

# Chapter 2

## Quantum Examples

In this chapter we review quantum theory (at the level of wave mechanics) and develop a toolbox of simple quantum mechanical examples that we will use, in the following chapters, to discuss a number of the issues raised in Chap. 1: locality, ontology, measurement, etc.

### 2.1 Overview

We begin with the (time-dependent) Schrödinger Equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi. \tag{2.1}$$

For a single particle of mass  $m$  moving in one dimension, the Hamiltonian operator  $\hat{H}$  is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \tag{2.2}$$

so that the time-dependent Schrödinger Equation reads:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x, t) \Psi(x, t). \tag{2.3}$$

We typically use this equation in the following sort of way: given some initial wave function  $\Psi(x, 0)$  (which we think of as having been created by a special *preparation* of the particle in question), we then solve Schrödinger’s Equation to find the wave function at some later time  $t$  when some kind of observation or measurement of the particle occurs. A second basic postulate of the theory – the “Born rule” – is then introduced to tell us what  $\Psi(x, t)$  implies about how the measurement will come

out. In its simplest form, corresponding to a measurement of the position  $x$  of the particle, the Born rule says that the probability of observing the particle at the point  $x$  is equal to the square of the wave function's modulus:

$$P(x) = |\Psi(x, t)|^2. \quad (2.4)$$

(Well, technically, this  $P(x)$  is a probability *density*, i.e., a probability-per-unit-length along the  $x$  axis. The precise statement is that the probability of finding the particle in a range of size  $dx$  near the point  $x$  is  $P(x)dx = |\Psi|^2 dx$ . Note also that we assume here that the wave function is properly normalized, i.e.,  $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$ .)

If some property of the particle other than its position is measured (for example, its momentum or energy) then we will use the “generalized Born rule”. This says that we should write  $\Psi(x, t)$  as a linear combination of *eigenstates* of the operator corresponding to the property in question. That is, we should write

$$\Psi(x, t) = \sum_i c_i \Psi_i(x, t) \quad (2.5)$$

(or perhaps instead an integral if the property in question has a continuous spectrum) where  $\Psi_i$  is an eigenstate of the operator  $\hat{A}$  with eigenvalue  $A_i$ :

$$\hat{A}\Psi_i(x, t) = A_i\Psi_i(x, t). \quad (2.6)$$

Then the probability that the measurement of  $A$  yields the value  $A_i$  is

$$P(A_i) = |c_i|^2. \quad (2.7)$$

As a simple example, suppose we measure the *momentum* of a particle at time  $t$ . The momentum operator is

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (2.8)$$

whose eigenstates are the plane waves

$$\psi_p(x) = e^{ipx/\hbar}. \quad (2.9)$$

(Note that there's a bit of funny business about normalization here, but let's ignore that for now.) Suppose our wave function at time  $t$  is  $\Psi(x, t) = \sqrt{2} \sin(kx)$ . We can write this as a linear combination of the momentum eigenstates as follows:

$$\Psi(x, t) = \sqrt{2} \sin(kx) = \frac{1}{\sqrt{2}i} e^{i(\hbar k)x/\hbar} - \frac{1}{\sqrt{2}i} e^{i(-\hbar k)x/\hbar}. \quad (2.10)$$

This is a linear combination of two momentum eigenstates, with eigenvalues  $p = +\hbar k$  and  $p = -\hbar k$ , and expansion coefficients  $c_{+\hbar k} = 1/\sqrt{2}i$  and  $c_{-\hbar k} = -1/\sqrt{2}i$

respectively. So evidently the probability that the momentum measurement has the outcome “ $p = +\hbar k$ ” is  $P(+\hbar k) = |1/\sqrt{2}i|^2 = 1/2$ , and the probability that the momentum measurement has the outcome “ $p = -\hbar k$ ” is  $P(-\hbar k) = |-1/\sqrt{2}i|^2$  which is also  $1/2$ .

Note that the original Born rule (for position measurements) can be understood as a special case of the “generalized Born rule” if we take  $\hat{A}$  to be the position operator  $\hat{x}$  with delta functions as eigenstates:

$$\hat{x}\delta(x - x') = x'\delta(x - x'). \quad (2.11)$$

We can then write any arbitrary state  $\Psi(x, t)$  as a linear combination of position eigenstates as follows:

$$\Psi(x, t) = \int \Psi(x', t)\delta(x - x') dx' \quad (2.12)$$

where the  $\Psi(x', t)$  should be understood as the expansion coefficient, like  $c_i$ . Thus, according to the generalized Born rule, the probability for a position measurement to yield the value  $x'$  should be the square of the expansion coefficient, i.e.,

$$P_t(x') = |\Psi(x', t)|^2 \quad (2.13)$$

just like in the original statement of the Born rule.

