2 The wave function and the uncertainty principle

In the previous chapter we discussed a number of phenomena which cannot be explained within the framework of classical physics. As a result of this experimental evidence, revolutionary concepts had to be introduced such as those of *quantisation* and of *wave–particle duality*.

Attempts to construct a theoretical structure which incorporates these concepts in a satisfactory way met first with great difficulties, until a new theory, called *quantum mechanics*, was elaborated between the years 1925 and 1930. Quantum mechanics provides a consistent description of matter on the microscopic scale, and can be considered as one of the greatest intellectual achievements of the twentieth century. Two equivalent formulations of the theory were proposed at nearly the same time. The first, known as *matrix mechanics*, was developed in the years 1925 and 1926 by W. Heisenberg, M. Born and P. Jordan. In this approach, only physically observable quantities appear, and to each physical quantity the theory associates a matrix. These matrices obey a non-commutative algebra, which is the essential difference between matrix mechanics and classical mechanics. The second form of quantum mechanics, called *wave mechanics*, was proposed in 1925 by E. Schrödinger, following the ideas put forward in 1923 by L. de Broglie about matter waves. The equivalence of matrix mechanics and wave mechanics was proved in 1926 by Schrödinger. In fact, both matrix mechanics and wave mechanics are particular forms of a general formulation of quantum mechanics, which was developed by P. A. M. Dirac in 1930.

The general formulation of quantum mechanics, as well as matrix mechanics, requires a certain amount of abstract mathematics, and hence we shall defer discussion of it until Chapter 5. Wave mechanics, on the other hand, is more suitable for a first contact with quantum theory, and this is the approach which we shall use in most of this book. In this chapter we shall discuss the fundamental ideas underlying quantum mechanics in their simplest form. We begin with an analysis of wave–particle duality, introducing the notion of a wave function and its probabilistic interpretation. We

then go on to construct wave functions corresponding to particles having a well-defined momentum, and to obtain localised wave functions by superposing plane waves into wave packets. Following this, we discuss the Heisenberg uncertainty relations which impose limits on the accuracy of simultaneous measurements of pairs of 'complementary' variables, such as position and momentum, or time and energy.

2.1 Wave–particle duality

In Chapter 1 we discussed several experiments which demonstrate conclusively that material particles possess wave-like properties, exhibiting interference and diffraction effects. On the other hand, we saw that electromagnetic radiation, which had been known for a long time to exhibit wave properties, can also show a particle-like behaviour. We shall now analyse this wave–particle duality in more detail.

Let us consider an idealised experiment in which monoenergetic particles, for example electrons, emitted by a source are directed on to a screen S_1 containing two slits A and B (see Fig. 2.1). At some distance beyond this screen a second screen S_2 is placed, incorporating detectors which can record each electron striking the screen S_2 at a given point. On detection, every electron exhibits purely particle-like properties, that is its mass and charge are localised, being never spread over more than one detector at a given time. In contrast, if after some time the total number of electrons arriving at the screen S_2 is plotted as a function of position, a diffraction pattern is found, which is characteristic of waves (see Fig. 2.2(a)). Thus, in a single experiment, both the particle and wave aspects of the electron are exhibited. A realisation of this ideal experiment by Jönsson has been described in Chapter 1. A similar experiment

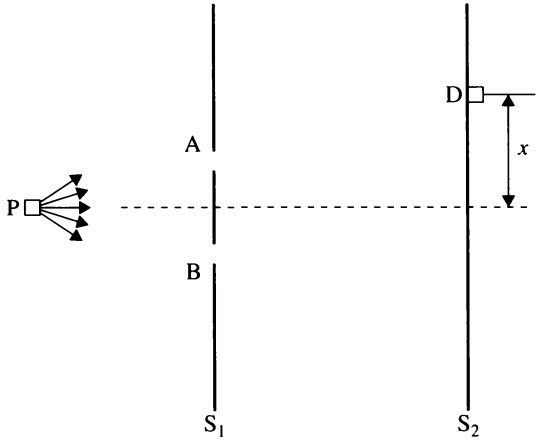

Figure 2.1 The two-slit experiment. Monoenergetic particles from a source at P fall on a screen S_1 containing slits at A and B. Detectors are placed on a second screen S_2 to record the number of particles arriving at each point. A particle detector D is indicated at a position x.

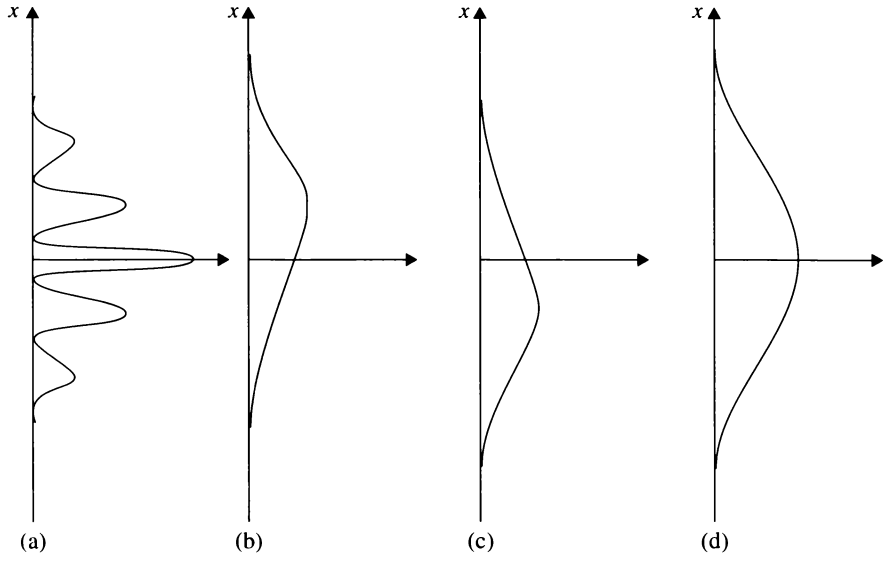

Figure 2.2 The intensity at a position x on the screen S_2 (see Fig. 2.1).
(a) A diffraction pattern characteristic of waves.
(b) The intensity with slit A open and B closed.
(c) The intensity with slit B open and A closed.
(d) An intensity distribution characteristic of classical particles when A and B are both open.

can be carried out with light. In this case the light can be detected by the photoelectric effect, showing its particle (photon) aspect, while the recorded intensity displays the diffraction pattern characteristic of the wave theory of light.

