

Chapter 2

Wave Functions

2.1 Classical and Quantum Particles

In classical Hamiltonian mechanics the *state* of a particle at a given instant of time is given by two vectors: $\mathbf{r} = (x, y, z)$ representing its position, and $\mathbf{p} = (p_x, p_y, p_z)$ representing its momentum. One can think of these two vectors together as determining a point in a six-dimensional *phase space*. As time increases the point representing the state of the particle traces out an *orbit* in the phase space. To simplify the discussion, consider a particle which moves in only one dimension, with position x and momentum p . Its phase space is the two-dimensional x, p plane. If, for example, one is considering a harmonic oscillator with angular frequency ω , the orbit of a particle of mass m will be an ellipse of the form

$$x = A \sin(\omega t + \phi), \quad p = mA\omega \cos(\omega t + \phi) \quad (2.1)$$

for some amplitude A and phase ϕ , as shown in Fig. 2.1.

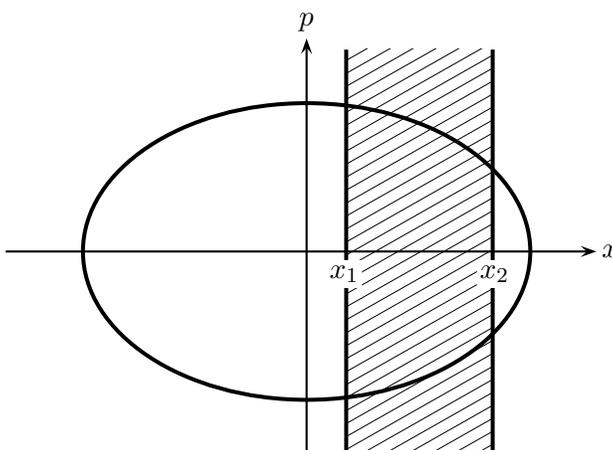


Figure 2.1: Phase space x, p for a particle in one dimension. The ellipse is a possible orbit for a harmonic oscillator. The cross-hatched region corresponds to $x_1 \leq x \leq x_2$.

A quantum particle at a single instant of time is described by a *wave function* $\psi(\mathbf{r})$, a complex function of position \mathbf{r} . Again in the interests of simplicity we will consider a quantum particle moving in one dimension, so that its wave function $\psi(x)$ depends on only a single variable, the position x . Some examples of real-valued wave functions, which can be sketched as simple graphs, are shown in Figs. 2.2 to 2.4. It is important to note that *all* of the information required to describe a quantum state is contained in the function $\psi(x)$. Thus this one function is the quantum analog of the pair of real numbers x and p used to describe a classical particle at a particular time.

In order to understand the physical significance of quantum wave functions, one needs to know that they belong to a *linear vector space* \mathcal{H} . That is, if $\psi(x)$ and $\phi(x)$ are any two wave functions belonging to \mathcal{H} , the *linear combination*

$$\omega(x) = \alpha\psi(x) + \beta\phi(x), \quad (2.2)$$

where α and β are any two complex numbers, also belongs to \mathcal{H} . The space \mathcal{H} is equipped with an *inner product* which assigns to any two wave functions $\psi(x)$ and $\phi(x)$ the complex number

$$\langle\phi|\psi\rangle = \int_{-\infty}^{+\infty} \phi^*(x)\psi(x) dx. \quad (2.3)$$

Here $\phi^*(x)$ denotes the complex conjugate of the function $\phi(x)$. (The notation used in (2.3) is standard among physicists, and differs in some trivial but annoying details from that generally employed by mathematicians.)

The inner product $\langle\phi|\psi\rangle$ is analogous to the dot product

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z \quad (2.4)$$

of two ordinary vectors \mathbf{a} and \mathbf{b} . One difference is that a dot product is always a real number, and $\mathbf{a} \cdot \mathbf{b}$ is the same as $\mathbf{b} \cdot \mathbf{a}$. By contrast, the inner product defined in (2.3) is in general a complex number, and interchanging $\psi(x)$ with $\phi(x)$ yields the complex conjugate:

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*. \quad (2.5)$$

Despite this difference, the analogy between a dot product and an inner product is useful in that it provides an intuitive geometrical picture of the latter.

