Finally, we note that in terms of the wave number k the ground state wave function is

$$A_0(k) = \frac{1}{\pi^{1/4} \sqrt{\alpha}} e^{-k^2/(2\alpha^2)}$$
(4.54)

and the uncertainty in the wave number  $\Delta k$  is

$$\Delta k = \frac{1}{\sqrt{2}}\alpha\tag{4.55}$$

so, in terms of x and k, the uncertainty relation is

$$\Delta x \Delta k = \begin{pmatrix} 1\\\sqrt{2\alpha} \end{pmatrix} \begin{pmatrix} 1\\\sqrt{2} \alpha \end{pmatrix}$$
(4.56)

$$=\frac{1}{2}$$
 (4.57)

# 4.5 Motion of a Wave Packet

We wish to investigate the fate of a wave packet with increasing time. To do this we must specify either  $\Psi(x, 0)$  or  $\Phi(p, 0)$  and find the time-dependent wave functions. To be definite we will assume that the initial wave functions are Gaussians. Our reasoning is that we already know that if the momentum wave function is Gaussian, the coordinate wave function is also Gaussian. Moreover, the values of the definite integrals involving Gaussian functions are known. Now, let us be clear that because we are starting with a Gaussian does not mean that we are starting with the ground state of the harmonic oscillator, an eigenstate (see Problem 22 of Chapter 3). How can we imagine the creation of such a packet? There is more than one way. Suppose that we have a bound system, for example a particle subjected to a harmonic oscillator potential. Suppose further that the particle is not in an eigenstate, but that the wave function is a Gaussian. This means that the constant  $\alpha = \sqrt{m\omega/\hbar}$  is not present in the exponent in the wave function. If the constant analogous to  $\alpha$  is designated  $\beta$  with the stipulation that  $\beta \neq \alpha$ , then the initial Gaussian wave packet cannot be an eigenfunction of the harmonic oscillator. There is another method of creating an initial Gaussian wave packet that is not the ground state wave function, in this case even if the system is initially in the ground state. This will be explained below. Our initial wave functions can be represented as linear combinations of the eigenstates of the harmonic oscillator. (Indeed, it can be represented as a linear combination of the eigenstates of any Hamiltonian provided the potential energy has the same boundary conditions as the harmonic oscillator potential.)

To create the initial conditions, we imagine a particle that is initially subjected to a harmonic oscillator potential and at t = 0 is described by a momentum wave function  $\Phi(p, 0)$  and a coordinate wave function  $\Psi(x, 0)$  that are Fourier

#### 4.5 Motion of a Wave Packet

transforms of each other. We specify, however, that they are each some form of Gaussian, but not the ground state of a harmonic oscillator. Physically, we may imagine the particle is attached to a spring and oscillating, but not in any eigenstate of the harmonic oscillator Hamiltonian. Thus, our Gaussian wave packet has been *created* while under the influence of a harmonic oscillator potential. At t = 0 we investigate the fate of the packet under three different circumstances.

- Case I. The spring is cut and nothing is done thereafter (it is a free packet/particle).
- Case II. The spring is cut and a constant field is turned on at t = 0.
- Case III. Nothing is done. That is, the packet remains under the influence of the spring.

In our treatment of these three cases we will tailor our initial Gaussian packet for computational convenience of the particular case. Before doing this we write the wave functions in coordinate space and momentum space for a general Gaussian packet. That is, suppose we imagine a Gaussian wave packet that is displaced from the origin by an amount  $x_0$  and given initial momentum  $p_0$ . The wave functions are Fourier transforms of each other and are given by

$$\Psi(x,0) = \frac{\sqrt{\beta}}{\pi^{1/4}} e^{-\beta^2 (x-x_0)^2/2} \cdot e^{ip_0 x/\hbar}$$
(4.58)

and

$$\Phi(p,0) = \frac{1}{\pi^{1/4} \sqrt{\beta\hbar}} e^{-(p-p_0)^2/2\beta^2\hbar^2} \cdot e^{-ipx_0/\hbar}$$
(4.59)

where we have used the constant  $\beta$  (rather than  $\alpha$  as defined in Equation 3.25) to emphasize that, even though it has the appearance of the ground state eigenfunction of the harmonic oscillator, the system is *not* in an eigenstate. It is easily shown that for these wave packets  $\Delta x_0 = 1/(\sqrt{2\beta})$  and  $\Delta p_0 = \beta \hbar/\sqrt{2}$  (see Problem 6). We may therefore write Equations 4.58 and 4.59 in terms of the uncertainties  $\Delta x_0$  and  $\Delta p_0$ :

