbar\frac{\hat{p}_x(t)}{m} \tag{6.149}$$

and

$$\left[\hat{p}_x(t), U\{\hat{x}(t)\}\right] = -i\hbar\frac{\partial U\{\hat{x}(t)\}}{\partial p_x(t)} \tag{6.150}$$

The Heisenberg equations of motion are then

$$\frac{d\hat{x}(t)}{dt} = \frac{\hat{p}_x(t)}{m} \tag{6.151}$$

and

$$\frac{d\hat{p}_x(t)}{dt} = -\frac{\partial U\{\hat{x}(t)\}}{\partial p_x(t)} \tag{6.152}$$

These are the familiar relations of nonrelativistic classical physics, the momentum is mass times velocity, and the time rate of change of the momentum is the force (Newton's second law).

The harmonic oscillator in the Heisenberg picture

We can illustrate the use of the Heisenberg picture by returning to an old friend, the harmonic oscillator. We will obtain the time dependences of the quantum mechanical operators $\hat{x}(t)$ and $\hat{p}_x(t)$ using this picture. We begin by applying Equation 6.152 to the potential energy function $U\{\hat{x}(t)\} = \frac{1}{2}m\omega^2\hat{x}(t)^2$. Of course, Equation 6.151 does not depend upon the potential energy. For simplicity of notation we eliminate the subscript on the momentum since this is a one-dimensional problem. The two equations of motion are therefore

$$\frac{d\hat{x}(t)}{dt} = \frac{\hat{p}(t)}{m} \tag{6.153}$$

and

$$\frac{d\hat{p}(t)}{dt} = -m\omega^2\hat{x}(t) \tag{6.154}$$

Uncoupling these two first-order differential equations we obtain two second-order equations,

$$\frac{d^2\hat{x}(t)}{dt^2} = -\omega^2\hat{x}(t) \tag{6.155}$$

and

$$\frac{d^2\hat{p}(t)}{dt^2} = -\omega^2\hat{p}(t) \tag{6.156}$$

the solutions to which are

$$\hat{x}(t) = \hat{x}(0)\cos\omega t + \frac{\hat{p}(0)}{m\omega}\sin\omega t \tag{6.157}$$

and

$$\hat{p}(t) = -m\omega\hat{x}(0)\sin\omega t + \hat{p}(0)\cos\omega t \tag{6.158}$$

where the constants of integration have been evaluated at $t = 0$, that is, $\hat{x}(0) = \hat{x}(t = 0)$ and $\hat{p}(0) = \hat{p}(t = 0)$.

We see then that the Heisenberg operators oscillate exactly as the classical quantities $x(t)$ and $p(t)$. In this context, however, they are not classical quantities, they are quantum mechanical operators, Heisenberg operators. In contrast, the operators $\hat{x}(t = 0)$ and $\hat{p}(t = 0)$ obtained from the boundary conditions are stationary operators. They are the Schrödinger operators. Moreover, the commutator $[\hat{x}(t), \hat{p}(t)] = i\hbar$ and it is independent of time (see Problem 11).

6.6 Spreading of Wave Packets

6.6.1 Spreading in the Heisenberg Picture

Because the Heisenberg operators are time-dependent, they are ideally suited for reexamining the spreading of wave packets as in Section 4.5. We examine Case I from that section, the case of a Gaussian wave packet subject to no external forces, a free particle. Recall that in this case we began with a minimum uncertainty wave packet and found that it spreads in time. We can employ Equation 6.109 with $A \rightarrow x(t)$ and $B \rightarrow \hat{x}(0)$ (which was called x_0 in Section 4.5). We therefore require the commutator $[\hat{x}(t), \hat{x}(0)]$. Before evaluating this commutator we must first find the equations of motion for a free particle in the Heisenberg picture.