If $\langle\phi|\psi\rangle = 0$, which in view of (2.5) is equivalent to $\langle\psi|\phi\rangle = 0$, the functions $\psi(x)$ and $\phi(x)$ are said to be *orthogonal* to each other. This is analogous to $\mathbf{a} \cdot \mathbf{b} = 0$, which means that \mathbf{a} and \mathbf{b} are perpendicular to each other. The concept of orthogonal (“perpendicular”) wave functions, along with certain generalizations of this notion, plays an extremely important role in the physical interpretation of quantum states. The inner product of $\psi(x)$ with itself,

$$\|\psi\|^2 = \int_{-\infty}^{+\infty} \psi^*(x)\psi(x) dx. \quad (2.6)$$

is a positive number whose (positive) square root $\|\psi\|$ is called the *norm* of $\psi(x)$. The integral must be less than infinity for a wave function to be a member of \mathcal{H} . Thus $\exp(-ax^2)$ for $a > 0$ is a member of \mathcal{H} , whereas $\exp(ax^2)$ is not.

A complex linear space \mathcal{H} with an inner product is known as a *Hilbert space* provided it satisfies some additional conditions which are discussed in texts on functional analysis and mathematical physics, but lie outside the scope of this book (see the remarks in Sec. 1.4). Because of the condition that the norm as defined in (2.6) be finite, the linear space of wave functions is called the *Hilbert space of square-integrable functions*, often denoted by L^2 .

2.2 Physical Interpretation of the Wave Function

The intuitive significance of the pair of numbers x, p used to describe a classical particle in one dimension at a particular time is relatively clear: the particle is located at the point x , and its velocity is p/m . The interpretation of a quantum wave function $\psi(x)$, on the other hand, is much more complicated, and an intuition for what it means has to be built up by thinking about various examples. We will begin this process in Sec. 2.3 below. However, it is convenient at this point to make some very general observations, comparing and contrasting quantum with classical descriptions.

Any point x, p in the classical phase space represents a possible state of the classical particle. In a similar way, almost every wave function in the space \mathcal{H} represents a possible state of a quantum particle. The exception is the state $\psi(x)$ which is equal to 0 for every value of x , and thus has norm $\|\psi\| = 0$. This is an element of the linear space, and from a mathematical point of view it is a very significant element. Nevertheless, it cannot represent a possible state of a physical system. All the other members of \mathcal{H} represent possible quantum states.

A point in the phase space represents the most precise description one can have of the state of a classical particle. If one knows both x and p for a particle in one dimension, that is all there is to know. In the same way, the quantum wave function $\psi(x)$ represents a complete description of a quantum particle, there is nothing more that can be said about it. To be sure, a classical “particle” might possess some sort of internal structure and in such a case the pair x, p , or \mathbf{r}, \mathbf{p} , would represent the position of the center of mass and the total momentum, respectively, and one would need additional variables in order to describe the internal degrees of freedom. Similarly, a quantum particle can possess an internal structure, in which case $\psi(x)$ or $\psi(\mathbf{r})$ provides a complete description of the center of mass, whereas ψ must also depend upon additional variables if it is to describe the internal structure as well as the center of mass. The quantum description of particles with internal degrees of freedom, and of collections of several particles is taken up in Ch. 6.

An important difference between the classical phase space and the quantum Hilbert space \mathcal{H} has to do with the issue of whether elements which are mathematically distinct describe situations which are physically distinct. Let us begin with the classical case, which is relatively straightforward. Two states (x, p) and (x', p') represent the same physical state if and only if

$$x' = x, \quad p' = p, \tag{2.7}$$

that is, if the two points in phase space coincide with each other. Otherwise they represent *mutually exclusive possibilities*: a particle cannot be in two different places at the same time, nor can it have two different values of momentum (or velocity) at the same time. To summarize, two states of a classical particle have the same *physical interpretation* if and only if they have the same *mathematical description*.

The case of a quantum particle is not nearly so simple. There are three different situations one needs to consider.

1. If two functions $\psi(x)$ and $\phi(x)$ are *multiples of each other*, that is, $\phi(x) = \alpha\psi(x)$ for some non-zero complex number α , then these two functions have *precisely the same* physical meaning. For example, all three functions in Fig. 2.2 have the same physical meaning. This is in marked contrast to the waves one is familiar with in classical physics, such as sound waves, or waves on the surface of water. Increasing the amplitude of a sound wave by a factor of two means that it carries four times as much energy, whereas multiplying a quantum wave function by two leaves its physical significance unchanged.