But enough about measurement. For now I just want to make sure you had heard of this so that you understand, in some practical terms, what solving the Schrödinger equation is *for*. There are a few Projects at the end of the chapter that will help you practice using Born’s rule and then we will return to discuss all of this more critically in Chap. 3.

For now, we return to Schrödinger’s equation. Given an initial wave function  $\Psi(x, 0)$ , how does one actually solve it? Our standard technique will take advantage of the fact that there exist “separable” solutions of the form

$$\Psi_n(x, t) = \psi_n(x)f_n(t). \quad (2.14)$$

If we plug this ansatz into the Schrödinger equation we find that the function  $\psi_n(x)$  should satisfy the “time-independent Schrödinger equation” (TISE),

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x)\psi_n(x) = E_n\psi_n(x) \quad (2.15)$$

where  $E_n$  is just a constant that we can think of as the energy of the solution in question. The function  $f_n(t)$  in turn satisfies

$$i\hbar \frac{df_n(t)}{dt} = E_n f_n(t) \quad (2.16)$$

which we can solve once and for all right now:

$$f_n(t) = e^{-iE_n t/\hbar}. \quad (2.17)$$

Now we can explain our basic strategy. For a given potential energy function  $V(x)$ , we solve the TISE to find the “energy eigenstates”  $\psi_n(x)$  and corresponding energy eigenvalues  $E_n$ . If we can find a way to write the given initial wave function as a linear combination of these “energy eigenstates”, as in

$$\Psi(x, 0) = \sum_n c_n \psi_n(x) \quad (2.18)$$

then we can construct a solution of the full time-dependent Schrödinger equation by simply tacking the appropriate time-dependent  $f_n(t)$  factor onto each term in the sum. That is:

$$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}. \quad (2.19)$$

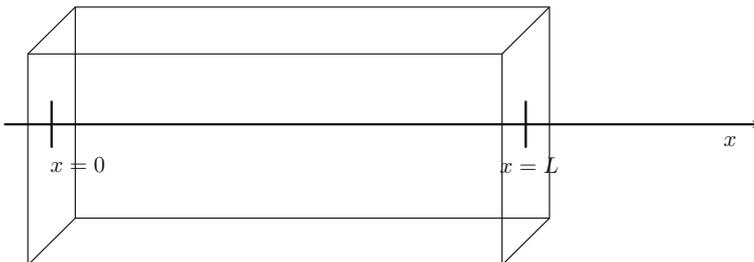
This is the basic technique we’ll now illustrate with a couple of examples.

## 2.2 Particle-in-a-Box

Suppose that a particle is absolutely confined to a certain region of the  $x$ -axis but is “free” within that region. That is, suppose

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \quad (2.20)$$

which we can (only somewhat misleadingly) think of as the particle being confined to a length- $L$  “box” as illustrated in Fig. 2.1.



**Fig. 2.1** The length- $L$  “box” that our “particle in a box” is confined to

Outside the box, where  $V = \infty$ , we need  $\psi = 0$ . Inside the box, where  $V = 0$ , the TISE takes on the simple form:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi \quad (2.21)$$

whose solution is

$$\psi(x) = A \sin(kx) + B \cos(kx). \quad (2.22)$$

But since the potential  $V$  goes to infinity abruptly at  $x = 0$  and  $x = L$ , the only way the TISE will be solved for all  $x$  (including  $x = 0$  and  $x = L$ ) is if  $\psi(x) = 0$  at  $x = 0$  and  $x = L$ . Requiring  $\psi = 0$  at  $x = 0$  means that we cannot have any of the cosine term, i.e.,  $B = 0$ . And then requiring  $\psi = 0$  at  $x = L$  puts a constraint on the wave number  $k$ : an integer number of half-wavelengths must fit perfectly in the box, i.e.,  $k = k_n$  where

$$k_n = \frac{n\pi}{L} \quad (2.23)$$

with  $n = 1, 2, 3, \dots$ . Good. So the “energy eigenfunctions” for the particle-in-a-box potential take the form

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right). \quad (2.24)$$

Note that the factor out front comes from requiring normalization:  $\int_0^L |\psi_n(x)|^2 dx = 1$ .