Using Equations 6.151 and 6.152 we find that

$$\frac{d\hat{x}(t)}{dt} = \frac{\hat{p}(t)}{m} \quad \text{and} \quad \frac{d\hat{p}(t)}{dt} = 0 \tag{6.159}$$

which lead to

$$\hat{x}(t) = \hat{x}(0) + \frac{\hat{p}(0)}{m}t \quad \text{and} \quad \hat{p}(t) = \hat{p}(0) \tag{6.160}$$

The commutator $[\hat{x}(t), \hat{x}(0)]$ is easily found to be

$$\begin{aligned}
[\hat{x}(t), \hat{x}(0)] &= \left[\left\{\hat{x}(0) + \frac{\hat{p}(0)}{m}t\right\}, \hat{x}(0)\right] \\
&= [\hat{p}_x(0), \hat{x}(0)]\frac{t}{m} \\
&= -\frac{i\hbar}{m}t
\end{aligned} \tag{6.161}$$

We can use this result in Equation 6.109 to obtain the standard deviation, the uncertainty, as a function of time $\Delta x(t)$. Let us clarify the meaning of the quantity ΔA in the present context. It is the standard deviation of the wave packet as a function of time beyond the initial standard deviation which at $t = 0$ is $\Delta x(0) = \Delta x_0$. Therefore, we will call the uncertainty in position that corresponds to ΔA in Equation 6.109 $\Delta x'(t)$ with the understanding that the $\Delta x(t)$ of Equation 4.74 is given by

$$\Delta x(t)^2 = \Delta x'(t)^2 + \Delta x_0^2 \tag{6.162}$$

Note that it is the variances, the squares of the standard deviations, that add, not the standard deviations themselves. We have then

$$\begin{aligned}
\left\{\Delta x'(t)\right\}^2 \{\Delta x(0)\}^2 &\geq -\frac{1}{4}\left\langle -\frac{i\hbar}{m}t\right\rangle^2 \\
&\geq \left(\frac{\hbar}{2m}\right)^2 t^2
\end{aligned} \tag{6.163}$$

and

$$\left\{\Delta x'(t)\right\}^2 \{\Delta x(0)\}^2 \geq -\frac{1}{4}\left\langle -\frac{i\hbar}{m}t\right\rangle^2$$

$$\Delta x'(t)^2 \geq \frac{1}{\Delta x(0)^2}\left(\frac{\hbar}{2m}\right)^2 t^2 \tag{6.164}$$

At $t = 0$ we had a minimum uncertainty wave packet so that $\Delta x'(t = 0) = 0$. Therefore, we must use the equal sign in Equation 6.164. Inserting this into Equation 6.162 we have

$$\Delta x(t)^2 = \frac{1}{\Delta x(0)^2}\left(\frac{\hbar}{2m}\right)^2 t^2 + \Delta x(0)^2 \tag{6.165}$$

$$= \Delta x(0)^2\left\{1 + \frac{1}{\Delta x(0)^4}\left(\frac{\hbar}{2m}\right)^2 t^2\right\} \tag{6.166}$$

from which we obtain

$$\Delta x(t) = \Delta x_0\sqrt{1 + \left(\frac{\hbar}{2m\Delta x_0^2}\right)^2 t^2} \tag{6.167}$$

which is indeed the same as Equation 4.74. As noted in Section 4.5, this time dependence of the uncertainty shows that a Gaussian wave packet subjected to no forces will rapidly expand in time.

When studying Case III, the case of a Gaussian wave packet subjected to a harmonic oscillator force, it was shown that the wave packet oscillates, but does not change shape. Thus, there should be no time dependence of the uncertainty product $\Delta x(t)\,\Delta p(t)$. We can verify this by finding the uncertainty product using the Heisenberg equations of motion, Equations 6.157 and 6.158.