It might at first be supposed that the diffraction pattern is in some way due to interference between electrons (or photons) passing through the two slits. However, if the incident intensity is reduced until at any instant there is no more than one particle between the source and the detecting screen, the interference pattern is still accumulated. This was demonstrated originally in 1909 by G. I. Taylor, who photographed the diffraction pattern formed by the shadow of a needle, using a very weak source such that the exposures lasted for months. It can be concluded that interference does not occur between photons, but is a property of a single photon. This was confirmed in more recent experiments performed in 1989 by A. Aspect, P. Grangier and G. Roger. Material particles such as electrons exhibit a similar behaviour, as was demonstrated directly in 1989 by A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki and H. Ezawa in two-slit experiments in which the accumulation of the interference pattern due to incoming single electrons was observed (see Fig. 2.3). It should be noted that if one slit is closed in a two-slit experiment, the diffraction pattern does not appear, so we may infer that when both slits are open the particle is not localised before it is detected, and hence must be considered as having passed through both slits!

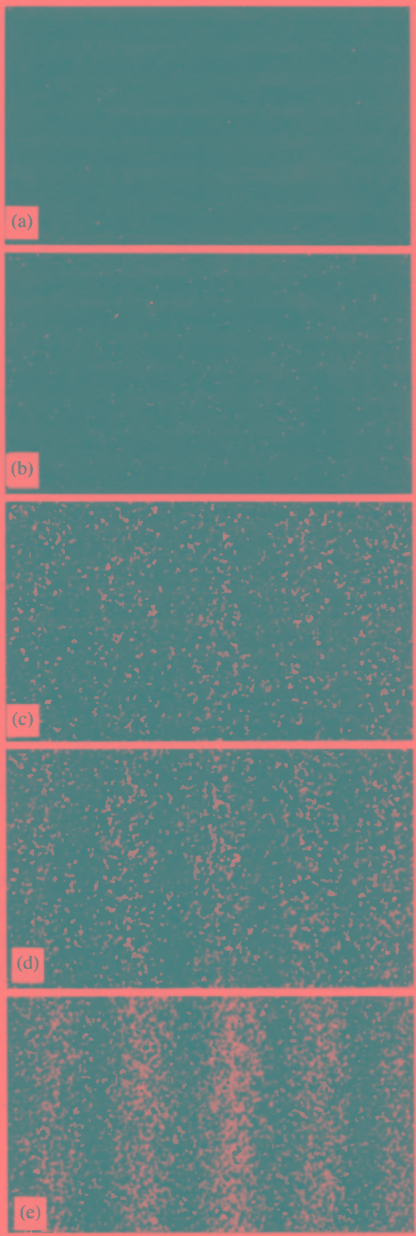

Figure 2.3 Buildup of an interference pattern by accumulating single electrons in the two-slit experiment of Tonomura *et al.*
(a) Number of electrons = 10; (b) number of electrons = 100;
(c) number of electrons = 3000; (d) number of electrons = 20 000; and
(e) number of electrons = 70 000.
(By courtesy of A. Tonomura.)

Another way of expressing these facts is to say that while in transit the electron or photon behaves like a wave, manifesting its particle-like property only on detection. This is of course in complete contradiction to the classical viewpoint, which would lead us to suppose that each particle being indivisible must pass either through one slit or the other. Let us put this to the test by detecting the particles as they pass through the slits. We can now record the particles which have passed through slit A and entered the detectors on screen S_2. Since all these particles passed through slit A, slit B might as well have been closed, in which case the intensity distribution will not show diffraction but will be as illustrated in Fig. 2.2(b). Similarly, if slit B is open and A is closed, the intensity distribution is that shown in Fig. 2.2(c). If we add the intensity distributions of Figs. 2.2(b) and 2.2(c) we obtain the intensity pattern shown in Fig. 2.2(d), which is very different from the diffraction pattern obtained in the absence of any knowledge about which slit the particles passed through (see Fig. 2.2(a)). Hence, if the particle nature of an electron, a photon, etc., is established by monitoring its trajectory, it cannot simultaneously behave like a wave. The wave and particle aspects of electrons, photons, etc., are *complementary*.

Let us now return to the case in which there is only one particle at a time transiting the apparatus and both slits are open. The place on the screen S_2 at which a given particle will be detected cannot be predicted, because if it could be predicted this would be equivalent to determining the trajectory, which we have seen would eliminate the diffraction pattern. What is predictable is the intensity distribution which builds up after a large number of individual events have occured. This suggests that for an individual particle the process is of a *statistical* nature, so that one can only determine the probability P that a particle will hit the screen S_2 at a certain point. By probability in this context we mean the number of times that an event occurs divided by the total number of events. The intensity of the pattern formed on the screen S_2, in the present case, is then proportional to the probability P.

In the classical theory of light, the intensity of light at each point is determined by the square of the amplitude of a wave. For example, in Young's two-slit experiment, the light intensity on the recording screen is given by the square of the amplitude of the wave formed by the *superposition* of the secondary waves arising from each slit. This classical wave theory cannot of course be used as it stands because it does not account for the particle aspect of light. However, it suggests, by analogy, that in quantum mechanics a *wave function* or *state function* $\Psi(x, y, z, t)$ can be introduced, which plays the role of a *probability amplitude*. We shall see later that in general the wave function Ψ is a *complex* quantity. We then expect that the probability $P(x, y, z, t)$ of finding the particle at a particular point within a volume V about the point with coordinates (x, y, z) at time t is proportional to $|\Psi|^2$:

$$P(x, y, z, t) \propto |\Psi(x, y, z, t)|^2. \tag{2.1}$$

Since probabilities are *real positive* numbers, we have associated in (2.1) the probability P with the square of the modulus of the wave function Ψ.

Let Ψ_A be the wave function at a particular point on the screen S_2 corresponding to waves spreading from the slit A. Similarly, let Ψ_B be the wave function at the same

point corresponding to waves spreading from the slit B. The two intensity distributions of Fig. 2.2(b) and (c) corresponding to experiments performed with only one open slit are determined respectively by the probability distributions

$$P_A \propto |\Psi_A|^2, \qquad P_B \propto |\Psi_B|^2. \tag{2.2}$$

On the other hand, when both slits are open, the wave function Ψ is taken to be the sum of the two contributions Ψ_A and Ψ_B,

$$\Psi = \Psi_A + \Psi_B. \tag{2.3}$$

The corresponding probability distribution

$$P \propto |\Psi_A + \Psi_B|^2 \tag{2.4}$$

then determines the intensity pattern illustrated in Fig. 2.2(a). It is important to notice that in (2.4) the probability amplitudes Ψ_A and Ψ_B have been added and not the probabilities P_A and P_B. If the latter were the case there would be no possibility of obtaining interference patterns characteristic of a wave theory.