$$\Psi(x,0) = \frac{1}{\pi^{1/4}} \begin{pmatrix} 1\\ 2^{1/4}\sqrt{\Delta x_0} \end{pmatrix} e^{-(x-x_0)^2/4\Delta x_0^2} \cdot e^{ip_0 x/\hbar}$$
(4.60)

$$\Phi(p,0) = \frac{1}{\pi^{1/4}} \begin{pmatrix} 1\\ 2^{1/4}\sqrt{\Delta p_0} \end{pmatrix} e^{-(p-p_0)^2/4\Delta p_0^2} \cdot e^{-ipx_0/\hbar}$$
(4.61)

Equations 4.60 and 4.61 illustrate an important property of Fourier transforms of Gaussian wave packets. Their uncertainties are equal in the sense that they occur in precisely the same form in each  $\Psi(x, 0)$  and  $\Phi(p, 0)$ . An alternative way of saying this is that if  $(x - x_0)$  and  $(p - p_0)$  are measured in units of their respective uncertainties, then the functions have decreased by the same amount. For example,

if  $(x - x_0) = 2\Delta x$ , then  $\Psi(x, 0)$  has decreased by one *e*-fold. In order for  $\Phi(p, 0)$  to decrease by one *e*-fold requires  $(p - p_0) = 2\Delta p$ .

It is actually more useful to have the absolute squares of  $\Psi(x, 0)$  and  $\Phi(p, 0)$  in terms of  $\Delta x_0$  and  $\Delta p_0$  at our disposal. They are

$$|\Psi(x,0)|^{2} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1\\ \Delta x_{0} \end{pmatrix} e^{-(x-x_{0})^{2}/2\Delta x_{0}^{2}}$$
(4.62)

$$|\Phi(p,0)|^{2} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1\\ \Delta p_{0} \end{pmatrix} e^{-(p-p_{0})^{2}/2\Delta p_{0}^{2}}$$
(4.63)

In what follows we will be interested in finding the time dependence of the uncertainties. It is a simple matter to include the time in the last two equations. We have

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{2\pi}} \left( \frac{1}{\Delta x(t)} \right) e^{-(x-x_{0})^{2}/2[\Delta x(t)]^{2}}$$
(4.64)

$$|\Phi(p,t)|^{2} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1\\ \Delta p(t) \end{pmatrix} e^{-(p-p_{0})^{2}/2[\Delta p(t)]^{2}}$$
(4.65)

## 4.5.1 Case I. The Free Packet/Particle

We choose to cut the spring at a time such that  $x_0 = 0$ . The packet will then have nonzero average momentum  $p_0$ . The Gaussian packet in momentum space at t = 0is therefore (see Equation 4.59)

$$\Phi(p,0) = \frac{1}{\pi^{1/4} \sqrt{\beta \hbar}} e^{-(p-p_0)^2/2\beta^2 \hbar^2}$$
(4.66)

Let us first ask what we expect. Certainly we expect the packet to propagate in the direction of  $p_0$ , +x or -x. We also expect the packet to change shape. The mathematics will tell us exactly how the packet propagates and how it reshapes after it is free. On the other hand, being a free particle we expect no change in the momentum so that the initial spread in momentum  $\Delta p$  cannot change in time.

First we will find the wave function in coordinate space  $\Psi(x, t)$ . Inserting  $\Phi(p, 0) = \phi(p)$  in Equation 4.34 we have

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}\pi^{1/4}\sqrt{\beta\hbar}} \int_{-\infty}^{\infty} e^{-(p-p_0)^2/(2\beta^2\hbar^2)} e^{ipx/\hbar} e^{-ip^2t/(2m\hbar)} dp \qquad (4.67)$$

Now, there is some unpleasant algebra in the exponent, but it is straightforward to complete the square and integrate. The result is

$$\Psi(x,t) = \frac{\beta^{1/2}}{\pi^{1/4}} \frac{1}{\sqrt{1 + \frac{i\beta^2\hbar t}{m}}} \\ \times \exp\left[-\frac{\beta^2 (x - p_0 t/m)^2}{2 (1 + i\beta^2\hbar t/m)}\right] \\ \times \exp\left[\frac{i}{\hbar} p_0 \left(x - \frac{p_0}{2m}t\right)\right]$$
(4.68)

The absolute square of the wave function, the probability density, tells us how the packet spreads. Squaring Equation 4.68 we obtain