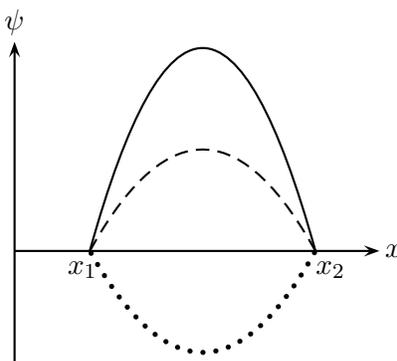


Figure 2.2: Three wave functions which have the same physical meaning.

Given any $\psi(x)$ with positive norm, it is always possible to introduce another function

$$\bar{\psi}(x) = \psi(x)/\|\psi\| \quad (2.8)$$

which has the same physical meaning as $\psi(x)$, but whose norm is $\|\bar{\psi}\| = 1$. Such *normalized* states are convenient when carrying out calculations, and for this reason quantum physicists often develop a habit of writing wave functions in normalized form, even when it is not really necessary. A normalized wave function remains normalized when it is multiplied by a complex constant $e^{i\phi}$, where the phase ϕ is some real number, and of course its physical meaning is not changed. Thus a normalized wave function representing some physical situation still has an *arbitrary phase*.

Warning! Although multiplying a wave function by a non-zero scalar does not change its physical significance, there are cases in which a careless use of this principle can lead to mistakes. Suppose that one is interested in a wave function which is a linear combination of two other functions,

$$\psi(x) = \phi(x) + \omega(x). \quad (2.9)$$

Multiplying $\phi(x)$ but not $\omega(x)$ by a complex constant α leads to a function

$$\tilde{\psi}(x) = \alpha\phi(x) + \omega(x) \quad (2.10)$$

which does *not*, at least in general, have the same physical meaning as $\psi(x)$, because it is not equal to a constant times $\psi(x)$.

2. Two wave functions $\phi(x)$ and $\psi(x)$ which are orthogonal to each other, $\langle\phi|\psi\rangle = 0$, represent *mutually exclusive* physical states: if one of them is true, in the sense that it is a correct description of the quantum system, the other is false, that is, an incorrect description of the quantum system. For example, the inner product of the two wave functions $\phi(x)$ and $\psi(x)$ sketched in Fig. 2.3 is zero, because at any x where one of them is finite, the other is zero, and thus the integrand in (2.3) is zero. As discussed in Sec. 2.3, if a wave function vanishes outside some finite interval, the quantum particle is located inside that interval. Since the two intervals $[x_1, x_2]$ and $[x_3, x_4]$ in Fig. 2.3 do not overlap, they represent mutually exclusive possibilities: if the particle is in one interval, it cannot be in the other.

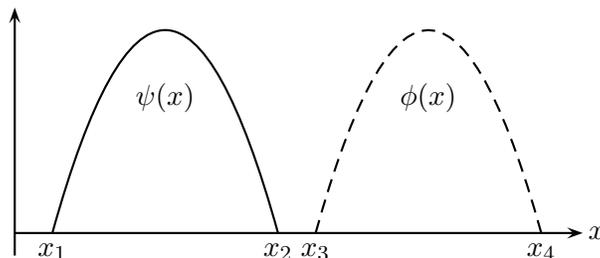


Figure 2.3: Two orthogonal wave functions.

In Fig. 2.4, $\psi(x)$ and $\phi(x)$ are the ground state and first excited state of a quantum particle in a smooth, symmetrical potential well (such as a harmonic oscillator). In this case the vanishing of $\langle\phi|\psi\rangle$ is not quite so obvious, but it follows from the fact that $\psi(x)$ is an even and $\phi(x)$ an odd function of x . Thus their product is an odd function of x , and the integral in (2.3) vanishes. From a physical point of view these two states are mutually exclusive possibilities because if a quantum particle has a definite energy, it cannot have some other energy.

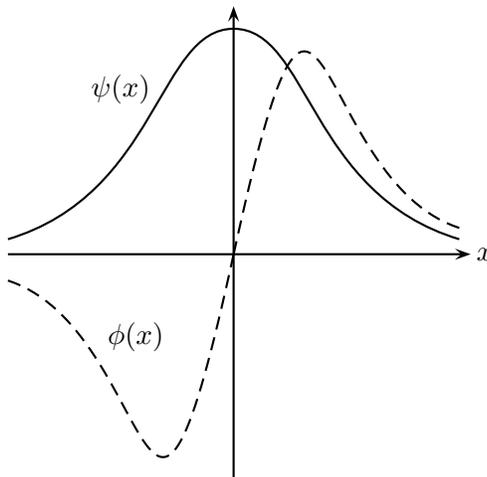


Figure 2.4: Two orthogonal wave functions.