2.2 The interpretation of the wave function

In analysing the two-slit experiment, we introduced the concept that the probability of finding a particle at a given location is proportional to the square of the modulus of the wave function associated with the particle. This concept may be restated more precisely in the form of a fundamental assumption made by M. Born in 1926, which can be formulated in the following way. Let us imagine a very large number of identical, independent systems, each of them consisting of a single particle moving under the influence of some given external force. All these systems are identically prepared, and this ensemble is assumed to be described by a single wave function $\Psi(x, y, z, t)$ which contains all the information that can be known about them. It is then postulated that if measurements of the position of the particle are made on each of the systems, the probability (that is the statistical frequency) of finding the particle within the volume element $\mathrm{d}\mathbf{r} \equiv \mathrm{d}x\mathrm{d}y\mathrm{d}z$ about the point $\mathbf{r} \equiv (x, y, z)$ at the time t is

$$P(\mathbf{r}, t)\mathrm{d}\mathbf{r} = |\Psi(\mathbf{r}, t)|^2 \mathrm{d}\mathbf{r} \tag{2.5}$$

so that

$$P(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 = \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t) \tag{2.6}$$

is the *position probability density*. Thus we see that the interpretation of the wave function introduced by Born is a statistical one. For convenience, we shall often speak of the wave function associated with a particular system, but it must always be understood that this is shorthand for the wave function associated with an ensemble of identical and identically prepared systems, as required by the statistical nature of the theory.

Since the probability of finding the particle somewhere must be unity, we deduce from (2.5) that the wave function $\Psi(\mathbf{r}, t)$ should be *normalised to unity*, so that

$$\int |\Psi(\mathbf{r}, t)|^2 \mathrm{d}\mathbf{r} = 1 \tag{2.7}$$

where the integral extends over all space. A wave function for which the integral on the left of (2.7) is finite is said to be *square integrable*: such a wave function can always be normalised to unity by multiplying it by an appropriate complex constant.

It is important to notice that since $|\Psi(\mathbf{r}, t)|^2$ is the physically significant quantity, two wave functions which differ from each other by a constant multiplicative factor of modulus one (that is, a constant phase factor of the form $\exp(\mathrm{i}\alpha)$, where α is a real number) are equivalent, and satisfy the same normalisation condition.

The superposition principle

As we have seen in the previous section, in order to account for interference effects, it must be possible to *superpose* wave functions. This means that if one possible state of an ensemble of identical systems is described by a wave function Ψ_1 and another state of this ensemble by a wave function Ψ_2, then any *linear combination*

$$\Psi = c_1\Psi_1 + c_2\Psi_2 \tag{2.8}$$

where c_1 and c_2 are complex constants, is also a wave function describing a possible state of the ensemble.

Let us write the (complex) wave functions Ψ_1 and Ψ_2 in the form

$$\Psi_1 = |\Psi_1|\mathrm{e}^{\mathrm{i}\alpha_1}, \qquad \Psi_2 = |\Psi_2|\mathrm{e}^{\mathrm{i}\alpha_2}. \tag{2.9}$$

Using (2.8), we find that the square of the modulus of Ψ is given by

$$|\Psi|^2 = |c_1\Psi_1|^2 + |c_2\Psi_2|^2 + 2\mathrm{Re}\{c_1c_2^*|\Psi_1||\Psi_2|\exp[\mathrm{i}(\alpha_1 - \alpha_2)]\} \tag{2.10}$$

so that, in general, $|\Psi|^2 \neq |c_1\Psi_1|^2 + |c_2\Psi_2|^2$, in keeping with the discussion of Section 2.1. It is worth stressing that although the quantity $|\Psi|^2$ is unaffected if Ψ is multiplied by an *overall* phase factor $\exp(\mathrm{i}\alpha)$ (where α is a real constant) it does depend on the *relative* phase $(\alpha_1 - \alpha_2)$ of Ψ_1 and Ψ_2 through the third term on the right of (2.10), which is an *interference* term.

Finally, we emphasise that unlike classical waves (such as sound waves or water waves) the wave function $\Psi(\mathbf{r}, t)$ is an *abstract* quantity, the interpretation of which is of a *statistical* nature. This wave function is assumed to provide a *complete* description of the dynamical state of an ensemble. Indeed, we shall see later that the knowledge of the wave function enables one to predict for each dynamical variable (position, momentum, energy and so on) a *statistical distribution* of values obtained in measurements.

2.3 Wave functions for particles having a definite momentum

In this section we begin to investigate how wave functions can be found, considering the simple case of *free* particles. The experiments exhibiting the corpuscular nature of the electromagnetic radiation, which we discussed in Chapter 1, require that with the electromagnetic field one associates a particle, the photon, whose energy E and magnitude p of momentum are related to the frequency ν and wavelength λ of the electromagnetic radiation by

$$E = h\nu, \qquad p = \frac{h}{\lambda}. \tag{2.11}$$

On the other hand, we have seen in Section 1.6 that de Broglie was led to associate matter waves with particles in such a way that the frequency ν and the wavelength λ of the wave were linked with the particle energy E and the magnitude p of its momentum by the same relations (2.11). The de Broglie relation $\lambda = h/p$ was confirmed by the results of a number of experiments exhibiting the wave nature of matter. Following de Broglie, we shall assume that the relations (2.11) hold for all types of particles and field quanta. Introducing the angular frequency $\omega = 2\pi\nu$, the wave number $k = 2\pi/\lambda$ and the reduced Planck constant $\hbar = h/2\pi$, we may write the relations (2.11) in the more symmetric form

$$E = \hbar\omega, \qquad p = \hbar k. \tag{2.12}$$

Let us consider a *free* particle of mass m, moving along the x-axis with a definite momentum $\mathbf{p} = p_x\hat{\mathbf{x}}$, where $\hat{\mathbf{x}}$ is a unit vector along the x-axis, and a corresponding energy E. Assuming that $p_x > 0$, so that the particle moves in the positive x-direction, we associate with this particle a wave travelling in the same direction with a fixed wave number k. Such a wave is a *plane wave* and can be written as

$$\Psi(x, t) = A\exp\{\mathrm{i}[kx - \omega(k)t]\} \tag{2.13a}$$

where A is a constant. This plane wave has a wavelength $\lambda = 2\pi/k$ and an angular frequency ω. Since from (2.12) $k = p/\hbar$ (with $p = p_x$) and $\omega = E/\hbar$, the wave function (2.13a) can be expressed as

$$\Psi(x, t) = A\exp\{\mathrm{i}[p_x x - E(p_x)t]/\hbar\}, \tag{2.13b}$$

In writing (2.13a,b) we have taken $\omega(k)$ and $E(p_x)$ as functions to be specified later. We note that the wave function (2.13) satisfies the two relations

$$-\mathrm{i}\hbar\frac{\partial}{\partial x}\Psi = p_x\Psi \tag{2.14}$$

and

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi = E\Psi \tag{2.15}$$

the significance of which will emerge shortly.