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{\pi}} \frac{\beta}{\sqrt{1+\frac{\beta^{4}\hbar^{2}t^{2}}{m^{2}}}} \exp\left\{-\beta^{2} \left[\frac{(x-p_{0}t/m)^{2}}{\left(1+\frac{\beta^{4}\hbar^{2}t^{2}}{m^{2}}\right)}\right]\right\}$$
(4.69)

or in terms of  $\Delta x_0 = 1/(\sqrt{2\beta})$ 

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{2\pi}} \frac{1}{\Delta x_{0}} \sqrt{1 + \frac{\hbar^{2}t^{2}}{4m^{2}\Delta x_{0}^{4}}} \exp\left\{-\left[\frac{(x - p_{0}t/m)^{2}}{2\Delta x_{0}^{2}\left(1 + \frac{\hbar^{2}t^{2}}{4m^{2}\Delta x_{0}^{4}}\right)}\right]\right\}$$
(4.70)

From Equation 4.69 we see that, because x and t occur in the combination x - vt, the probability packet travels with group velocity  $v_g = p_0/m = \langle p \rangle / m$  which corresponds to the classical particle velocity. Moreover,  $\langle x(t) \rangle = (p_0/m)t$  which corresponds to the particle position. Additionally, the phase factor in Equation 4.68 shows that the phase velocity  $v_p = p_0/(2m)$ .

Comparing Equation 4.69 with Equation 4.64, we see that the uncertainty as a function of time is given by

$$\Delta x(t) = \Delta x_0 \sqrt{1 + \left(\frac{\hbar t}{2\Delta x_0^2 m}\right)^2}$$
(4.71)

so that, in terms of  $\Delta x$  (t), Equation 4.70 may be written more compactly as

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{2\pi}} \frac{1}{\Delta x(t)} \exp\left\{-\left[\frac{(x-p_{0}t/m)^{2}}{2\Delta x(t)^{2}}\right]\right\}$$
(4.72)

Notice that comparison with Equation 4.64 provides a double check because  $\Delta x(t)$  occurs in both the exponent and the preexponential factor. From Equation 4.71

- -

it is seen that, in coordinate space, the packet spreads as it moves along. On the other hand, this is a free particle so  $\Delta p$  must be independent of time. This may be seen quantitatively by examining the appropriate integrals. Because the only time dependence in the momentum wave function is in the imaginary exponent, the time will not appear in the integrand of either  $\langle p^2 \rangle$  or  $\langle p \rangle$ . The time appears in  $\Delta x$  because x and  $x^2$  must be changed to their momentum notation, derivatives, which operate on the time-dependent part of the imaginary exponent. Thus, the uncertainty product  $\Delta x \Delta p$ , while initially its minimum value, grows with time. Figure 4.2 illustrates the motion in time of the packet.

Another feature of this packet is that the amplitude of the probability density decreases as indicated by the preexponential factor. This decrease in amplitude is compensated by the spreading with time of  $\Delta x(t)$ . The normalization of  $\Psi(x, t)$  is preserved in time as may be seen by evaluating the integral of  $|\Psi(x, t)|^2$  (see Problem 8). Thus, while the Gaussian wave packet propagates and spreads with increasing time, the area under it remains constant. Note that if we imagine the packet to have originated from cutting the spring when the particle was in an eigenstate of the harmonic oscillator so that  $\langle p \rangle = 0$ , the packet would not propagate because  $v_g = 0$ . The packet would, however, spread just as described by Equation 4.71 because the momentum does not enter into this result. In other words, the concave up parabola that is U(x) disintegrates and the Gaussian ground state in coordinate space would spread symmetrically forever.

The probability density represented in Equation 4.69 may be more revealing if it is cast in terms of the initial uncertainty in position  $\Delta x$  (t = 0) =  $\Delta x_0 = 1/(\sqrt{2\beta})$ , which is identical with Equation 4.52 with  $\alpha \rightarrow \beta$ . Rewriting Equation 4.71 and letting

$$t_0 = \frac{2m}{\hbar} \Delta x_0^2 \tag{4.73}$$

we have

$$\Delta x(t) = \Delta x_0 \sqrt{1 + \frac{t^2}{t_0^2}}$$
(4.74)