First, the packet used in Case III, the wave function of which at $t = 0$, was given by Equation 4.95, which we reproduce here, is

$$\Psi(x, 0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\alpha^2(x-x_0)^2/2} \tag{6.168}$$

has initial momentum zero and initial displacement x_0. Therefore, the expectation values of momentum and position at $t = 0$ are given by

$$\langle \hat{x}(0)\rangle = x_0 \quad \text{and} \quad \langle \hat{p}(0)\rangle = 0 \tag{6.169}$$

The uncertainties are then

$$\Delta\hat{x}(t)^2 = \left\langle \hat{x}(t)^2\right\rangle - \langle \hat{x}(t)\rangle^2 \quad \text{and} \quad \Delta\hat{p}(t)^2 = \left\langle \hat{p}(t)^2\right\rangle - \langle \hat{p}(t)\rangle^2 \tag{6.170}$$

where, from Equation 6.158,

$$\langle \hat{p}(t) \rangle = -m\omega \langle \hat{x}(0) \rangle \sin \omega t \tag{6.171}$$

and, from Equation 6.157,

$$\langle \hat{x}(t) \rangle = \langle \hat{x}(0) \rangle \cos \omega t = x_0 \cos \omega t \tag{6.172}$$

Also,

$$\Delta \hat{x}(0)^2 = \left\langle \hat{x}(0)^2 \right\rangle - x_0^2 \quad \text{and} \quad \Delta \hat{p}(0)^2 = \left\langle \hat{p}(0)^2 \right\rangle \tag{6.173}$$

Next we compute $\left\langle \hat{p}(t)^2 \right\rangle$:

$$\begin{aligned} \left\langle \hat{p}(t)^2 \right\rangle &= \left\langle \hat{p}(0)^2 \right\rangle \cos^2 \omega t + m^2\omega^2 \left\langle \hat{x}(0)^2 \right\rangle \\ &\quad - m\omega \sin \omega t \cos \omega t \left\langle \hat{p}(0)\hat{x}(0) + \hat{x}(0)\hat{p}(0) \right\rangle \\ &= \left\langle \hat{p}(0)^2 \right\rangle \cos^2 \omega t + m^2\omega^2 \left\langle \hat{x}(0)^2 \right\rangle \\ &\quad - m\omega \sin \omega t \cos \omega t \left\langle 2\hat{x}(0)\hat{p}(0) - i\hbar \right\rangle \end{aligned} \tag{6.174}$$

where we have used the commutator $[\hat{x}(0), \hat{p}(0)] = i\hbar$.

Now, it can be shown that $\langle 2\hat{x}(0)\hat{p}(0) - i\hbar \rangle = 0$ (see Problem 12) so that

$$\Delta \hat{p}(t)^2 = \left\langle \hat{p}(0)^2 \right\rangle \cos^2 \omega t + m^2\omega^2 \left\langle \hat{x}(0)^2 \right\rangle \sin^2 \omega t - m^2\omega^2 \langle \hat{x}(0) \rangle^2 \sin^2 \omega t \tag{6.175}$$

which may be written in terms of the uncertainties

$$\begin{aligned} \Delta \hat{p}(t)^2 &= \Delta \hat{p}(0)^2 \cos^2 \omega t + \left\{ \left\langle \hat{x}(0)^2 \right\rangle - \langle \hat{x}(0) \rangle^2 \right\} m^2\omega^2 \sin^2 \omega t \\ &= \Delta \hat{p}(0)^2 \cos^2 \omega t + \Delta \hat{x}(0)^2 m^2\omega^2 \sin^2 \omega t \end{aligned} \tag{6.176}$$

Because, however, the wave packet had minimum uncertainty at $t = 0$ we must have

$$\Delta \hat{x}(0)^2 \Delta \hat{p}(0)^2 = \frac{\hbar^2}{4} \tag{6.177}$$

which we may use to eliminate $\Delta \hat{p}(0)$ from Equation 6.176 leading to

$$\Delta \hat{p}(t)^2 = \frac{\hbar^2}{4\Delta \hat{x}(0)^2} \cos^2 \omega t + \Delta \hat{x}(0)^2 m^2\omega^2 \sin^2 \omega t \tag{6.178}$$