This one-dimensional treatment is easily extended to three dimensions. To a free particle of mass m, having a well-defined momentum $\mathbf{p}$ and an energy E, we now associate a plane wave

$$\begin{aligned}\Psi(\mathbf{r},t) &= A\exp\{\mathrm{i}[\mathbf{k}.\mathbf{r}-\omega(k)t]\}\\ &= A\exp\{\mathrm{i}[\mathbf{p}.\mathbf{r}-E(p)t]/\hbar\}\end{aligned} \tag{2.16}$$

where the propagation vector (or wave vector) $\mathbf{k}$ is related to the momentum $\mathbf{p}$ by

$$\mathbf{p}=\hbar\mathbf{k} \tag{2.17}$$

with

$$k=|\mathbf{k}|=\frac{|\mathbf{p}|}{\hbar}=\frac{2\pi}{\lambda} \tag{2.18}$$

and the angular frequency ω is related to the energy by $\omega = E/\hbar$. Again, the functions $\omega(k)$ and $E(p)$ will be specified later. The equation (2.15) remains unchanged for the plane wave (2.16), while (2.14) is now replaced by its obvious generalisation

$$-\mathrm{i}\hbar\nabla\Psi=\mathbf{p}\Psi \tag{2.19}$$

where ∇ is the gradient operator, having Cartesian components $(\partial/\partial x, \partial/\partial y, \partial/\partial z)$. The relations (2.15) and (2.19) show that for a free particle the energy and momentum can be represented by the differential operators

$$E_{\mathrm{op}}=\mathrm{i}\hbar\frac{\partial}{\partial t},\qquad \mathbf{p}_{\mathrm{op}}=-\mathrm{i}\hbar\nabla \tag{2.20}$$

acting on the wave function Ψ. It is a *postulate* of wave mechanics that when the particle is not free the dynamical variables E and $\mathbf{p}$ are still represented by these differential operators.

According to the discussion of Section 2.2, wave functions should be normalised to unity if the probability interpretation is to be maintained. For one-dimensional systems, the normalisation condition (2.7) reduces to

$$\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\mathrm{d}x=1. \tag{2.21}$$

However, the plane wave (2.13) does not satisfy this requirement, since the integral on the left of (2.21) is given in this case by

$$\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\mathrm{d}x=|A|^2\int_{-\infty}^{+\infty}\mathrm{d}x \tag{2.22}$$

and hence does not exist. Similarly, the three-dimensional plane wave (2.16) cannot be normalised according to (2.7). There are two ways out of this difficulty. The first is to give up the concept of *absolute* probabilities when dealing with wave functions such as (2.13) or (2.16) which are not square integrable. Instead, $|\Psi(\mathbf{r},t)|^2\mathrm{d}\mathbf{r}$ is then interpreted as the *relative* probability of finding the particle at time t in a volume element $\mathrm{d}\mathbf{r}$ centred about $\mathbf{r}$, so that the ratio $|\Psi(\mathbf{r}_1,t)|^2/|\Psi(\mathbf{r}_2,t)|^2$ gives the probability of finding the particle within a volume element centred around $\mathbf{r}=\mathbf{r}_1$,

compared with that of finding it within the same volume element at $\mathbf{r} = \mathbf{r}_2$. For the particular case of the plane wave (2.16), we see that $|\Psi|^2 = |A|^2$, so that there is an equal chance of finding the particle at any point. The plane wave (2.16) therefore describes the *idealised* situation of a free particle having a perfectly well-defined momentum, but which is completely '*delocalised*'. This suggests a second way out of the difficulty, which is to give up the requirement that the free particle should have a precisely defined momentum, and to superpose plane waves corresponding to different momenta to form a localised *wave packet*, which can be normalised to unity. It is to this question that we now turn our attention.

2.4 Wave packets

We have seen in the preceding section that plane waves such as (2.13) or (2.16) associated with free particles having a definite momentum are completely delocalised. To describe a particle which is confined to a certain spatial region, a *wave packet* can be formed by superposing plane waves of different wave numbers. Of course, in this case the momentum no longer has a precise value, but we shall construct a wave packet which 'represents' a particle having fairly precise values of both momentum and position.

Let us begin by considering the one-dimensional case. In order to describe a free particle confined to a region of the x-axis, we superpose plane waves of the form (2.13), where we now allow $p_x = \hbar k$ to be either positive or negative. The most general superposition of this kind is then given by the integral

$$\Psi(x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i[p_x x - E(p_x)t]/\hbar} \phi(p_x) dp_x \tag{2.23}$$

where the factor $(2\pi\hbar)^{-1/2}$ in front of the integral has been chosen for future convenience. The function $\phi(p_x)$ is the amplitude of the plane wave corresponding to the momentum p_x. In general it is a complex function, but it is sufficient for our present purposes to discuss only the case for which $\phi(p_x)$ is real.

Let us assume that $\phi(p_x)$ is sharply peaked about some value $p_x = p_0$, falling rapidly to zero outside an interval $(p_0 - \Delta p_x, p_0 + \Delta p_x)$. Writing (2.23) in the form

$$\Psi(x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i\beta(p_x)/\hbar} \phi(p_x) dp_x \tag{2.24}$$

where

$$\beta(p_x) = p_x x - E(p_x)t \tag{2.25}$$

we see that $|\Psi(x, t)|$ is largest when $\beta(p_x)$ is nearly constant in the vicinity of $p_x = p_0$. Indeed, if $\beta(p_x)$ were varying significantly over the interval $(p_0 - \Delta p_x, p_0 + \Delta p_x)$, the factor $\exp[i\beta(p_x)/\hbar]$ would oscillate rapidly, so that the value of the integral on

the right of (2.24) would be small. Thus $|\Psi(x, t)|$ will only be significant in a limited region, its maximum value occurring when the *stationary phase condition*

$$\left[\frac{\mathrm{d}\beta(p_x)}{\mathrm{d}p_x}\right]_{p_x=p_0} = 0 \tag{2.26}$$

is satisfied. This condition determines the *centre of the wave packet*, which upon using (2.25) is seen to travel according to the law

$$x = v_g t \tag{2.27}$$

where

$$v_g = \left[\frac{\mathrm{d}E(p_x)}{\mathrm{d}p_x}\right]_{p_x=p_0}. \tag{2.28}$$