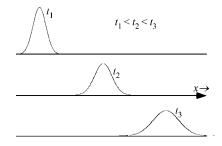


Fig. 4.2 A free Gaussian wave packet shown at three different times. Note that the width of the packet increases in time, but the area under the curve remains constant We see from Equation 4.74 that  $\Delta x(t) > \Delta x_0$  for t > 0. Naturally, we expect this effect to be evident only at the microscopic level. For a free electron we can assume the initial uncertainty to be the order of the Compton wavelength  $\hbar/(m_e c)$  so that

$$t_{0} = \frac{2\hbar}{m_{e}c^{2}}$$
  
=  $\frac{2(6.58 \times 10^{-16} \text{eV} \cdot \text{s})}{0.51 \times 10^{6} \text{eV}}$   
=  $2.6 \times 10^{-21} \text{s}$  (4.75)

Thus, the probability density representing a *free* electron initially confined to a region of space comparable with its own Compton wavelength spreads very rapidly. On the other hand, if it is a macroscopic particle of mass say  $10^{-4}$ kg having diameter  $10^{-3}$ m, appreciable spreading takes more than  $10^{17}$ s, roughly the age of the universe.

### 4.5.2 Case II. The Packet/Particle Subjected to a Constant Field

At t = 0 the Gaussian packet is subjected to a constant force  $\varphi$ . How could such a situation arise? If the particle of mass *m* carries an electrical charge and if it is in a region of constant electric field, then the force is the product of the charge and the electric field. It would also occur if a particle oscillating on a hanging spring were suddenly set free by cutting the spring. After cutting the spring the particle is subjected to the constant gravitational force.

Without specifying the origin of the force we may write the potential as

$$U(x) = -\varphi x; \quad -\infty < x < \infty \tag{4.76}$$

To simplify the mathematics we take the Gaussian packet to be one for which the average momentum and average displacement are zero. In momentum space the initial packet is described by

$$\Phi(p,0) = \frac{1}{\pi^{1/4} \sqrt{\beta\hbar}} e^{-p^2/2\beta^2\hbar^2}$$
(4.77)

The TDSE with the potential energy of Equation 4.76 can be solved exactly in coordinate space (see Section 5.5), but for the present purpose it is convenient to write the TDSE in momentum space. Using Equation 4.38 to replace  $x \rightarrow (i\hbar) \partial/\partial p$  in the TDSE with a linear potential, we have

$$\frac{p^2}{2m}\Phi(p,t) - i\hbar\varphi \frac{\partial\Phi(p,t)}{\partial p} = i\hbar \frac{\partial\Phi(p,t)}{\partial t}$$
(4.78)

This partial differential equation may be solved by making the substitution

$$\Phi(p,t) = \Theta(p') f(p) \text{ where } p' = p - \varphi t$$
(4.79)

which leads to a differential equation for the function f(p)

$$\varphi \frac{df(p)}{dp} = \frac{p^2}{2m(i\hbar)} f(p) \tag{4.80}$$

the solution to which is

$$f(p) = \exp\left(-\frac{ip^3}{6m\hbar\varphi}\right) \tag{4.81}$$

so that

$$\Phi(p,t) = \Theta(p - \varphi t) \exp\left(-\frac{ip^3}{6m\hbar\varphi}\right)$$
(4.82)

where  $\Theta(p - \varphi t)$  is any function of  $(p - \varphi t)$  (see Problem 12). Initial conditions fix  $\Theta(p - \varphi t)$ .

To determine the  $\Theta(p - \varphi t)$  that corresponds to the wave packet in Equation 4.77 we set t = 0 in Equation 4.82 and equate the result to the wave function representing the initial Gaussian wave packet, Equation 4.77. This permits determination of  $\Theta(p)$  which can immediately be converted to  $\Theta(p - \varphi t)$  because this function can contain p and t in only the combination  $(p - \varphi t)$  (see Problem 13). We obtain

$$\Theta(p - \varphi t) = \begin{pmatrix} 1\\ \pi^{1/4} \sqrt{\beta \hbar} \end{pmatrix} \exp\left(-\frac{(p - \varphi t)^2}{2\beta^2 \hbar^2} + \frac{i(p - \varphi t)^3}{6m\hbar\varphi}\right)$$
(4.83)