We can find the corresponding energy eigenvalues by plugging  $\psi_n$  into Eq. (2.15). The result is

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}. \quad (2.25)$$

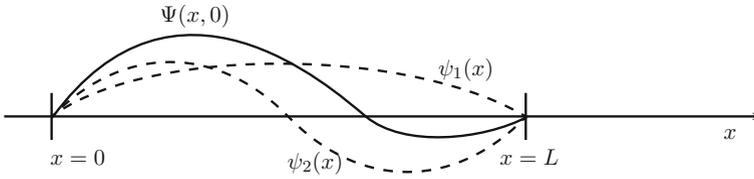
The general solution of the time-dependent Schrödinger equation can thus be written

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}. \quad (2.26)$$

Let’s illustrate with a simple example. Suppose the wave function of a particle in a box is given, at  $t = 0$ , by

$$\Psi(x, 0) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x). \quad (2.27)$$

This function is plotted in Fig. 2.2. Notice that there is constructive interference between  $\psi_1$  and  $\psi_2$  on the left hand side of the box, giving rise to a  $\Psi$  with a large modulus there, but (partial) destructive interference on the right. So at  $t = 0$  the



**Fig. 2.2** The initial wave function (*solid curve*) for a particle-in-a-box that is in a superposition of the two lowest energy eigenstates (shown individually as *dashed curves*)

particle is much more likely to be found (if looked for!) on the left hand side of the box.

How, then, does  $\Psi$  evolve in time? Here we don't have to do any work to write the initial wave function as a linear combination of energy eigenstates. Equation (2.27) already gave it to us in that form! So then it is trivial to write down an equation for the wave function at time  $t$ :

$$\Psi(x, t) = \frac{1}{\sqrt{2}}\psi_1(x)e^{-iE_1t/\hbar} + \frac{1}{\sqrt{2}}\psi_2(x)e^{-iE_2t/\hbar} \quad (2.28)$$

or, writing everything out in full explicit glory,

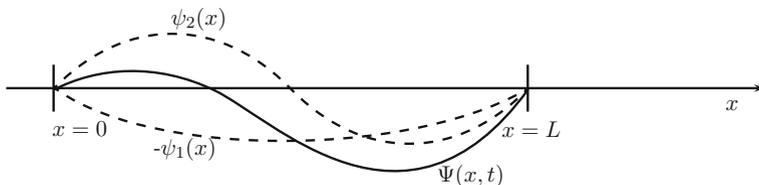
$$\Psi(x, t) = \frac{1}{\sqrt{L}} \sin\left(\frac{\pi x}{L}\right) e^{-i\hbar\pi^2 t/2mL^2} + \frac{1}{\sqrt{L}} \sin\left(\frac{2\pi x}{L}\right) e^{-4i\hbar\pi^2 t/2mL^2}. \quad (2.29)$$

Notice that each term has an  $e^{-iE_n t/\hbar}$  factor, but that the frequencies ( $\omega_n = E_n/\hbar$ ) are different for the two terms. In particular, the frequency of the  $n = 2$  term is four times as big as the frequency of the  $n = 1$  term. And so, for example, in a time  $t = T_1/2 = \pi/\omega_1 = \hbar\pi/E_1 = 2mL^2/\hbar\pi$  equal to half the period of the  $n = 1$  factor (so that the  $n = 1$  factor is  $-1$ ), the  $n = 2$  factor will have gone through two complete oscillations and will therefore be back to its original value of unity. At this time, the overall wave function will therefore look like the one shown in Fig. 2.3: there will now be constructive interference (and hence a high probability of finding the particle) *on the right*.

Thus, already in this simple example, we see an interesting non-trivial dynamics: the (probability of finding the) particle in some sense “sloshes back and forth” in the box.

### 2.3 Free Particle Gaussian Wave Packets

Let us now turn our attention to a second simple example – the “free particle”. This is the same as the particle-in-a-box, but with the edges of the box (which in the previous section were at  $x = 0$  and  $L$ ) pushed back to  $\pm\infty$ . So in principle we could jump in



**Fig. 2.3** The wave function for the same situation but after a time equal to half the period of the  $n = 1$  state. The frequency of the  $n = 2$  state is four times higher, so in the same amount of time that makes  $e^{-iE_1t/\hbar} = -1$ , we have that  $e^{-iE_2t/\hbar} = +1$ . So the  $n = 2$  term in the superposition looks the same as it did at  $t = 0$ , but the  $n = 1$  term is now “upside down”. This produces destructive interference on the *left* and constructive interference on the *right*

by saying that the general solution to the TISE is just Eq. (2.22) again:

$$\psi(x) = A \sin(kx) + B \cos(kx) \quad (2.30)$$

but where now there is no reason that  $B$  needs to be zero, and no constraint at all on the wave number  $k$ .