It follows from (2.27) that the centre of the wave packet moves with the constant velocity v_g, which is known as the *group velocity* of the packet. From (2.28) and the fact that $E = \hbar\omega$, and $p_x = \hbar k$, we see that the group velocity can also be written as

$$v_g = \left[\frac{\mathrm{d}\omega(k)}{\mathrm{d}k}\right]_{k=k_0} \tag{2.29}$$

with $k_0 = p_0/\hbar$. We remark that this velocity is, in general, different from the *phase velocity* v_{ph}, which is the velocity of propagation of the individual plane waves (2.13) and is given for a particular plane wave $A\exp[\mathrm{i}(k_0 x - \omega(k_0)t)]$ by

$$v_{ph} = \frac{\omega(k_0)}{k_0} = \frac{E(p_0)}{p_0}. \tag{2.30}$$

In the macroscopic limit the motion of a particle must be governed by the laws of classical mechanics, in accordance with the correspondence principle (see Section 1.4). In this limit the extension of the wave packet is negligible so that the group velocity v_g can be identified with the classical velocity $v = p_0/m$ of the particle

$$v_g = v = \frac{p_0}{m}. \tag{2.31}$$

Combining this result with (2.28) allows us to determine the functional dependence of $E(p_x)$ on p_x. We have

$$\frac{\mathrm{d}E(p_x)}{\mathrm{d}p_x} = \frac{p_x}{m} \tag{2.32}$$

so that $E(p_x) = p_x^2/2m +$ constant. We may set the constant of integration equal to zero because the zero of energy can be chosen arbitarily, only *energy differences* being of physical interest. Hence we have

$$E(p_x) = \frac{p_x^2}{2m}. \tag{2.33}$$

It should be noted that since $E = h\nu$, the absolute value of the frequency has no physical significance in quantum mechanics, in contrast with classical wave theory

(e.g. sound waves). We remark that since in our case $E(p_0) = p_0^2/2m$, the phase velocity (2.30) is given by

$$v_{\text{ph}} = \frac{p_0^2/2m}{p_0} = \frac{p_0}{2m} = \frac{v_g}{2}. \tag{2.34}$$

Let us return to the expression (2.23) of the wave packet and express $E(p_x) = p_x^2/2m$ in the form

$$\begin{aligned} E(p_x) &= \frac{p_0^2}{2m} + \frac{p_0}{m}(p_x - p_0) + \frac{(p_x - p_0)^2}{2m} \\ &= E(p_0) + v_g(p_x - p_0) + \frac{(p_x - p_0)^2}{2m}. \end{aligned} \tag{2.35}$$

Since the function $\phi(p_x)$ in (2.23) is negligible except in the interval $(p_0 - \Delta p_x, p_0 + \Delta p_x)$ we can neglect the third term on the right of (2.35), provided t is small enough so that

$$\frac{1}{2m\hbar}(\Delta p_x)^2 t \ll 1. \tag{2.36}$$

Indeed, if the condition (2.36) is satisfied, the quantity $\exp[-\mathrm{i}(p_x - p_0)^2 t/2m\hbar]$ which occurs in the integrand on the right of (2.23) is approximately equal to unity. Making this approximation, equation (2.23) reduces to

$$\Psi(x, t) = \mathrm{e}^{\mathrm{i}[p_0 x - E(p_0)t]/\hbar} F(x, t) \tag{2.37}$$

where

$$F(x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}(p_x - p_0)(x - v_g t)/\hbar} \phi(p_x) \mathrm{d}p_x. \tag{2.38}$$

The wave packet (2.37) is the product of a plane wave of wavelength $\lambda_0 = h/|p_0|$ and angular frequency $\omega_0 = E(p_0)/\hbar$ times a *modulating* amplitude or *envelope* function $F(x, t)$ such that $|\Psi(x, t)|^2 = |F(x, t)|^2$. Since

$$F(x, t = 0) = F(x + v_g t, t) \tag{2.39}$$

this envelope function propagates *without change of shape* with the group velocity v_g (see Fig. 2.4). It should be borne in mind that this is only true for times t satisfying the condition (2.36); at later times the shape of the wave packet will change as it propagates.

Fourier transforms and momentum space wave function

Looking back at the wave packet (2.23), defining $\psi(x) \equiv \Psi(x, t = 0)$ and using the results of Appendix A, we see that the functions

$$\psi(x) = (2\pi\hbar)^{-1/2} \int \mathrm{e}^{\mathrm{i}p_x x/\hbar} \phi(p_x) \mathrm{d}p_x \tag{2.40}$$

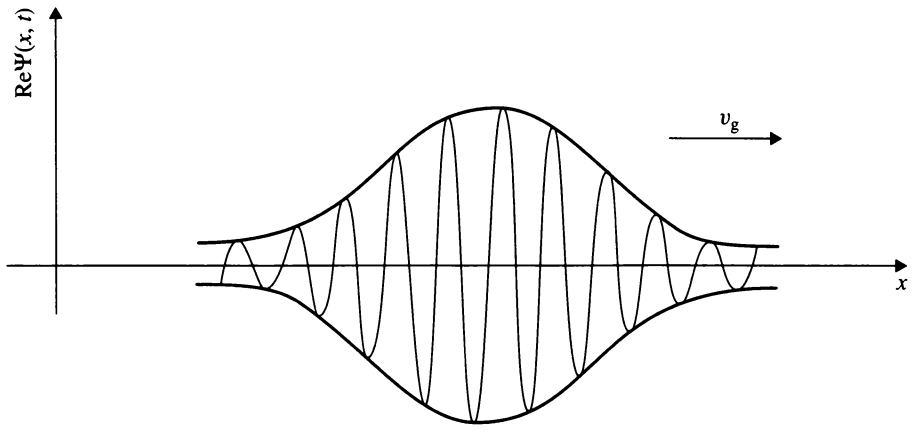

Figure 2.4 The function $\mathrm{Re}\Psi(x, t)$ for a wave packet propagating along the x-axis, with a group velocity v_g.

and

$$\phi(p_x) = (2\pi\hbar)^{-1/2} \int \mathrm{e}^{-\mathrm{i}p_x x/\hbar} \psi(x) \mathrm{d}x \tag{2.41}$$

are *Fourier transforms* of each other. More generally, at time t, we can introduce a function $\Phi(p_x, t)$ such that

$$\Psi(x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}p_x x/\hbar} \Phi(p_x, t) \mathrm{d}p_x \tag{2.42}$$

and

$$\Phi(p_x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}p_x x/\hbar} \Psi(x, t) \mathrm{d}x \tag{2.43}$$

are also mutual Fourier transforms. The function $\Phi(p_x, t)$ is called the *wave function in momentum space*, and we see that $\phi(p_x) = \Phi(p_x, t = 0)$. The definition of the momentum space wave function given by (2.43) is completely general and holds for all types of wave function $\Psi(x, t)$, including the free particle wave packets which we have been considering.