Substituting Equation 4.83 into Equation 4.82 we obtain the time-dependent wave function in momentum space for a Gaussian wave packet:

$$\Phi(p,t) = \begin{pmatrix} 1\\ \pi^{1/4}\sqrt{\beta\hbar} \end{pmatrix} \exp\left(-\frac{(p-\varphi t)^2}{2\beta^2\hbar^2}\right) \exp\left[i\left(\frac{(p-\varphi t)^3 - p^3}{6m\hbar\varphi}\right)\right]$$
(4.84)

and the probability density in momentum space is

$$\left|\Phi\left(p,t\right)\right|^{2} = \begin{pmatrix}1\\\sqrt{\pi\beta\hbar}\end{pmatrix} \exp\left[-\frac{(p-\varphi t)^{2}}{\beta^{2}\hbar^{2}}\right]$$
(4.85)

or in terms of  $\Delta p_0 = \beta \hbar / \sqrt{2}$ 

$$\left|\Phi\left(p,t\right)\right|^{2} = \begin{pmatrix}1\\\sqrt{2\pi}\Delta p_{0}\end{pmatrix}\exp\left[-\frac{\left(p-\varphi t\right)^{2}}{2\Delta p_{0}^{2}}\right]$$
(4.86)

Comparing Equation 4.85 with Equation 4.65 reveals that

$$\Delta p\left(t\right) = \Delta p_0 \tag{4.87}$$

which contains no time dependence. Thus, as for the free particle Gaussian wave packet, this packet does not spread in momentum. Why is this? After all, there is a force applied. The force is, however, constant so all momentum components are affected equally. The packet moves as a unit in momentum space, but it does not spread.

It is straightforward to extract the time-dependent expectation values  $\langle x(t) \rangle$  and  $\langle p(t) \rangle$  (see Problem 15). We obtain

$$\langle x(t) \rangle = \frac{\varphi t^2}{2m} \text{ and } \langle p(t) \rangle = \varphi t$$
 (4.88)

both of which are consistent with the Ehrenfest equations. Note that  $\langle x(t) \rangle$  has the familiar  $t^2$  dependence of any particle under the influence of a constant force because, by Newton's second law, the acceleration is  $\varphi/m$ . The expectation value of the momentum is indeed Newton's second law because the force is the time rate of change of the (average) momentum.

Consider now the uncertainty in position  $\Delta x(t)$ . We already know  $\langle x(t) \rangle$  so one method of obtaining  $\Delta x(t)$  is to compute  $\langle x(t)^2 \rangle$  using the momentum space wave function, Equation 4.84, and replacing  $x^2$  in the integral with  $\hbar^2 d^2/dp^2$ . Alternatively, we could obtain  $\Psi(x, t)$  by performing a Fourier transform on the momentum wave function, squaring, and identifying  $\Delta x(t)$  by comparing with Equation 4.64. The Fourier transform yields

$$\Psi(x,t) = \frac{1}{\pi^{1/4}} \sqrt{\frac{\beta}{\gamma}} \exp\left[\frac{i\varphi t}{\hbar} \left(x - \frac{\varphi t^2}{6m}\right)\right] \cdot \exp\left\{-\frac{\left[x - \varphi t^2/(2m)\right]^2}{\left(2\gamma/\beta^2\right)}\right\}$$
(4.89)

where, defining  $t_0 = m / (\hbar \beta^2)$  as in Equation 4.73,

$$\gamma = 1 + \frac{it}{t_0}$$
 and  $t_0 = \frac{m}{\hbar\beta^2} = \frac{2m}{\hbar}\Delta x_0^2$  (4.90)

4 Time-Dependent States in One Dimension

The probability density in coordinate space is then

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{\pi}} \begin{pmatrix} 1\\ \sqrt{|\gamma|^{2}/\beta^{2}} \end{pmatrix} \exp\left\{-\frac{\left[x - \varphi t^{2}/(2m)\right]^{2}}{\left(|\gamma|^{2}/\beta^{2}\right)}\right\}$$
(4.91)

Comparing Equation 4.91 with Equation 4.64 we see that

$$2\Delta x (t)^{2} = \frac{|\gamma|^{2}}{\beta^{2}}$$
(4.92)

so that in terms of  $\Delta x(t)$  we have

$$|\Psi(x,t)|^{2} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1\\ \Delta x(t) \end{pmatrix} \exp\left\{-\frac{\left[x - \varphi t^{2}/(2m)\right]^{2}}{2\Delta x(t)^{2}}\right\}$$
(4.93)

where, recalling that  $\Delta x_0 = 1/(\sqrt{2\beta})$ 

$$\Delta x (t) = \Delta x_0 \left( 1 + \frac{t^2}{t_0^2} \right)^{1/2}$$
(4.94)

which is identical to Equation 4.71, again a consequence of the constant force being applied.