This would be fine, actually, but it turns out to be a little nicer to instead use the so-called plane-wave states

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \quad (2.31)$$

which are also perfectly good solutions of the free-particle TISE and which, as mentioned earlier, can be understood as eigenstates of the momentum operator  $\hat{p} = -i\hbar \partial/\partial x$  with eigenvalue  $p_k = \hbar k$ . They are also of course energy eigenstates with

$$E_k = \frac{p_k^2}{2m} = \frac{\hbar^2 k^2}{2m}. \quad (2.32)$$

(Note that – like the “position eigenstates” we mentioned earlier in the chapter – these momentum eigenstates are not properly normalized, and indeed not technically normalizable at all! As long as we include the pre-factor of  $\frac{1}{\sqrt{2\pi}}$  in our definition of the  $\psi_k$  states, however, their normalization is in a certain sense consistent with the normalization of the  $\delta$ -function position eigenstates, and we won’t run into trouble.)

Let’s again focus on a concrete example: suppose that the wave function of a free particle is initially given by the Gaussian function

$$\Psi(x, 0) = N e^{-x^2/4\sigma^2} \quad (2.33)$$

where  $N$  is a normalization constant. What, exactly,  $N$  is is not that important, but it will be a useful exercise to calculate it here. The idea is to choose  $N$  so that

$$1 = \int |\Psi(x, 0)|^2 dx = |N|^2 \int_{-\infty}^{\infty} e^{-x^2/2\sigma^2} dx. \quad (2.34)$$

There is a cute trick to evaluate Gaussian integrals like that appearing here on the right hand side. Let's define the "standard Gaussian integral" as

$$J = \int_{-\infty}^{\infty} e^{-Ax^2} dx. \quad (2.35)$$

Then we can write  $J^2$  as a double integral like this:

$$\begin{aligned} J^2 &= \left( \int_{-\infty}^{\infty} e^{-Ax^2} dx \right)^2 \\ &= \left( \int_{-\infty}^{\infty} e^{-Ax^2} dx \right) \left( \int_{-\infty}^{\infty} e^{-Ay^2} dy \right) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-Ax^2} e^{-Ay^2} dx dy. \end{aligned} \quad (2.36)$$

One can think of this as integrating a two-dimensional Gaussian function over the entire  $x - y$ -plane. But we can rewrite this integral using polar coordinates ( $r^2 = x^2 + y^2$ ) as follows:

$$J^2 = \int_0^{\infty} e^{-Ar^2} 2\pi r dr. \quad (2.37)$$

But then this integral can be done (using a substitution,  $u = Ar^2$ , so  $2\pi r dr = \pi du/A$ ) to give

$$J^2 = \frac{\pi}{A} \quad (2.38)$$

so that

$$J = \sqrt{\frac{\pi}{A}}. \quad (2.39)$$

Using this general result to simplify the right hand side of Eq. (2.34) gives

$$1 = |N|^2 \int_{-\infty}^{\infty} e^{-x^2/2\sigma^2} dx = |N|^2 \sigma \sqrt{2\pi}. \quad (2.40)$$

so

$$|N| = \frac{1}{\sqrt{J}} = \frac{1}{\sqrt{\sigma\sqrt{2\pi}}}. \quad (2.41)$$

We might as well choose  $N$  to be real and positive, so now we know how to write a properly-normalized Gaussian initial wave function:

$$\Psi(x, 0) = \frac{1}{\sqrt{\sigma\sqrt{2\pi}}} e^{-x^2/4\sigma^2}. \quad (2.42)$$

But of course the real question is: how does this state evolve in time?

To find out, we need to follow the general procedure: write the initial state  $\Psi(x, 0)$  as a linear combination of the energy eigenstates, then just tack on the appropriate  $e^{-iEt/\hbar}$  factor to each term in the linear combination.