3. If $\phi(x)$ and $\psi(x)$ are *not* multiples of each other, and $\langle\phi|\psi\rangle$ is *not* equal to zero, the two

wave functions represent *incompatible* states of affairs, a relationship which will be discussed in Sec. 4.6. Figure 2.5 shows a pair of incompatible wave functions. It is obvious that $\phi(x)$ cannot be a multiple of $\psi(x)$, because there are values of x at which ϕ is positive and ψ is zero. On the other hand, it is also obvious that the inner product $\langle\phi|\psi\rangle$ is not zero, for the integrand in (2.3) is positive, and non-zero over a finite interval.

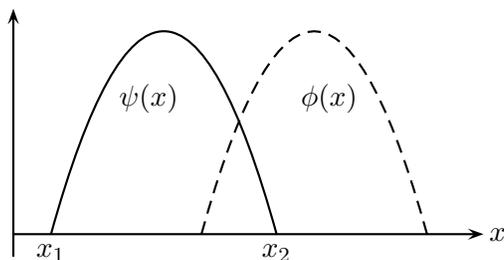


Figure 2.5: Two incompatible wave functions.

There is nothing in classical physics corresponding to descriptions which are incompatible in the quantum sense of the term. This is one of the main reasons why quantum theory is hard to understand: there is no good classical analogy for the situation shown in Fig. 2.5. Instead, one has to build up one's physical intuition for this situation using examples that are quantum mechanical. It is important to keep in mind that quantum states which are *incompatible* stand in a very different relationship to each other than states which are *mutually exclusive*; one must not confuse these two concepts!

2.3 Wave Functions and Position

The quantum wave function $\psi(x)$ is a function of x , and in classical physics x is simply the position of the particle. But what can one say about the position of a quantum particle described by $\psi(x)$? In classical physics wave packets are used to describe water waves, sound waves, radar pulses, and the like. In each of these cases the wave packet does not have a precise position; indeed, one would not recognize something as a wave if it were not spread out to some extent. Thus there is no reason to suppose that a quantum particle possesses a precise position if it is described by a wave function $\psi(x)$, since the wave packet itself, thought of as a mathematical object, is obviously not located at a precise position x .

In addition to waves, there are many objects, such as clouds and cities, which do not have a precise location. These, however, are made up of other objects whose location is more definite: individual water droplets in a cloud, or individual buildings in a city. However, in the case of a quantum wave packet, a more detailed description in terms of smaller (better localized) physical objects or properties is not possible. To be sure, there is a very localized *mathematical* description: at each x the wave packet takes on some precise value $\psi(x)$. But there is no reason to suppose that this represents a corresponding physical "something" located at this precise point. Indeed, the discussion in Sec. 2.2 above suggests quite the opposite. To begin with, the value of $\psi(x_0)$ at a particular point x_0 cannot in any direct way represent the value of some physical quantity, since one

can always multiply the function $\psi(x)$ by a complex constant to obtain another wave function with the same physical significance, and thus altering $\psi(x_0)$ in an arbitrary fashion (unless, of course, $\psi(x_0) = 0$). Furthermore, in order to see that the mathematically distinct wave functions in Fig. 2.2 represent the same physical state of affairs, and that the two functions in Fig. 2.4 represent distinct physical states, one cannot simply carry out a point-by-point comparison; instead it is necessary to consider each wave function “as a whole”.

It is probably best to think of a quantum particle as *delocalized*, that is, as not having a position which is more precise than that of the wave function representing its quantum state. The term “delocalized” should be understood as meaning that no precise position can be defined, and not as suggesting that a quantum particle is in two different places at the same time. Indeed, we shall show in Sec. 4.5, there is a well-defined sense in which a quantum particle *cannot* be in two (or more) places at the same time.

Things which do not have precise positions, such as books and tables, can nonetheless often be assigned *approximate* locations, and it is often useful to do so. The situation with quantum particles is similar. There are two different, though related, approaches to assigning an approximate position to a quantum particle in one dimension (with obvious generalizations to higher dimensions). The first is mathematically quite “clean”, but can only be applied for a rather limited set of wave functions. The second is mathematically “sloppy”, but is often of more use to the physicist. Both of them are worth discussing, since each adds to one’s physical understanding of the meaning of a wave function.