# 4.5.3 Case III. The Packet/Particle Subjected to a Harmonic Oscillator Potential

In this case we assume that we have a Gaussian wave packet that is a linear superposition of harmonic oscillator eigenstates and that we know the wave function in coordinate space  $\Psi(x, 0)$ . To be specific we choose an initial wave function of the form

$$\Psi(x,0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\alpha^2 (x-x_0)^2/2}$$
(4.95)

where, in this case,  $\alpha = \sqrt{m\omega/\hbar}$ , the same constant that appears in the eigenfunctions of the harmonic oscillator. The inclusion of a nonzero average displacement, however, assures us that Equation 4.95 is not an eigenfunction of the harmonic oscillator Hamiltonian. Of course, it may be expanded upon the complete set of harmonic oscillator eigenfunctions. Despite not being an eigenfunction, Equation 4.95 is nonetheless a Gaussian distribution with average displacement  $x_0$  and zero initial momentum which (classically) is equivalent to pulling the particle to  $x = x_0$  and releasing it with no initial momentum. Such a state is sometimes referred to as a displaced ground state. In the case studied here, the particle remains under the influence of the potential energy  $U(x) = \frac{1}{2}kx^2$ .

We wish to find the function  $\Psi(x, t)$  so that we may determine the time dependence of the probability distribution  $|\Psi(x, t)|^2$ . There is no need to determine the momentum space wave function so we do not require any Fourier transforms. Using the superposition theorem we write

$$\Psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-i(E_n/\hbar)t}$$
(4.96)

Of course, it makes sense to choose as our complete set, the  $\psi_n(x)$ , the harmonic oscillator eigenfunctions; the  $E_n$  in the exponents are then the corresponding harmonic oscillator energy eigenvalues. To complete the task we would have to multiply both sides by  $\Psi(x, 0)$  and integrate, taking advantage of the orthogonality of the eigenfunctions. In this particular case, however, there is an easier way. It involves using the generating function for the Hermite polynomials. Although generating functions may seem intimidating, this exercise will illustrate the friendliness of such functions. Recall that for the Hermite polynomials the generating function is (see Table 3.2)

$$e^{2\mu\xi-\mu^2} = \sum_{n=0}^{\infty} \frac{H_n(\xi)\,\mu^n}{n!} \tag{4.97}$$

For simplicity of notation let us temporarily use the scaled distance  $\xi = \alpha x$ . The initial packet is

$$\Psi(\xi,0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-(\xi - \xi_0)^2/2}$$
(4.98)

which, with a prescient eye toward using the generating function we let  $\xi_0 = 2\mu$  so that

$$\Psi(\xi, 0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} \exp\left[-\frac{\xi^2}{2} + 2\mu\xi - 2\mu^2\right]$$
$$= \frac{\sqrt{\alpha}}{\pi^{1/4}} \exp\left[-\frac{\xi^2}{2} - \mu^2 + 2\mu\xi - \mu^2\right]$$
$$= \frac{\sqrt{\alpha}}{\pi^{1/4}} \exp\left[-\left(\frac{\xi^2}{2} + \mu^2\right)\right] \cdot \exp\left(2\mu\xi - \mu^2\right)$$
(4.99)

In this form, the last term is recognized as the generating function of the Hermite polynomials. We may therefore replace it using Equation 4.97:

4 Time-Dependent States in One Dimension

$$\Psi(\xi,0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} \exp\left[-\left(\frac{\xi^2}{2} + \mu^2\right)\right] \sum_{n=0}^{\infty} \frac{H_n(\xi) \mu^n}{n!}$$
$$= \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\mu^2} \sum_{n=0}^{\infty} \frac{\mu^n}{n!} \left\{ e^{-\xi^2/2} H_n(\xi) \right\}$$
(4.100)

Notice, however, that the terms in the brackets in Equation 4.100 are precisely the harmonic oscillator eigenfunctions. Comparing Equation 4.100 with Equation 4.96 we see that we have "accidentally" calculated the expansion coefficients, the  $a_n$ .

To include the time in the wave function we multiply each harmonic oscillator eigenfunction in the summation by an exponential that contains the corresponding energy eigenvalue. Inserting the time dependence into Equation 4.100 we have

$$\Psi(\xi,t) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\mu^2} \sum_{n=0}^{\infty} \frac{\mu^n}{n!} \left\{ e^{-\xi^2/2} H_n(\xi) \right\} \exp\left[ -i\left(n+\frac{1}{2}\right) \omega t \right]$$
$$= \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\mu^2} e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{\mu^n}{n!} \left\{ e^{-\xi^2/2} H_n(\xi) \right\} e^{-in\omega t}$$
(4.101)