From Parseval's theorem (see equation (A.43) of Appendix A), we infer that if the wave function $\phi(p_x)$ is normalised to unity in the sense that

$$\int_{-\infty}^{+\infty} |\phi(p_x)|^2 \mathrm{d}p_x = 1 \tag{2.44}$$

then the wave function $\psi(x) \equiv \Psi(x, t = 0)$ given by (2.40) is also normalised to unity. Moreover, once $\Psi(x, t)$ is normalised to unity at $t = 0$, it remains normalised

to unity at all times. Indeed,

$$\begin{aligned}\int_{-\infty}^{+\infty}\Psi^*(x,t)\Psi(x,t)\mathrm{d}x &= (2\pi\hbar)^{-1}\int_{-\infty}^{+\infty}\mathrm{d}x\int_{-\infty}^{+\infty}\mathrm{d}p_x\int_{-\infty}^{+\infty}\mathrm{d}p'_x\mathrm{e}^{\mathrm{i}[(p_x-p'_x)x]/\hbar}\\ &\quad\times\mathrm{e}^{-\mathrm{i}[E(p_x)-E(p'_x)]t/\hbar}\phi^*(p'_x)\phi(p_x)\\ &= \int_{-\infty}^{+\infty}\mathrm{d}p_x\int_{-\infty}^{+\infty}\mathrm{d}p'_x\delta(p_x-p'_x)\mathrm{e}^{-\mathrm{i}[E(p_x)-E(p'_x)]t/\hbar}\phi^*(p'_x)\phi(p_x)\\ &= \int_{-\infty}^{+\infty}\phi^*(p_x)\phi(p_x)\mathrm{d}p_x\\ &= 1 \end{aligned} \tag{2.45}$$

where in the second line we have introduced the Dirac delta function $\delta(p_x - p'_x)$ such that (see (A.18))

$$\begin{aligned}(2\pi\hbar)^{-1}\int_{-\infty}^{+\infty}\mathrm{e}^{\mathrm{i}[(p_x-p'_x)x]/\hbar}\mathrm{d}x &= (2\pi)^{-1}\int_{-\infty}^{+\infty}\mathrm{e}^{\mathrm{i}[(p_x-p'_x)x']}\mathrm{d}x'\\ &= \delta(p_x-p'_x)\end{aligned} \tag{2.46}$$

and used the property (A.26) in the third line. The result (2.45) expresses the *conservation of probability*, which is clearly a requirement of the theory. We note that if $\Psi(x,t)$ is normalised to unity, so is also the momentum space wave function $\Phi(p_x,t)$.

Gaussian wave packet

As an example, we shall now study the particular case in which the function $\phi(p_x)$ is a Gaussian function peaked about the value p_0

$$\phi(p_x) = C\exp\left[-\frac{(p_x-p_0)^2}{2(\Delta p_x)^2}\right] \tag{2.47}$$

where Δp_x, which we call the width of the distribution in p_x, is a constant such that $|\phi(p_x)|^2$ drops to $1/\mathrm{e}$ of its maximum value at $p_x = p_0 \pm \Delta p_x$ (see Fig. 2.5(a)). The constant C in (2.47) is a *normalisation constant* which we shall choose in such a way that the normalisation condition (2.44) is satisfied. Using the known result

$$\int_{-\infty}^{+\infty}\mathrm{e}^{-\alpha u^2}\mathrm{e}^{-\beta u}\mathrm{d}u = \left(\frac{\pi}{\alpha}\right)^{1/2}\mathrm{e}^{\beta^2/4\alpha} \tag{2.48}$$

with $u = p_x - p_0$, $\alpha = (\Delta p_x)^{-2}$ and $\beta = 0$, we have

$$\int_{-\infty}^{+\infty}|\phi(p_x)|^2\mathrm{d}p_x = |C|^2\pi^{1/2}\Delta p_x. \tag{2.49}$$

The normalisation condition (2.44) is therefore fulfilled by taking

$$|C|^2 = \pi^{-1/2}(\Delta p_x)^{-1}. \tag{2.50}$$

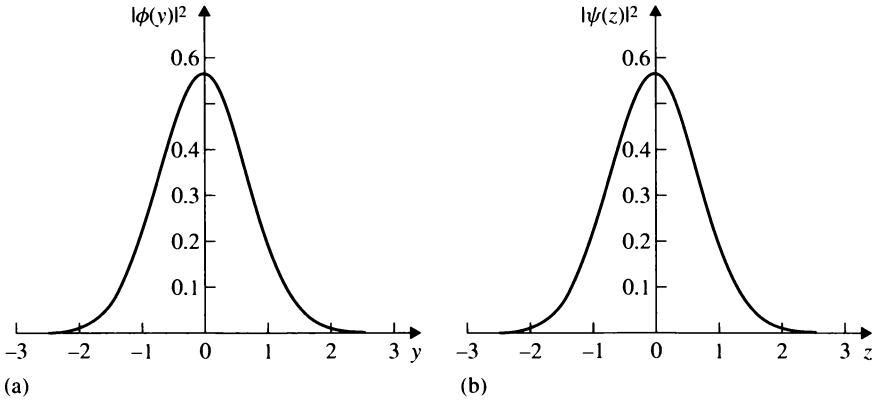

Figure 2.5 (a) The function $|\phi(y)|^2 = \pi^{-1/2}\exp(-y^2)$, where $y = (p_x - p_0)/\Delta p_x$. (b) The function $|\psi(z)|^2 = \pi^{-1/2}\exp(-z^2)$, where $z = (\Delta p_x/\hbar)x$.

The constant C is determined by (2.50) apart from a phase factor of unit modulus, which can be set equal to one, so that we can take C to be given by

$$C = \pi^{-1/4}(\Delta p_x)^{-1/2}. \tag{2.51}$$

Substituting $\phi(p_x)$ given by (2.47) into (2.40) and using (2.48) and (2.51), we find that

$$\psi(x) \equiv \Psi(x, t = 0) = \pi^{-1/4}\hbar^{-1/2}(\Delta p_x)^{1/2}e^{ip_0x/\hbar}e^{-(\Delta p_x)^2x^2/2\hbar^2}. \tag{2.52}$$

Apart from the phase factor $\exp(ip_0x/\hbar)$, this function is again a Gaussian. We remark that $|\psi(x)|^2$ has a maximum at $x = 0$ and falls to $1/e$ of its maximum value at $x = \pm\Delta x$, where $\Delta x = \hbar/\Delta p_x$ is the width of the distribution in the x variable (see Fig. 2.5(b)). Given the above definitions of the 'widths' Δx and Δp_x, we see that for a Gaussian wave packet $\Delta x \Delta p_x = \hbar$. Thus if we decrease Δp_x so that the wave function in momentum space, $\phi(p_x)$, is more sharply peaked about $p_x = p_0$, then Δx will increase and $\psi(x)$ becomes increasingly 'delocalised'. Conversely, if Δp_x is increased, so that $\phi(p_x)$ is 'delocalised' in momentum space, then $\psi(x)$ will become more strongly localised about $x = 0$. We shall return shortly to this important property, which is of a general nature. We note from (2.40) and (A.26) that in the limit in which $\phi(p_x)$ is the delta function $\delta(p_x - p_0)$, the wave function $\psi(x)$ becomes the plane wave $(2\pi\hbar)^{-1/2}\exp(ip_0x/\hbar)$, which is completely delocalised.