Now, it is easily shown that (see Problem 14)

$$\Delta \hat{x}(0)^2 = \frac{1}{2\alpha^2} \tag{6.179}$$

so that (using $\alpha^2 = m\omega/\hbar$)

$$\Delta\hat{p}\,(t)^2 = \frac{\hbar^2}{4}\left(2\alpha^2\right)\cos^2\omega t + \left(\frac{1}{2\alpha^2}\right)m^2\omega^2\sin^2\omega t$$
$$= \frac{\hbar^2\alpha^2}{2} \tag{6.180}$$

Returning now to $\Delta x\,(t)$ we have

$$\begin{aligned}\Delta\hat{x}\,(t)^2 &= \left\langle \hat{x}\,(t)^2\right\rangle - \langle\hat{x}\,(t)\rangle^2 \\ &= \left\langle \hat{x}\,(0)^2\right\rangle\cos^2\omega t + \frac{\left\langle \hat{p}\,(0)^2\right\rangle}{m^2\omega^2}\sin^2\omega t - \langle\hat{x}\,(0)\rangle^2\cos^2\omega t \\ &= \left\{\left\langle \hat{x}\,(0)^2\right\rangle - \langle\hat{x}\,(0)\rangle^2\right\}\cos^2\omega t + \left(\frac{\hbar^2\alpha^2}{2}\right)\frac{1}{\hbar^2\alpha^4}\sin^2\omega t \\ &= \Delta\hat{x}\,(0)^2\cos^2\omega t + \frac{1}{2\alpha^2}\sin^2\omega t \\ &= \frac{1}{2\alpha^2}\end{aligned} \tag{6.181}$$

where we have again used the fact that $\langle 2\hat{x}\,(0)\,\hat{p}\,(0) - i\hbar\rangle = 0$ and used Equation 6.179. Combining Equations 6.180 and 6.181 we can write the time dependence of the uncertainty product $\Delta\hat{x}\,(t)\,\Delta\hat{p}\,(t)$. We have

$$\Delta\hat{x}\,(t)\,\Delta\hat{p}\,(t) = \frac{\hbar}{2} \tag{6.182}$$

which is independent of time.

These results show that not only is the uncertainty product constant in time (see Problem 11), but so too are the individual uncertainties. That is, neither $\Delta\hat{x}\,(t)$ nor $\Delta\hat{p}\,(t)$ contains the time. This means that the spread in both position and momentum remain constant for a Gaussian packet subject to a harmonic force. Of course, we have already deduced this in Section 4.5 (see Equation 4.106), but the use of the Heisenberg picture presents a more nearly classical approach.

6.6.2 Spreading in the Schrödinger Picture

Because the time evolution operator converts a wave function at a fixed time to its time-dependent form, the new wave function is necessarily a representation in the Schrödinger picture. As an exercise in the use of the time evolution operator, in this section we will use it to derive the probability densities for the free particle wave packet and the wave packet under the influence of a constant force, Cases I and II in Section 4.5. Calculation of the time evolution operator for a harmonic oscillator potential is beyond the intended scope of this book so we defer reexamination of

Case III until Section 7.2 when we will have the tools to circumvent the use of this operator.

The Free Particle

It was shown in Section 6.3.2, Postulate VI that the state ket $|\Psi(x,t)\rangle$ may be obtained by applying the time evolution operator, $e^{-i\hat{H}(t-t_0)/\hbar}$ (see Equation 6.116) to the state ket at a fixed time $|\Psi(x,t_0)\rangle$. Therefore, if we consider the free particle Gaussian wave packet (Case I of Section 4.5.1) we may apply the time evolution operator to the wave function at $t=0$ and compare the result with that obtained in Section 4.5.1. In terms of wave functions

$$\begin{aligned}\Psi(x,t) &= \langle x\,|\Psi(x,t)\rangle \\ &= e^{-i\hat{p}^2 t/(2m\hbar)}\Psi(x,0)\end{aligned} \tag{6.183}$$