Removing  $e^{-\xi^2/2}$  from the summation and regrouping the terms we have

$$\Psi(\xi,t) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\mu^2} e^{-i\omega t/2} e^{-\xi^2/2} \sum_{n=0}^{\infty} \left[ \frac{(\mu e^{-i\omega t})^n}{n!} H_n(\xi) \right]$$
(4.102)

Incredibly, the summation is the generating function for the Hermite polynomials with  $\mu \rightarrow \mu e^{-i\omega t}$  as is easily seen from Equation 4.97. That is,

$$\sum_{n=0}^{\infty} \frac{H_n\left(\xi\right) \left(\mu e^{-i\omega t}\right)^n}{n!} = \exp\left[2\xi\mu e^{-i\omega t} - \left(\mu e^{-i\omega t}\right)^2\right]$$
(4.103)

so that, after substituting  $\mu = \xi_0/2$ , Equation 4.102 becomes

$$\Psi(\xi,t) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-i\omega t/2} \exp\left[-\left(\frac{\xi^2}{2} + \frac{\xi_0^2}{4}\right)\right] \cdot \exp\left[\xi_0 \xi e^{-i\omega t} - \frac{\xi_0^2}{4} e^{-2i\omega t}\right]$$
(4.104)

Converting to sines and cosines, we have

$$\Psi(\xi, t) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-i\omega t/2} \exp\left[-\frac{1}{2}\left(\xi^2 + \frac{\xi_0^2}{2}\left(1 + \cos 2\omega t\right) - 2\xi_0\xi\cos\omega t\right)\right] \\ \times \exp\left[\frac{i}{2}\left(\frac{\xi_0^2}{2}\sin 2\omega t - 2\xi_0\xi\sin\omega t\right)\right]$$
(4.105)

106

Finally, the time-dependent probability density is

$$|\Psi(\xi, t)|^{2} = \frac{\alpha}{\sqrt{\pi}} \exp\left\{-\left[\xi^{2} + \frac{\xi_{0}^{2}}{2}\left(1 + \cos 2\omega t\right) - 2\xi_{0}\xi\cos\omega t\right]\right\}$$
$$= \frac{\alpha}{\sqrt{\pi}} \exp\left[-\left(\xi - \xi_{0}\cos\omega t\right)^{2}\right]$$
(4.106)

or, in terms of the coordinate x,

$$|\Psi(x,t)|^2 = \frac{\alpha}{\sqrt{\pi}} \exp\left[-\alpha^2 \left(x - x_0 \cos \omega t\right)^2\right]$$
(4.107)

Equation 4.107 shows that the wave packet oscillates about x = 0 so the expectation value of position as a function of time is (see Problem 18)

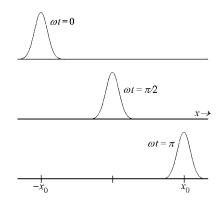
$$\langle x(t) \rangle = x_0 \cos \omega t \tag{4.108}$$

Comparison with Equation 4.64 shows that the uncertainty in position is

$$\Delta x(t) = \frac{1}{\sqrt{2\alpha}} = \Delta x_0 \tag{4.109}$$

which is time-independent. The packet oscillates without any change in shape! (Remember, the harmonic oscillator is special.) This was first pointed out by Schr<sup>2</sup>odinger in 1926 and is often referred to as *the* coherent state, but, in truth, it is really *a* coherent state. We will return to this state in a future chapter. The reason for this special behavior is that the energy levels are equally spaced. There are few other systems that exhibit such a feature. The behavior is illustrated in Fig. 4.3 at three different values of the time.

There are some other interesting features of this wave packet. Rewriting  $\Psi(\xi, 0)$  from Equation 4.100 we have



**Fig. 4.3** A Gaussian wave packet under the influence of a harmonic oscillator potential shown at three different times. Note that the shape of the packet does not change

4 Time-Dependent States in One Dimension

$$\Psi(\xi,0) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\xi_0^2/4} \sum_{n=0}^{\infty} \frac{(\xi_0/2)^n}{n!} e^{-\xi^2/2} H_n(\xi)$$
$$= \sum_{n=0}^{\infty} \binom{\xi_0^n e^{-\xi_0^2/4}}{\sqrt{2^n n!}} \left[ \sqrt{\frac{\alpha}{2^n n!}} \frac{1}{\pi^{1/4}} e^{-\xi^2/2} H_n(\xi) \right]$$
(4.110)