OK, so, first step: write the initial state as a linear combination of the energy eigenstates. Here there is a continuous infinity of energy eigenstates (parameterized by the wave number  $k$ ) so the linear combination will involve an integral rather than a sum. It should look like this:

$$\Psi(x, 0) = \int_{-\infty}^{\infty} \phi(k) \frac{e^{ikx}}{\sqrt{2\pi}} dk. \quad (2.43)$$

The (continuously infinite collection of!) numbers  $\phi(k)$  are the “expansion coefficients”. How do we find them? One way is to recognize that the last equation says:  $\phi(k)$  is just the Fourier transform of  $\Psi(x, 0)$ . So if that’s a familiar thing, there you go! If not, though, here’s how to extract them. This procedure is sometimes called “Fourier’s trick”. The idea is to use the fact that the different energy eigenstates (here, the plane waves) are *orthogonal* in the following sense: if you multiply one of them ( $k$ ) by the complex conjugate of a different one ( $k'$ ) the result is oscillatory and its integral is zero – unless  $k = k'$  in which case the product is just 1 and you get a giant infinity. Formally:

$$\int \left( \frac{e^{ikx}}{\sqrt{2\pi}} \right) \left( \frac{e^{ik'x}}{\sqrt{2\pi}} \right)^* dx = \delta(k - k'). \quad (2.44)$$

We can use this property to isolate the expansion coefficients  $\phi(k)$  in Eq. (2.43). Just multiply both sides by  $e^{-ik'x}/\sqrt{2\pi}$  and then integrate both sides with respect to  $x$ . The result of the  $x$ -integral on the right is a delta function that we can use to do the  $k$ -integral. When the dust settles, the result is

$$\phi(k') = \int \left( \frac{e^{-ik'x}}{\sqrt{2\pi}} \right) \Psi(x, 0) dx. \quad (2.45)$$

So far we have avoided plugging in our Gaussian state for the initial wave function so this result is completely general. But let’s now plug in Eq. (2.42) and proceed as follows:

$$\begin{aligned}
\phi(k) &= \frac{1}{\sqrt{2\pi}} \int e^{-ikx} \Psi(x, 0) dx \\
&= \frac{N}{\sqrt{2\pi}} \int e^{-ikx} e^{-x^2/4\sigma^2} dx \\
&= \frac{N}{\sqrt{2\pi}} \int e^{-\frac{1}{4\sigma^2}(x^2+4ik\sigma^2x)} dx \\
&= \frac{N}{\sqrt{2\pi}} \int e^{-\frac{1}{4\sigma^2}[x^2+4ik\sigma^2x+(2ik\sigma^2)^2-(2ik\sigma^2)^2]} dx \\
&= \frac{N}{\sqrt{2\pi}} \int e^{-\frac{1}{4\sigma^2}[(x+2ik\sigma^2)^2-(2ik\sigma^2)^2]} dx \\
&= \frac{N}{\sqrt{2\pi}} e^{\frac{(2ik\sigma^2)^2}{4\sigma^2}} \int e^{-\frac{1}{4\sigma^2}(x+2ik\sigma^2)^2} dx \\
&= \frac{N}{\sqrt{2\pi}} e^{-k^2\sigma^2} \int e^{-x^2/4\sigma^2} dx
\end{aligned} \tag{2.46}$$

which is just another “standard Gaussian integral”. Using our general formula to perform it, we arrive at:

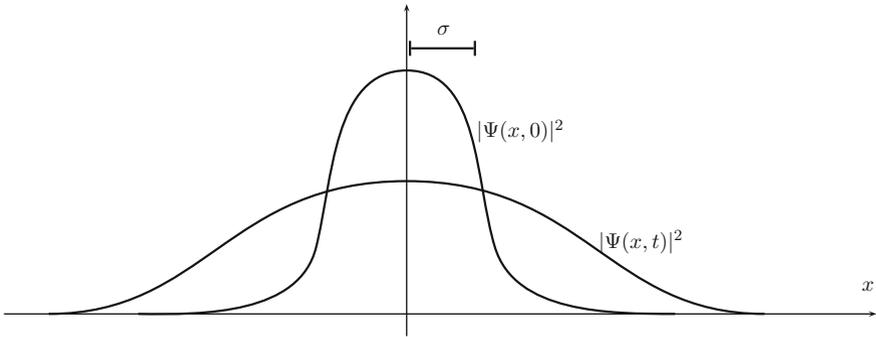
$$\phi(k) = \sqrt{2}N\sigma e^{-k^2\sigma^2}. \tag{2.47}$$