The first-order of business is to convert the initial momentum wave function $\Phi(p,0)$ of Equation 4.66 to the coordinate space wave function $\Psi(x,0)$. This can be done by taking the Fourier transform. The present calculation will be simplified by using the wave function in the form of the Fourier transformed wave functions given in Equations 4.60 and 4.61. Moreover, it was assumed in Section 4.5.1 that the initial state has $p(0)=p_0$ and $x(0)=0$, but the calculation can be further simplified by assuming that both $p(0)$ and $x(0)$ vanish. Comparison with the previous results will not suffer from this simplification. The initial wave function in coordinate space is therefore

$$\Psi(x,0) = \frac{1}{\pi^{1/4}}\left(\frac{1}{2^{1/4}\sqrt{\Delta x_0}}\right)e^{-x^2/4\Delta x_0^2} \tag{6.184}$$

The second thing that we must do is to determine the action of the time evolution operator $\hat{U}(t,0)$ on $\Psi(x,0)$. Letting $p\to(\hbar/i)\,\partial/\partial x$ to convert $\hat{U}(t,0)$ to coordinate space representation, this operator is

$$\begin{aligned}\hat{U}(t,0) &= e^{-i\hat{p}^2 t/(2m\hbar)} \\ &= \exp\left(\frac{i\hbar t}{2m}\frac{\partial^2}{\partial x^2}\right)\end{aligned} \tag{6.185}$$

which is difficult to apply to an arbitrary wave function. Because, however, the initial wave packet has Gaussian form, it has been shown that the action of $\hat{U}(t,0)$ can be deduced using an ingenious mathematical trick [1]. Letting $\Delta x_0^2 = z$ to simplify Equation 6.184, it can be verified that

$$\frac{\partial^2}{\partial x^2}\left[\frac{1}{\sqrt{z}}e^{-x^2/4z}\right] = \frac{\partial}{\partial z}\left[\frac{1}{\sqrt{z}}e^{-x^2/4z}\right] \tag{6.186}$$

Expressing $\Psi(x,0)$ in terms of z and Δx_0 we have

$$\Psi(x,0) = \frac{\sqrt{\Delta x_0}}{(2\pi)^{1/4}} \frac{1}{\sqrt{z}} e^{-x^2/4z} \tag{6.187}$$

Now, using the identity given in Equation 6.186 we are in a position to apply the time evolution operator to $\Psi(x,0)$:

$$\begin{aligned}\hat{U}(t,0)\Psi(x,0) &= \frac{\sqrt{\Delta x_0}}{(2\pi)^{1/4}} \exp\left(\frac{i\hbar t}{2m}\frac{\partial^2}{\partial x^2}\right)\left[\frac{1}{\sqrt{z}}e^{-x^2/4z}\right] \\ &= \frac{\sqrt{\Delta x_0}}{(2\pi)^{1/4}}\left[\exp\left(\frac{i\hbar t}{2m}\frac{\partial}{\partial z}\right)\right]\left[\frac{1}{\sqrt{z}}e^{-x^2/4z}\right]\end{aligned} \tag{6.188}$$

Comparing the last line of Equation 6.188 with the translation operator as given in Equation L.11 we see that $i\hbar t/(2m) = x_0$, the distance by which the translation is made. We see then that the action of the free particle time development operator, Equation 6.185, operating on an arbitrary function $f(x)$ is

$$\begin{aligned}\hat{U}(t,0) f(x) &= e^{-i\hat{p}^2 t/(2m\hbar)} f(x) \\ &= \exp\left[\left(-\frac{i\hbar t}{2m}\right)\frac{\partial}{\partial x}\right] f(x) \\ &= f\left(x + \frac{i\hbar t}{2m}\right)\end{aligned} \tag{6.189}$$

Letting z return to Δx_0^2 we see that $\Psi(x,t)$ is found by letting $z \to \Delta x_0^2 + i\hbar t/(2m)$ after applying the translation operator. We have

$$\begin{aligned}\Psi(x,t) &= \frac{\sqrt{\Delta x_0}}{(2\pi)^{1/4}} \frac{1}{\sqrt{\Delta x_0^2 + \frac{i\hbar t}{2m}}} \exp\left[-\frac{x^2}{4\left(\Delta x_0^2 + \frac{i\hbar t}{2m}\right)}\right] \\ &= \frac{1}{(2\pi)^{1/4}\sqrt{\Delta x_0}} \frac{1}{\sqrt{1 + \frac{i\hbar t}{2m\Delta x_0^2}}} \exp\left[-\frac{x^2}{4\left(\Delta x_0^2 + \frac{i\hbar t}{2m}\right)}\right]\end{aligned} \tag{6.190}$$