It is sometimes the case, as in the examples in Figs. 2.2, 2.3 and 2.5, that the quantum wave function is non-zero only in some finite interval

$$x_1 \leq x \leq x_2. \tag{2.11}$$

In such a case it is safe to assert that the quantum particle is *not* located *outside* this interval, or, equivalently, that it is inside this interval, provided the latter is not interpreted to mean that there is some precise point inside the interval where the particle is located. In the case of a classical particle, the statement that it is not outside, and therefore inside the interval (2.11) corresponds to asserting that the point x, p representing the state of the particle falls somewhere inside the region of its phase space indicated by the crosshatching in Fig. 2.1. To be sure, since the actual position of a classical particle must correspond to a single number x , we know that if it is inside the interval (2.11), then it is actually located at a definite point in this interval, even though we may not know what this precise point is. By contrast, in the case of any of the wave functions in Fig. 2.2 it is incorrect to say that the particle has a location which is more precise than is given by the interval (2.11), because the wave packet cannot be located more precisely than this, and the particle cannot be located more precisely than its wave packet.

There is a quantum analog of the cross-hatched region of the phase space in Fig. 2.1: it is the collection of all wave functions in \mathcal{H} with the property that they vanish outside the interval $[x_1, x_2]$. There are, of course, a very large number of wave functions of this type, a few of which are indicated in Fig. 2.6. Given a wave function which vanishes outside (2.11), it still has this property if multiplied by an arbitrary complex number. And the sum of two wave functions of this type will also vanish outside the interval. Thus the collection of all functions which vanish outside $[x_1, x_2]$ is itself a linear space. If in addition we impose the condition that the allowable functions have a finite norm, the corresponding collection of functions \mathcal{X} is part of the collection \mathcal{H} of all allowable

wave functions, and because \mathcal{X} is a linear space, it is a *subspace* of the quantum Hilbert space \mathcal{H} . As we shall see in Ch. 4, a *physical property* of a quantum system can always be associated with a subspace of \mathcal{H} , in the same way that a physical property of a classical system corresponds to a subset of points in its phase space. In the case at hand, the physical property of being located inside the interval $[x_1, x_2]$ corresponds in the classical case to the crosshatched region in Fig. 2.1, and in the quantum case to the subspace \mathcal{X} which has just been defined.

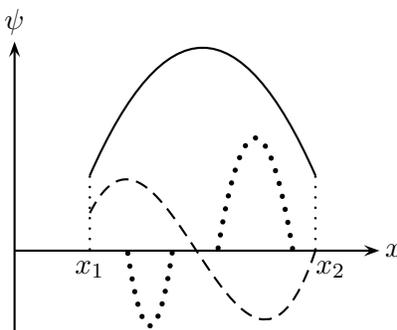


Figure 2.6: Some of the many wave functions which vanish outside the interval $x_1 \leq x \leq x_2$.

The notion of approximate location discussed above has limited applicability, because one is often interested in wave functions which are never equal to zero, or at least do not vanish outside some finite interval. An example is the Gaussian wave packet

$$\psi(x) = \exp[-(x - x_0)^2/4(\Delta x)^2], \quad (2.12)$$

centered at $x = x_0$, where Δx is a constant, with the dimensions of a length, that provides a measure of the width of the wave packet. The function $\psi(x)$ is never equal to zero. However, when $|x - x_0|$ is large compared to Δx , $\psi(x)$ is very small, and so it seems sensible, at least to a physicist, to suppose that for this quantum state, the particle is located “near” x_0 , say within an interval

$$x_0 - \lambda\Delta x \leq x \leq x_0 + \lambda\Delta x, \quad (2.13)$$

where λ might be set equal to 1 when making a rough back-of-the-envelope calculation, or perhaps 2 or 3 or more if one is trying to be more careful or conservative.