Qualitatively, the important thing here is that the Fourier transform of a Gaussian (in  $x$ ) is another Gaussian (in  $k$ ). And notice in particular that the “width” of  $\phi(k)$  is (something like)  $1/\sigma$  – the inverse of the width of the original Gaussian in position space. This illustrates an important qualitative principle of Fourier analysis, that to make a sharply peaked function in position space requires superposing plane-waves with a very broad range of wave numbers, whereas you only need a narrower range of wave numbers to construct a more spread out function in position space. In the context of quantum mechanics this idea is intimately related to the Heisenberg uncertainty principle: the width of a wave packet in position space is essentially “the uncertainty in its position”,  $\Delta x$ , whereas the “width” in  $k$ -space is (since  $p = \hbar k$ ) “the uncertainty in its momentum” divided by  $\hbar$ . These being inverses of each other therefore means that the position uncertainty and the momentum uncertainty are inversely related:  $\Delta x \sim \hbar/\Delta p$ .

See the end-of-chapter Projects for some further (and more careful) exploration of this connection.

Let’s step back and remember why we’re doing all this math. We want to start with a nice Gaussian wave packet and see how it evolves in time according to Schrödinger’s equation. To do that, we needed to first figure out how to write the initial Gaussian packet as a superposition of the energy eigenstates – here, the plane-wave states. That’s what we’ve just accomplished! That is, we figured out that we can write

$$\Psi(x, 0) = \int \phi(k) \frac{e^{ikx}}{\sqrt{2\pi}} dk \tag{2.48}$$



**Fig. 2.4** A wave function that is a Gaussian with half-width  $\sigma$  at  $t = 0$  spreads out in time

where

$$\phi(k) = \sqrt{2}N\sigma e^{-k^2\sigma^2}. \tag{2.49}$$

Now the whole reason we wanted to write  $\Psi(x, 0)$  in this special form, is that doing so makes it easy to write down an equation for the state at a later time  $t$ : we just tack the  $e^{-iEt/\hbar}$  factor on each term. So let's do that! The result is:

$$\begin{aligned} \Psi(x, t) &= \int \phi(k) \frac{e^{ikx}}{\sqrt{2\pi}} e^{-iE_k t/\hbar} dk \\ &= \frac{\sigma N}{\sqrt{\pi}} \int e^{-k^2\sigma^2} e^{ikx} e^{-i\hbar k^2 t/2m} dk. \end{aligned} \tag{2.50}$$

Now, with the same sort of massaging we did before (“completing the square” in the argument of the exponential, etc.) we can do this integral. I’ll leave that as a Project if you want to go through it and just quote the result here:

$$\Psi(x, t) = N \frac{\sigma}{\sqrt{\sigma^2 + \frac{i\hbar t}{2m}}} e^{-\frac{x^2}{4(\sigma^2 + i\hbar t/2m)}}. \tag{2.51}$$

Phew!

This function is Gaussian-ish... You could think of it as a Gaussian with a time-dependent, complex width (whatever that means!). But if you multiply it by its complex conjugate, to get the probability density for finding the particle, that is definitely Gaussian:

$$P_t(x) = |\Psi(x, t)|^2 = \frac{N^2}{\sqrt{1 + \frac{\hbar^2 t^2}{4m^2\sigma^4}}} \exp \left[ \frac{-x^2}{2\sigma^2 \left(1 + \frac{\hbar^2 t^2}{4m^2\sigma^4}\right)} \right]. \tag{2.52}$$

Notice in particular that the *width* of this Gaussian (i.e., the uncertainty in the position of the particle) grows with time:

$$\Delta x(t) = \sigma \sqrt{1 + \frac{\hbar^2 t^2}{4m^2 \sigma^4}}. \quad (2.53)$$

See Fig. 2.4 for an illustration. Initially (for times small compared to  $2m\sigma^2/\hbar$ ) the width grows slowly, but then later (for times long compared to  $2m\sigma^2/\hbar$ ) the width grows linearly in time. So the uncertainty in the position of the particle grows and grows as time evolves. Interestingly, the uncertainty in the momentum never changes: the first line of Eq. (2.50) can be understood as saying that the complex *phases* of the momentum “expansion coefficients” change with time, but their magnitudes stay the same. So the probability distribution for momentum values, and hence  $\Delta p$ , is independent of time. This makes sense, if you think about it, since we’re talking about a free particle, i.e., a particle on which no forces act. Anyway, this nicely illustrates the fact that the Heisenberg uncertainty principle takes the form of an inequality: the product of  $\Delta x$  and  $\Delta p$  can be arbitrarily large, but there’s a smallest possible value.