Let us now examine how the Gaussian wave packet evolves in time. Using (2.23), (2.33), (2.47), (2.51) and (2.48) we find that

$$\Psi(x,t) = \pi^{-1/4}\left[\frac{\Delta p_x/\hbar}{1 + i(\Delta p_x)^2 t/m\hbar}\right]^{1/2} \times \exp\left[\frac{ip_0x/\hbar - (\Delta p_x/\hbar)^2x^2/2 - ip_0^2t/2m\hbar}{1 + i(\Delta p_x)^2t/m\hbar}\right] \tag{2.53}$$

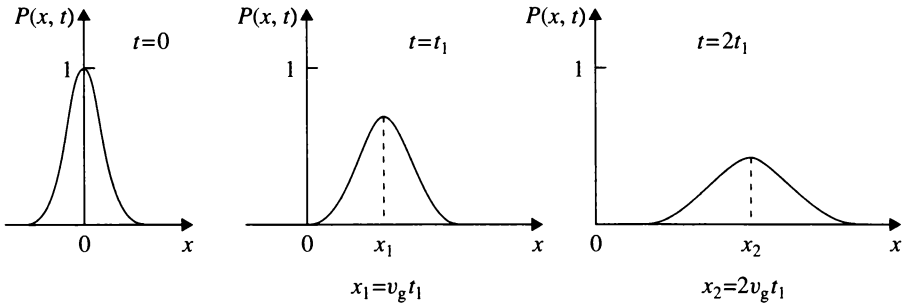

Figure 2.6 The position probability density $P(x, t) = |\Psi(x, t)|^2$ for a Gaussian wave packet at times $t = 0$, $t = t_1$ and $t = 2t_1$, plotted in arbitrary units.

and the corresponding position probability density is

$$P(x,t) = |\Psi(x,t)|^2 = \pi^{-1/2}\frac{\Delta p_x/\hbar}{[1+(\Delta p_x)^4 t^2/m^2\hbar^2]^{1/2}} \times \exp\left[-\frac{(\Delta p_x/\hbar)^2(x-v_g t)^2}{1+(\Delta p_x)^4 t^2/m^2\hbar^2}\right] \tag{2.54}$$

where we recall that $v_g = p_0/m$ is the group velocity of the packet. It is clear from (2.54) that the centre of the wave packet moves uniformly with the velocity v_g. The width of the packet, defined so that $P(x, t)$ falls to $1/e$ of its maximum value at the points $x - v_g t = \pm\Delta x$, is given by

$$\Delta x(t) = \frac{\hbar}{\Delta p_x}\left[1+\frac{(\Delta p_x)^4}{m^2\hbar^2}t^2\right]^{1/2} \tag{2.55}$$

and hence increases with time. However, if the time is sufficiently small so that

$$t \ll t_1 = \frac{m\hbar}{(\Delta p_x)^2} \tag{2.56}$$

the second term in brackets in (2.55) is very small and the wave packet propagates without changing its width appreciably. This is in accordance with our general discussion (see (2.36)–(2.39)). The spreading of the probability density (2.54) is illustrated in Fig. 2.6, where $P(x, t)$ is shown for times $t = 0$, $t = t_1$ and $t = 2t_1$.

To take a particular case, consider a Gaussian wave packet associated with an electron which at time $t = 0$ is localised to within a distance 10^{-10} m characteristic of atomic dimensions, so that $\Delta p_x = \hbar/\Delta x \simeq 10^{-24}$ kg m s^{-1}. According to (2.55) the wave packet will have spread to twice its size at time $t = \sqrt{3}t_1 \simeq 10^{-16}$ s (see Problem 2.7). On the other hand, for a macroscopic object having a mass of 1 g, whose position is initially defined within an accuracy $\Delta x \simeq 10^{-6}$ m, we find that the width of the packet doubles after a time $t \simeq 10^{19}$ s, which is larger than the estimated age of the universe.

A word of caution should be said about the interpretation of these results. Let us suppose that we have a wave packet representing an electron, which is spread so that the width of the packet is, for example, $\Delta x = 1$ km at a given time. If an electron detector is placed at a particular position at that time, it will record the presence or absence of the 'complete' electron, since when the electron manifests itself in the detection process it is indivisible. Before the electron is detected the wave function determines the *probability* that the electron will be found at a certain place, at a given time. As soon as the electron has been detected, its location is of course known to within a precision $\Delta x' \ll \Delta x$, so that a new wave function must describe the situation. This change of the wave function upon measurement is called the '*collapse of the wave packet*'. A more careful analysis of this measurement problem can be based on the study of the combined wave function of the measured system and the measuring apparatus. Using this approach, it will be shown in Chapter 17 that the idea of an instantaneous 'collapse' of 'reduction' of the wave function on measurement can be avoided.

Wave packets in three dimensions

Our discussions of one-dimensional free-particle wave packets can easily be extended to three dimensions. By superposing plane waves of the form (2.16) we obtain the wave packet

$$\begin{aligned}\Psi(\mathbf{r},t) &= (2\pi\hbar)^{-3/2}\int_{-\infty}^{+\infty}\mathrm{d}p_x\int_{-\infty}^{+\infty}\mathrm{d}p_y\int_{-\infty}^{+\infty}\mathrm{d}p_z\mathrm{e}^{\mathrm{i}[\mathbf{p}.\mathbf{r}-E(p)t]/\hbar}\phi(\mathbf{p})\\ &= (2\pi\hbar)^{-3/2}\int\mathrm{e}^{\mathrm{i}[\mathbf{p}.\mathbf{r}-E(p)t]/\hbar}\phi(\mathbf{p})\mathrm{d}\mathbf{p}\end{aligned} \tag{2.57}$$

where $\mathrm{d}\mathbf{p} = \mathrm{d}p_x\mathrm{d}p_y\mathrm{d}p_z$ is the volume element in momentum space. Writing $\psi(\mathbf{r}) \equiv \Psi(\mathbf{r}, t=0)$ we see from Appendix A that

$$\psi(\mathbf{r}) = (2\pi\hbar)^{-3/2}\int\mathrm{e}^{\mathrm{i}\mathbf{p}.\mathbf{r}/\hbar}\phi(\mathbf{p})\mathrm{d}\mathbf{p} \tag{2.58}$$

and

$$\phi(\mathbf{p}) = (2\pi\hbar)^{-3/2}\int\mathrm{e}^{-\mathrm{i}\mathbf{p}.\mathbf{r}/\hbar}\psi(\mathbf{r})\mathrm{d}\mathbf{r} \tag{2.59}$$