What the physicist is, in effect, doing in such circumstances is approximating the Gaussian wave packet in (2.12) by a function which has been set equal to zero for x lying outside the interval (2.13). Once the “tails” of the Gaussian packet have been eliminated in this manner, one can employ the ideas discussed above for functions which vanish outside some finite interval. To be sure, “cutting off the tails” of the original wave function involves an approximation, and as with all approximations, this requires the application of some judgment as to whether or not one will be making a serious mistake, and this will in turn depend upon the sort of questions which are being addressed. Since approximations are employed in all branches of theoretical physics (apart from those which are indistinguishable from pure mathematics), it would be quibbling to deny this possibility to the quantum physicist. Thus it makes physical sense to say that the wave packet (2.12) represents a quantum particle with an approximate location given by (2.13), as long as λ is

not too small. Of course, similar reasoning can be applied to other wave packets which have long tails.

It is sometimes said that the meaning, or at least one of the meanings of the wave function $\psi(x)$ is that

$$\rho(x) = |\psi(x)|^2 / \|\psi\|^2 \quad (2.14)$$

is a probability distribution density for the particle to be located at the position x , or found to be at the position x by a suitable measurement. Wave functions can indeed be used to calculate probability distributions, and in certain circumstances (2.14) is a correct way to do such a calculation. However, in quantum theory it is necessary to differentiate between $\psi(x)$ as representing a *physical property* of a quantum system, and $\psi(x)$ as a *pre-probability*, a mathematical device for calculating probabilities. It is necessary to look at examples to understand this distinction, and we shall do so in Ch. 9, following a general discussion of probabilities in quantum theory in Ch. 5.

2.4 Wave Functions and Momentum

The state of a classical particle in one dimension is specified by giving both x and p , while in the quantum case the wave function $\psi(x)$ depends upon only one of these two variables. From this one might conclude that quantum theory has nothing to say about the momentum of a particle, but this is not correct. The information about the momentum provided by quantum mechanics is contained in $\psi(x)$, but one has to know how to extract it. A convenient way to do so is to define the *momentum wave function*

$$\hat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \exp[-ipx/\hbar] \psi(x) dx, \quad (2.15)$$

as the Fourier transform of $\psi(x)$.

Note that $\hat{\psi}(p)$ is completely determined by the position wave function $\psi(x)$. On the other hand, (2.15) can be inverted by writing

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \exp[+ipx/\hbar] \hat{\psi}(p) dp, \quad (2.16)$$

so that, in turn, $\psi(x)$ is completely determined by $\hat{\psi}(p)$. Therefore $\psi(x)$ and $\hat{\psi}(p)$ contain precisely the same information about a quantum state; they simply express this information in two different forms. Whatever may be the physical significance of $\psi(x)$, that of $\hat{\psi}(p)$ is exactly the same. One can say that $\psi(x)$ is the *position representation* and $\hat{\psi}(p)$ the *momentum representation* of the *single* quantum state which describes the quantum particle at a particular instant of time. (As an analogy, think of a novel published simultaneously in two different languages: the two editions represent exactly the same story, assuming the translator has done a good job.) The inner product (2.3) can be expressed equally well using either the position or the momentum representation:

$$\langle \phi | \psi \rangle = \int_{-\infty}^{+\infty} \phi^*(x) \psi(x) dx = \int_{-\infty}^{+\infty} \hat{\phi}^*(p) \hat{\psi}(p) dp. \quad (2.17)$$

Information about the momentum of a quantum particle can be obtained from the momentum wave function in the same way that information about its position can be obtained from the position

wave function, as discussed above in Sec. 2.3. A quantum particle, unlike a classical particle, does not possess a well-defined momentum. However, if $\hat{\psi}(p)$ vanishes outside an interval

$$p_1 \leq p \leq p_2, \quad (2.18)$$

it possesses an *approximate* momentum in that the momentum does *not* lie *outside* the interval (2.18); equivalently, the momentum lies inside this interval, though it does not have some particular precise value inside this interval.

Even when $\hat{\psi}(p)$ does not vanish outside any interval of the form (2.18), one can still assign an approximate momentum to the quantum particle in the same way that one can assign an approximate position when $\psi(x)$ has non-zero tails, as in (2.12). In particular, in the case of a Gaussian wave packet

$$\hat{\psi}(p) = \exp[-(p - p_0)^2/4(\Delta p)^2], \quad (2.19)$$

it is reasonable to say that the momentum is “near” p_0 in the sense of lying in the interval

$$p_0 - \lambda\Delta p \leq p \leq p_0 + \lambda\Delta p, \quad (2.20)$$

with λ on the order of 1 or larger. The justification for this is that one is approximating (2.19) with a function which has been set equal to zero outside the interval (2.20). Whether or not “cutting off the tails” in this manner is an acceptable approximation is a matter of judgment, just as in the case of the position wave packet discussed earlier in Sec. 2.3.