Setting $\Delta x_0 = 1/\left(\sqrt{2}\beta\right)$ in Equation 6.190 and $p_0 = 0$ in Equation 4.68 makes it clear that the present treatment is consistent with our earlier formulation.

Constant Field

In Section 4.5.2, Case II, a wave packet under the influence of a constant field, we derived the probability density and the spreading of the packet in momentum space. In this section we will treat the same problem, but we will use the time evolution operator and derive the probability density in coordinate space. For simplicity, we begin with the initial wave function given in Equation 6.184. We will follow the treatment of Robinett [2].

The Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} - Fx \tag{6.191}$$

so the time evolution operator is

$$\hat{U}(t,0) = \exp\left[-i\left(\frac{\hat{p}^2}{2m} - Fx\right)\left(\frac{t}{\hbar}\right)\right] \tag{6.192}$$

Because $\hat{p}$ and x are operators we cannot naively apply the usual rules of algebra to this exponential expression. Rather, we must use the BCH formula of Appendix L in the form of Equation L.1 and L.2:

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{C}} \tag{6.193}$$

where

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2}\left[\hat{A}, \hat{B}\right] + \frac{1}{12}\left\{\left[\left[\hat{A}, \hat{B}\right], \hat{B}\right] + \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right]\right\} + \cdots \tag{6.194}$$

Notice that when one of the commutators vanishes, all subsequent commutators vanish. In the special case in which $\left[\hat{A}, \hat{B}\right] = 0$ the usual rules of exponents apply. Unfortunately, in the present case $\left[\hat{A}, \hat{B}\right] \neq 0$ so we must use Equation 6.194.

Letting

$$\hat{A} = -i\frac{tFx}{\hbar} \quad \text{and} \quad \hat{B} = -i\frac{\hat{H}t}{\hbar} = -i\frac{t}{\hbar}\left(\frac{\hat{p}^2}{2m} - Fx\right) \tag{6.195}$$

so that

$$\left[\hat{A}, \hat{B}\right] = -i\frac{Ft^2}{m\hbar}\hat{p} \quad \text{and} \quad \left[\left[\hat{A}, \hat{B}\right], \hat{B}\right] = -i\frac{F^2t^3}{m\hbar} = \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] \tag{6.196}$$

Because $\left[\left[\hat{A}, \hat{B}\right], \hat{B}\right] \propto \hat{I}$, the remaining commutators vanish. Therefore,

$$\hat{C} = -i\frac{\hat{p}^2 t}{2m\hbar} - i\frac{Ft^2}{2m\hbar}\hat{p} - \frac{1}{6}\left(i\frac{F^2t^3}{m\hbar}\right) \tag{6.197}$$

To find the time development operator for a wave packet subjected to a constant force we multiply Equation 6.193 on the left by $e^{-\hat{A}}$ to obtain

$$\begin{aligned} e^{-i\hat{H}t/\hbar} &= e^{\hat{B}} \\ &= e^{-\hat{A}}e^{\hat{C}} \\ &= e^{iFtx/\hbar}\exp\left[-i\frac{\hat{p}^2t}{2m\hbar} - i\frac{Ft^2}{2m\hbar}\hat{p} - \frac{1}{6}\left(i\frac{F^2t^3}{m\hbar}\right)\right] \\ &= \exp\left[i\frac{Ft}{\hbar}\left(x - \frac{Ft^2}{6m}\right)\right]\cdot\exp\left[-i\frac{Ft^2}{2m\hbar}\hat{p}\right]\cdot\exp\left[-i\frac{\hat{p}^2t}{2m\hbar}\right] \end{aligned} \tag{6.198}$$

An operator ($\hat{p}$ in this case) commutes with any function of that operator, so the exponential containing $\hat{p}$ may be written as a simple product.