## 2.4 Diffraction and Interference

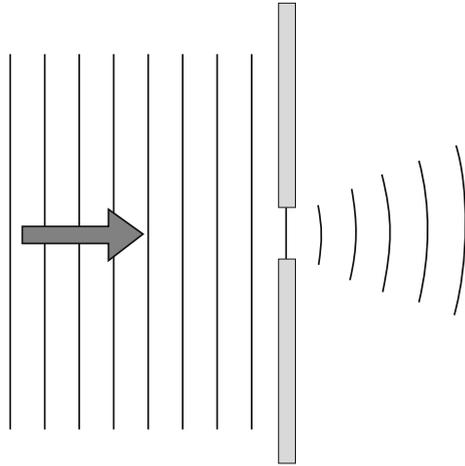
The spreading of an initial wave packet is closely related to the phenomenon of *diffraction*. Imagine, for example, a particle that is incident on a barrier with a slit: the barrier simply blocks/absorbs the part of the particle’s wave function that hits it, so that just downstream of the barrier and along the direction transverse to the direction of propagation of the particle, the wave function has a packet-shaped profile like the ones we were discussing in the last section. And the evolution of the packet-shape with *position*, downstream of the slit, is (approximately) the same as the evolution of the one-dimensional packets (discussed in the previous section) with *time*. In particular, as we saw in the last section, the wave packet will *spread* in this transverse direction as it propagates downstream. This is the phenomenon, illustrated in Fig. 2.5, of *diffraction*.

Of course, for a literal slit (which absorbs everything that hits it, and transmits whatever part of the incident wave goes through the slit) the transverse profile of the wave function (just downstream of the barrier) would be something like this:

$$\Psi(x, 0) = \begin{cases} N & \text{for } -\frac{L}{2} < x < \frac{L}{2} \\ 0 & \text{otherwise} \end{cases} \quad (2.54)$$

with the constant  $N$  evidently being  $1/\sqrt{L}$  to ensure proper normalization. As it turns out, the sharp edges (at  $x = -L/2$  and  $x = L/2$ ) of this function produce a Fourier transform  $\phi(k)$  that diverges at  $k = 0$  and this makes it slightly tricky to work with. See the Projects for a work-around that allows one to deal with this situation.

**Fig. 2.5** An incident wave passes through a slit and diffracts



But just to understand the process conceptually, we can contemplate a “Gaussian slit”, i.e., a barrier with a “transmission profile” (i.e., fraction of incident wave function that transmits rather than being absorbed) equal to a Gaussian. Then – basically by definition – the transverse profile of the beam just downstream of the barrier is a Gaussian, as in Eq. (2.42). If we make the approximation that the wave just steadily propagates to the right at some speed  $v = \frac{\hbar k}{m}$  then we can relate the coordinate  $y$  along the direction of propagation to the time via  $y = vt$ . (This approximation is explained and developed further in the Projects.) And so we can immediately use, for example, Eq. (2.52) to write down an expression for the “intensity” (i.e., probability density) for finding the particle in the two-dimensional region behind the barrier:

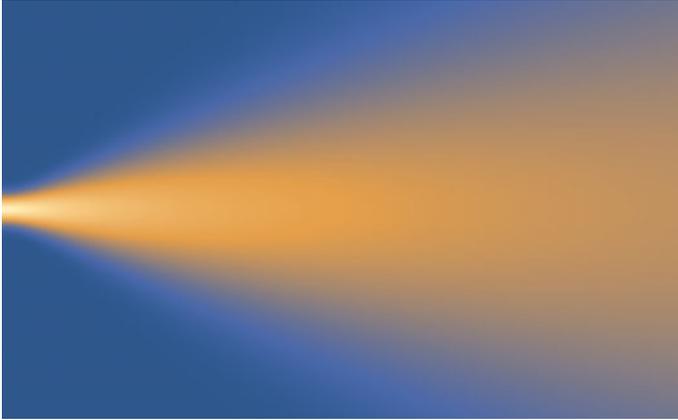
$$I(x, y) \sim |\Psi(x, y)|^2 \sim \frac{1}{\sqrt{1 + \frac{\hbar^2 y^2}{4m^2 v^2 \sigma^4}}} e^{-x^2/2\left(\sigma^2 + \frac{\hbar^2 y^2}{4m^2 v^2 \sigma^4}\right)}. \quad (2.55)$$

I used Mathematica to make a nice density plot of this function; the result is shown in Fig. 2.6.