The momentum wave function can be used to calculate a probability distribution density

$$\hat{\rho}(p) = |\hat{\psi}(p)|^2 / \|\psi\|^2 \quad (2.21)$$

for the momentum p in much the same way as the position wave function can be used to calculate a similar density for x , (2.14). See the remarks following (2.14): it is important to distinguish between $\hat{\psi}(p)$ as representing a physical property, which is what we have been discussing, and as a pre-probability, which is its role in (2.21). If one sets $x_0 = 0$ in the Gaussian wave packet (2.12) and carries out the Fourier transform (2.15), the result is (2.19) with $p_0 = 0$ and $\Delta p = \hbar/2\Delta x$. As shown in introductory textbooks, it is quite generally the case that for any given quantum state,

$$\Delta p \cdot \Delta x \geq \hbar/2, \quad (2.22)$$

where $(\Delta x)^2$ is the variance of the probability distribution density (2.14), and $(\Delta p)^2$ the variance of the one in (2.21). Probabilities will be taken up later in the book, but for present purposes it suffices to regard Δx and Δp as convenient, albeit somewhat crude measures of the widths of the wave packets $\psi(x)$ and $\hat{\psi}(p)$, respectively. What the inequality tells us is that the narrower the position wave packet $\psi(x)$, the broader the corresponding momentum wave packet $\hat{\psi}(p)$ has got to be, and vice versa.

The inequality (2.22) expresses the well-known *Heisenberg uncertainty principle*. This principle is often discussed in terms of *measurements* of a particle’s position or momentum, and the difficulty of simultaneously measuring both of these quantities. While such discussions are not without merit—and we shall have more to say about measurements later in this book—they tend to put the emphasis in the wrong place, suggesting that the inequality somehow arises out of peculiarities

associated with measurements. But in fact (2.22) is a consequence of the decision by quantum physicists to use a Hilbert space of wave packets in order to describe quantum particles, and to make the momentum wave packet for a particular quantum state equal to the Fourier transform of the position wave packet for the same state. In the Hilbert space there are, as a fact of mathematics, no states for which the widths of the position and momentum wave packets violate the inequality (2.22). Hence if this Hilbert space is appropriate for describing the real world, no particles exist for which the position and momentum can even be approximately defined with a precision better than that allowed by (2.22). If measurements can accurately determine the properties of quantum particles—another topic to which we shall later return—then the results cannot, of course, be more precise than the quantities which are being measured. To use an analogy, the fact that the location of the city of Pittsburgh is uncertain by several kilometers has nothing to do with the lack of precision of surveying instruments. Instead a city, as an extended object, does not have a precise location.

2.5 Toy Model

The Hilbert space \mathcal{H} for a quantum particle in one dimension is extremely large; viewed as a linear space it is infinite-dimensional. Infinite-dimensional spaces provide headaches for physicists and employment for mathematicians. Most of the conceptual issues in quantum theory have nothing to do with the fact that the Hilbert space is infinite dimensional, and therefore it is useful, in order to simplify the mathematics, to replace the continuous variable x with a discrete variable m which takes on only a *finite number of integer values*. That is to say, we will assume that the quantum particle is located at one of a finite collection of sites arranged in a straight line, or, if one prefers, it is located in one of a finite number of boxes or cells. It is often convenient to think of this system of sites as having “periodic boundary conditions” or as placed on a circle, so that the last site is adjacent to (just in front of) the first site. If one were representing a wave function numerically on a computer, it would be sensible to employ a discretization of this type. However, our goal is not numerical computation, but physical insight. Temporarily shunting mathematical difficulties out of the way is part of a useful “divide and conquer” strategy for attacking difficult problems. Our aim will not be realistic descriptions, but instead *simple* descriptions which still contain the essential features of quantum theory. For this reason, the term “toy model” seems appropriate.