The form of this last equation isolates the expansion coefficients  $a_n$  in Equation 4.96 because the expression in the square brackets represents the normalized harmonic oscillator eigenfunctions (see Equation 3.49). Thus,

$$a_{n} = \frac{\xi_{0}^{n} e^{-\xi_{0}^{2}/4}}{\sqrt{2^{n} n!}}$$
$$= \frac{\alpha^{n} x_{0}^{n} e^{-\alpha^{2} x_{0}^{2}/4}}{\sqrt{2^{n} n!}}$$
(4.111)

As  $x_0 \rightarrow 0$  it is clear from the form of the initial wave packet that it approaches the ground state of the harmonic oscillator, a stationary state. It might be said that the packet oscillates about x = 0 with zero amplitude. Thus, we expect that  $a_0 = 1$ and all other expansion coefficients vanish. Note that in Equation 4.111 the limit as  $x_0 \rightarrow 0$  for n = 0 is indeterminate because zero to the zero power is indeterminate. On the other hand,

$$\lim_{x_0 \to 0} a_n \equiv 0 \text{ for all } n \ge 1 \tag{4.112}$$

so we conclude that, in this case, indeed, the mathematics yield  $a_0 = 1$ .

In the opposite extreme the correspondence principle tells us that the motion should emulate that of a classical oscillator. In that case it can be shown that for large  $x_0$  high harmonic oscillator eigenstates make significant contributions. Moreover, for high *n* the maximum contribution to the admixture comes from the state that has the same energy as the classical oscillator having amplitude  $x_0$  (see Problem 19).

#### 4.6 Retrospective

Wave packets provide the crucial link between classical and quantum physics. Understanding of this concept should not be obscured by the morass of Fourier transforms attendant to the mathematical description of wave packets. While quantum mechanics permits particles to retain their pointlike properties, the probabilistic nature of quantum physics manifests itself via constructive and destructive interference of probability waves that produce localized probability distributions, thus emulating the characteristics of a classical particle. As we have seen, however, the Problems

price that Mr. Heisenberg exacts from us for having precise knowledge of position is that we must ante up by relinquishing knowledge of the particle's momentum. On the other hand, a pure de Broglie wave is the antithesis of such a particle. Here we have precise knowledge of the momentum so we must pay by having no idea of the particle's position. Such is the life of a quantum mechanic. Mathematically, Fourier transforms account for the Heisenberg uncertainty principle, but physical comprehension should trump mathematical quagmires.

# **Problems**

- 1. Derive the Ehrenfest equation that is the relationship between the expectation values of the time rate of change of momentum and the force.
- 2. To see how the superposition of waves can cause the probability density to cluster, add two waves of differing frequencies and make a plot of their sum as a function of time at a fixed value of x. For ease of computation use  $\Psi_1(x, t) =$  $15x \cos t$  and  $\Psi_2(x, t) = -3x \cos(17t)$ . The trigonometric identity  $\cos A - 4x \cos(17t)$  $\cos B = 2 \sin \left[\frac{1}{2}(A+B)\right] \sin \left[\frac{1}{2}(B-A)\right]$  will be helpful. 3. Find  $(\Delta x)^2 = \langle x^2 \rangle$  and  $(\Delta p)^2 = \langle p^2 \rangle$  for the ground state of the harmonic
- oscillator to show that, indeed,  $\Delta x \Delta p \equiv \frac{1}{2}\hbar$  for a Gaussian wave function.
- 4. For the wave functions

$$\Psi(x,0) = \frac{\sqrt{\beta}}{\pi^{1/4}} e^{-\beta^2 (x-x_0)^2/2} e^{ip_0 x/\hbar}$$

and

$$\Phi(p,0) = \frac{1}{\pi^{1/4} \sqrt{\beta \hbar}} e^{-(p-p_0)^2/2\beta^2 \hbar^2} \cdot e^{-ipx_0/\hbar}$$

show that  $\langle x \rangle = x_0$  and  $\langle p \rangle = p_0$ . Do the calculations in both coordinate and momentum space.

- 5. (a) Show that for  $\phi(p) = \frac{1}{\pi^{1/4} \sqrt{\hbar\beta}} e^{-(p-p_0)^2/(2\beta^2\hbar^2)}, \langle p \rangle = p_0 \text{ and } \langle p^2 \rangle =$  $\frac{\beta^2 \hbar^2}{2} + p_0^2 \text{ so that } (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\beta^2 \hbar^2}{2}.$ (b) Show that both of these average values are independent of time.
- 6. Show that for the Gaussian wave packet

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

the uncertainty in position and momentum at t = 0 are  $\Delta x = 1/(\sqrt{2\beta})$  and  $\Delta p = \left(\beta \hbar / \sqrt{2}\right).$