Now, this time evolution operator looks somewhat formidable, but we have already done most of the work required to apply it. The exponential containing $\hat{p}^2$ is simply the free particle time evolution operator, Equation 6.189. As shown above, it causes a free particle to spread in time. This spreading is effected by making the conversion $\Delta x_0^2 \to \Delta x_0^2 + i\hbar t/(2m)$ in Equation 6.184. Moreover, the exponential that contains the first power of the momentum is also a translation operator (see above and Appendix L). This operator causes the conversion $x \to x - Ft^2/(2m\hbar)$. The effect of the time development operator on the initial wave function, Equation 6.184, results in Equation 6.190 so we have

$$\begin{aligned} \Psi(x,t) &= \exp\left[i\frac{Ft}{\hbar}\left(x - \frac{Ft^2}{6m}\right)\right]\cdot\exp\left[-i\frac{Ft^2}{2m\hbar}\hat{p}\right] \\ &\quad\times\frac{1}{(2\pi)^{1/4}\sqrt{\Delta x_0}}\frac{1}{\sqrt{1+\dfrac{i\hbar t}{2m\Delta x_0^2}}}\exp\left[-\frac{x^2}{4\left(\Delta x_0^2 + \dfrac{i\hbar t}{2m}\right)}\right] \\ &= \exp\left[i\frac{Ft}{\hbar}\left(x - \frac{Ft^2}{6m}\right)\right]\frac{1}{(2\pi)^{1/4}\sqrt{\Delta x_0}}\frac{1}{\sqrt{1+\dfrac{i\hbar t}{2m\Delta x_0^2}}} \\ &\quad\times\exp\left[-\frac{\left(x - \dfrac{Ft^2}{2m\hbar}\right)^2}{4\Delta x_0^2\left(1+\dfrac{i\hbar t}{2m\Delta x_0^2}\right)}\right] \end{aligned} \tag{6.199}$$

Notice that because x and $\hat{p}$ do not commute, the exponential operator in Equation 6.198 remains to the left of the exponential operators containing $\hat{p}$. As a consequence, the x in that operator does not get shifted by the other operators.

Squaring Equation 6.199, the probability density is

$$
\begin{aligned}
|\Psi(x,t)|^2 &= \frac{1}{\sqrt{2\pi}\Delta x_0} \frac{1}{\sqrt{1+\left(\frac{t}{t_0}\right)^2}} \exp\left[-\frac{\left(x-\frac{Ft^2}{2m\hbar}\right)^2}{2\Delta x_0^2\left(1+\left(\frac{t}{t_0}\right)^2\right)}\right] \\
&= \frac{1}{\sqrt{2\pi}\Delta x(t)} \exp\left[-\frac{\left(x-\frac{Ft^2}{2m\hbar}\right)^2}{2\Delta x(t)^2}\right]
\end{aligned}
\tag{6.200}
$$

where, as in Section 4.5,

$$
t_0 = \frac{2m}{\hbar}\Delta x_0^2 \quad \text{and} \quad \Delta x(t) = \Delta x_0\sqrt{1+\left(\frac{t}{t_0}\right)^2} \tag{6.201}
$$

Clearly Equation 6.201 is identical with the result obtained previously using Fourier transforms, Equation 4.94.

6.7 Retrospective

While a great deal of time and effort has been spent in this chapter on the properties of operators, especially Hermitian operators, the most important point for understanding quantum physics is the introduction of the postulates and their consequences. Although the discussion of the postulates may seem rather abstract and, in some cases, off the point of the chapter, the introduction of quantum mechanical concepts within the framework of abstract vector spaces makes it possible to reexamine problems treated in earlier chapters of this book with new insight. Moreover, once having mastered the formulation of quantum mechanics within the framework of vector spaces, many problems become simpler to solve, a good example being the harmonic oscillator as formulated in the next chapter of this book.