Let us suppose that the quantum wave function is of the form $\psi(m)$, with m an integer in the range

$$-M_a \leq m \leq M_b, \quad (2.23)$$

where M_a and M_b are fixed integers, so m can take on $M = M_a + M_b + 1$ different values. Such wave functions form an M -dimensional Hilbert space. For example, if, $M_a = 1 = M_b$, the particle can be at one of the three sites, $m = -1, 0, 1$, and its wave function is completely specified by the $M = 3$ complex numbers $\psi(-1)$, $\psi(0)$ and $\psi(1)$. The inner product of two wave functions is given by

$$\langle \phi | \psi \rangle = \sum_m \phi^*(m) \psi(m), \quad (2.24)$$

where the sum is over those values of m allowed by (2.23), and the norm of ψ is the positive square

root of

$$\|\psi\|^2 = \sum_m |\psi(m)|^2. \quad (2.25)$$

The toy wave function χ_n defined by

$$\chi_n(m) = \delta_{mn} = \begin{cases} 1 & \text{if } m = n, \\ 0 & \text{for } m \neq n, \end{cases} \quad (2.26)$$

where δ_{mn} is the Kronecker delta function, has the physical significance that the particle is at site n (or in cell n). Now suppose that $M_a = 3 = M_b$, and consider the wave function

$$\psi(m) = \chi_{-1}(m) + 1.5\chi_0(m) + \chi_1(m). \quad (2.27)$$

It is sketched in Fig. 2.7, and one can think of it as a relatively coarse approximation to a continuous function of the sort shown in Fig. 2.2, with $x_1 = -2$, $x_2 = +2$. What can one say about the location of the particle whose quantum wave function is given by (2.27)?

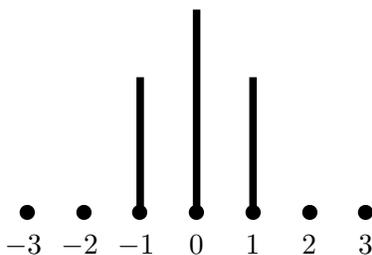


Figure 2.7: The toy wave packet (2.27).

In light of the discussion in Sec. 2.3 above it seems sensible to interpret $\psi(m)$ as signifying that the position of the quantum particle is not outside the interval $[-1, +1]$, where by $[-1, +1]$ we mean the three values -1 , 0 , and $+1$. The circumlocution “not outside the interval” can be replaced with the more natural “inside the interval” provided the latter is not interpreted to mean “at a particular site inside this interval”, since the particle described by (2.27) cannot be said to be at $m = -1$ or at $m = 0$ or at $m = 1$. Instead it is delocalized, and its position cannot be specified any more precisely than by giving the interval $[-1, +1]$. There is no concise way of stating this in English, which is one reason we need a mathematical notation in which quantum properties can be expressed in a precise way—this will be introduced in Ch. 4.

It is important not to look at a wave function written out as a sum of different pieces whose physical significance one understands, and interpret it in physical terms as meaning the quantum system has one or the other of the properties corresponding to the different pieces. In particular, one should not interpret (2.27) to mean that the particle is at $m = -1$ or at $m = 0$ or at $m = 1$. A simple example which illustrates how such an interpretation can lead one astray is obtained by writing χ_0 in the form

$$\chi_0(m) = (1/2)[\chi_0(m) + i\chi_2(m)] + (1/2)[\chi_0(m) + (-i)\chi_2(m)]. \quad (2.28)$$

If we carelessly interpret “+” to mean “or”, then both of the functions in square brackets on the right side of (2.28), and therefore also their sum, have the interpretation that the particle is at 0 or 2, whereas in fact $\chi_0(m)$ means that the particle is at 0 and *not* at 2. The correct quantum-mechanical way to use “or” will be discussed in Secs. 4.5, 4.6 and 5.2.

Just as $\psi(m)$ is a discrete version of the position wave function $\psi(x)$, there is also a discrete version $\hat{\psi}(k)$ of the momentum wave function $\hat{\psi}(p)$, given by the formula

$$\hat{\psi}(k) = \frac{1}{\sqrt{M}} \sum_m \exp[-2\pi i k m / M] \psi(m), \quad (2.29)$$

where k is an integer which can take on the same set of values as m , (2.23). The inverse transformation is

$$\psi(m) = \frac{1}{\sqrt{M}} \sum_k \exp[2\pi i k m / M] \hat{\psi}(k). \quad (2.30)$$

The inner product of two states, (2.24), can equally well be written in terms of momentum wave functions:

$$\langle \phi | \psi \rangle = \sum_k \hat{\phi}^*(k) \hat{\psi}(k). \quad (2.31)$$

These expressions are similar to those in (2.15) to (2.17). The main difference is that integrals have been replaced by sums. The reason \hbar has disappeared from the toy model expressions is that position and momentum are being expressed in dimensionless units.