are three-dimensional *Fourier transforms* of each other. Paralleling our discussion of the one-dimensional case, a *momentum space wave function* $\Phi(\mathbf{p}, t)$ can be introduced as the Fourier transform of the wave function $\Psi(\mathbf{r}, t)$, so that

$$\Psi(\mathbf{r},t) = (2\pi\hbar)^{-3/2}\int\mathrm{e}^{\mathrm{i}\mathbf{p}.\mathbf{r}/\hbar}\Phi(\mathbf{p},t)\mathrm{d}\mathbf{p} \tag{2.60}$$

and

$$\Phi(\mathbf{p},t) = (2\pi\hbar)^{-3/2}\int\mathrm{e}^{-\mathrm{i}\mathbf{p}.\mathbf{r}/\hbar}\Psi(\mathbf{r},t)\mathrm{d}\mathbf{r} \tag{2.61}$$

and we note that $\phi(\mathbf{p}) = \Phi(\mathbf{p}, t = 0)$. As in the one-dimensional case (see (2.43)) this definition of the momentum space wave function is completely general, and holds for all types of wave functions $\Psi(\mathbf{r}, t)$. If $\phi(\mathbf{p})$ is normalised to unity, then $\Psi(\mathbf{r}, t)$ is also normalised to unity at all times, i.e. satisfies (2.7). The momentum space wave function $\Phi(\mathbf{p}, t)$ will then also be normalised to unity, satisfying

$$\int |\Phi(\mathbf{p}, t)|^2 \mathrm{d}\mathbf{p} = 1. \tag{2.62}$$

As a result, the quantity

$$\Pi(\mathbf{p}, t)\mathrm{d}\mathbf{p} = |\Phi(\mathbf{p}, t)|^2 \mathrm{d}\mathbf{p} = \Phi^*(\mathbf{p}, t)\Phi(\mathbf{p}, t)\mathrm{d}\mathbf{p} \tag{2.63}$$

is the probability at time t that the momentum of the particle lies within the momentum space volume element $\mathrm{d}\mathbf{p} \equiv \mathrm{d}p_x \mathrm{d}p_y \mathrm{d}p_z$ about the point $\mathbf{p} \equiv (p_x, p_y, p_z)$.

A three-dimensional wave packet associated with a free particle having fairly well determined values of both position coordinates (x, y, z) and momentum coordinates (p_x, p_y, p_z) can be constructed analogously to the one-dimensional case. Assuming that the function $\phi(\mathbf{p})$ in (2.57) is peaked about $\mathbf{p} = \mathbf{p}_0$, and setting

$$\beta(\mathbf{p}) = \mathbf{p}.\mathbf{r} - E(p)t \tag{2.64}$$

one finds (Problem 2.8) that the centre of the wave packet, defined by the condition[1]

$$[\nabla_{\mathbf{p}}\beta(\mathbf{p})]_{\mathbf{p}=\mathbf{p}_0} = 0 \tag{2.65}$$

travels with a uniform motion according to the law

$$\mathbf{r} = \mathbf{v}_{\mathrm{g}} t \tag{2.66}$$

where

$$\mathbf{v}_{\mathrm{g}} = [\nabla_{\mathbf{p}} E(p)]_{\mathbf{p}=\mathbf{p}_0} \tag{2.67}$$

is the *group velocity* of the wave packet. Equations (2.66) and (2.67) are the generalisations of equations (2.27) and (2.28), respectively. In the classical limit the group velocity $\mathbf{v}_{\mathrm{g}}$ must be equal to the velocity $\mathbf{v} = \mathbf{p}_0/m$ of the particle, from which we find that the functional relation between E and p is given by

$$E(p) = \frac{p^2}{2m} \tag{2.68}$$

apart from an additive constant which can be chosen to be zero.

[1] In equation (2.65), $\nabla_{\mathbf{p}}\beta(\mathbf{p})$ is a vector having Cartesian components $\partial\beta(p_x, p_y, p_z)/\partial p_x$, $\partial\beta(p_x, p_y, p_z)/\partial p_y$ and $\partial\beta(p_x, p_y, p_z)/\partial p_z$.

Wave packets in a slowly varying potential

The general idea we have developed for the motion of a free-particle wave packet in the classical limit can be extended to describe the motion of a particle in a potential $V(\mathbf{r})$ provided that the potential does not vary appreciably over a distance comparable to the de Broglie wavelength of the particle. In this case the centre of the wave packet travels along the trajectory followed by a classical particle moving in the potential $V(\mathbf{r})$. As the centre of the wave packet moves along this trajectory, the de Broglie wavelength changes slowly, being determined by the relation

$$\lambda = \frac{h}{p} = \frac{h}{[2m(E - V(\mathbf{r}))]^{1/2}} \tag{2.69}$$

where $p = [2m(E - V(\mathbf{r}))]^{1/2}$ is the classical local momentum of the particle.

2.5 The Heisenberg uncertainty principle

We have shown in the case of a one-dimensional Gaussian wave packet that the 'width' Δx of the distribution in the position variable x is linked with the 'width' Δp_x of the distribution in the momentum p_x by the relation $\Delta x \Delta p_x \geqslant \hbar$. In fact, it is a general property of Fourier transforms that 'widths' in position and momentum satisfy the relation

$$\Delta x \Delta p_x \gtrsim \hbar \tag{2.70}$$

where the sign $\gtrsim$ means 'greater than or of the order of'. In the context of quantum mechanics this is called the *Heisenberg uncertainty relation for position and momentum*, according to which a state cannot be prepared in which both the position and momentum of a particle can be defined simultaneously to arbitrary accuracy. In fact, the product of the uncertainty Δx in the precision with which the position can be defined with the uncertainty Δp_x in the precision with which the momentum can be defined, cannot be made smaller than a quantity of order $\hbar$. At this point we have not given a precise definition of the uncertainties Δx and Δp_x, but this will be done later, in Chapter 5.

The relation (2.70) is easily generalised to three dimensions by using the properties of three-dimensional Fourier transforms. The three-dimensional form of the Heisenberg uncertainty relations for position and momentum is

$$\Delta x \Delta p_x \gtrsim \hbar, \qquad \Delta y \Delta p_y \gtrsim \hbar, \qquad \Delta z \Delta p_z \gtrsim \hbar. \tag{2.71}$$

It should be noted that there is no relation between the uncertainty in one Cartesian component of the position vector of a particle, for example Δx, and the uncertainty in a *different* Cartesian component of the momentum, for example Δp_y. The only restrictions are on the 'complementary' pairs: Δx, Δp_x; Δy, Δp_y; and Δz, Δp_z.

It is worth stressing that the Heisenberg uncertainty relations do not place any restriction on the precision with which a position measurement of a particle can be