While the Schrödinger picture is the most often used in quantum mechanical calculations at the level of this book, the Heisenberg picture provides a clearer link between classical and quantum physics. This is because the time-dependent operators (the observables) of the Heisenberg picture are closely related to their classical analogs, while the wave functions of the Schrödinger picture have no classical counterpart. The equivalence of the two pictures should make the results obtained using the Schrödinger picture more credible to the student, especially the first time around the quantum mechanical block.

6.8 References

1. S. M. Blinder, "Evolution of a Gaussian wavepacket," Am. J. Phys., **36**, 525-526 (1968).
2. R. W. Robinett, "Quantum mechanical time-development operator for the uniformly accelerated particle," Am. J. Phys., **64**, 803-808 (1996).

Problems

1. Show that the unit vectors $1/\sqrt{2}\,(\hat{\boldsymbol{\imath}}+\hat{\boldsymbol{\jmath}})$; $1/\sqrt{2}\,(\hat{\boldsymbol{\imath}}-\hat{\boldsymbol{\jmath}})$; $\hat{\boldsymbol{k}}$ given in Equation 6.3 constitute an orthonormal basis set.
2. Show that $\left[\hat{A},\hat{B}^{-1}\right]=-\hat{B}^{-1}\left[\hat{A},\hat{B}\right]\hat{B}^{-1}$. Begin with $\left[\hat{A},\hat{B}\hat{B}^{-1}\right]=\left[\hat{A},\hat{I}\right]=0$.
3. Show that the product of two Hermitian operators $\hat{A}$ and $\hat{B}$ is non-Hermitian unless $\left[\hat{A},\hat{B}\right]=0$.
4. Show that the expectation value of a Hermitian operator is real.
5. Show that the projection operator is Hermitian.
6. For the time evolution operator $e^{-i\hat{H}t/\hbar}$

   (a) Show that the eigenvectors are the same as those of the Hamiltonian.
   (b) What are the eigenvalues of $e^{-i\hat{H}t/\hbar}$?
   (c) Are the eigenvalues of $e^{-i\hat{H}t/\hbar}$ necessarily real? If not, why not?

7. Show that if the Schrödinger operators $\hat{A}$ and $\hat{B}$ obey $\left[\hat{A},\hat{B}\right]=\hat{C}$, then the Heisenberg operators $\hat{A}(t)$ and $\hat{B}(t)$ obey $\left[\hat{A}(t),\hat{B}(t)\right]=\hat{C}(t)$.
8. Show that the eigenvectors of the Hamiltonian are also eigenvectors of the time evolution operator $e^{-i\hat{H}t/\hbar}$. What are the eigenvalues?
9. Verify Equation 6.157 for the time dependence of the $\hat{x}(t)$ for the harmonic oscillator using the fundamental definition of a Heisenberg operator in terms of the time evolution operator and the equivalent Schrödinger operator. That is, show that

$$\begin{aligned}\hat{x}(t)&=e^{i\hat{H}t/\hbar}\hat{x}(t=0)\,e^{-i\hat{H}t/\hbar}\\&=\hat{x}(t=0)\cos\omega t+\frac{\hat{p}_x(t=0)}{m\omega}\sin\omega t\end{aligned}$$

   The Baker–Campbell–Hausdorff lemma, which will be needed, is

$$e^{i\lambda\hat{C}}\hat{A}e^{-i\lambda\hat{C}}=\hat{A}+i\lambda\left[\hat{C},\hat{A}\right]+\frac{i^2\lambda^2}{2!}\left[\hat{C},\left[\hat{C},\hat{A}\right]\right]+\cdots$$

10. Using $[x,\hat{p}_x]=i\hbar\hat{I}$ and mathematical induction show that

$$\left[x,\hat{p}_x^n\right]=i\hbar n\hat{p}_x^{n-1}$$

11. Show that the commutator $[\hat{x}(t),\hat{p}(t)]=i\hbar$ for the harmonic oscillator.