One of the nice reasons for setting this up, however, is that it provides a simple way to examine the structure of the wave function behind a *double slit* barrier. The classic two-slit interference pattern was first identified by Thomas Young as crucial evidence that light was a *wave*. And then of course the identification that “particles” (such as electrons) also exhibit interference, played and continues to play a crucial role in our understanding of the quantum nature of the sub-atomic realm.

So, then, imagine a barrier with not one but *two* “Gaussian slits” centered, say, at  $x = a$  and  $x = -a$ . Then, the transverse profile of the wave function just behind the barrier will be given by

$$\Psi(x, 0) \sim \Psi_G(x - a, 0) + \Psi_G(x + a, 0) \quad (2.56)$$



**Fig. 2.6** Density plot of  $|\Psi(x, y)|^2$  from Eq. (2.55) illustrating the intensity of a wave, diffracting as it propagates to the right having emerged from a “Gaussian slit” on the *left* edge of the image

i.e., a superposition of two Gaussians, one centered at  $x = a$  and one centered at  $x = -a$ .

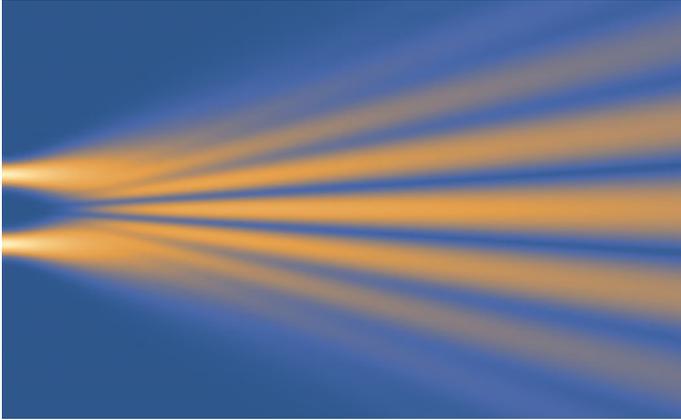
Each Gaussian term just spreads out in time in the way we analyzed in the previous section. (Formally, we can say that since the Schrödinger equation is *linear* in  $\Psi$ , the solution  $\Psi(x, t)$  for this initial state – a superposition of two Gaussians – is just the corresponding superposition of the solutions for the two superposed terms individually.) Thus, using Eq. (2.51) twice (but with one small tweak each time) we can write

$$\Psi(x, t) \sim \Psi_G(x - a, t) + \Psi_G(x + a, t) \sim \frac{1}{\sqrt{\sigma^2 + \frac{i\hbar t}{2m}}} \left[ e^{-\frac{(x-a)^2}{4(\sigma^2 + i\hbar t/2m)}} + e^{-\frac{(x+a)^2}{4(\sigma^2 + i\hbar t/2m)}} \right] \quad (2.57)$$

or, converting this into an expression for the wave function in the two-dimensional region in the way that we did before,

$$\Psi(x, y) \sim \frac{1}{\sqrt{\sigma^2 + \frac{i\hbar y}{2mv}}} \left[ e^{-\frac{(x-a)^2}{4(\sigma^2 + i\hbar y/2mv)}} + e^{-\frac{(x+a)^2}{4(\sigma^2 + i\hbar y/2mv)}} \right]. \quad (2.58)$$

This is slightly messy to work with, but the idea qualitatively is that, as the two individual Gaussians begin to spread, they start to overlap. But then there can be either constructive or destructive interference depending on the relative *phases* in the region of overlap. For example, along the symmetry line,  $x = 0$ , the phases of the two terms will always match and we will therefore always have constructive interference, corresponding to a large value of  $|\Psi|^2$ , i.e., a high probability for the particle (if looked for) to be detected. But if we move a little bit to the side (say, in the positive  $x$ -direction) we are moving *toward* the central peak of one of the



**Fig. 2.7** Density plot of  $|\Psi|^2$  from Eq. (2.58). A classic interference pattern emerges in the intensity of the wave downstream from the “double Gaussian slit” barrier at the *left* edge of the image

Gaussians and *away* from the central peak of the other, and so the phases of the two terms change at different rates, and eventually we find a spot where there is (at least for large  $y$ , nearly complete) destructive interference, corresponding to  $|\Psi|^2 = 0$ . Moving even farther in the positive  $x$ -direction eventually yields another spot where there is constructive interference, and so on.

The intensity pattern that results is shown in Fig. 2.7, which is again a Mathematica density plot of  $|\Psi(x, y)|^2$ , with  $\Psi(x, y)$  given by Eq. (2.58). It is the classic two-slit interference pattern.

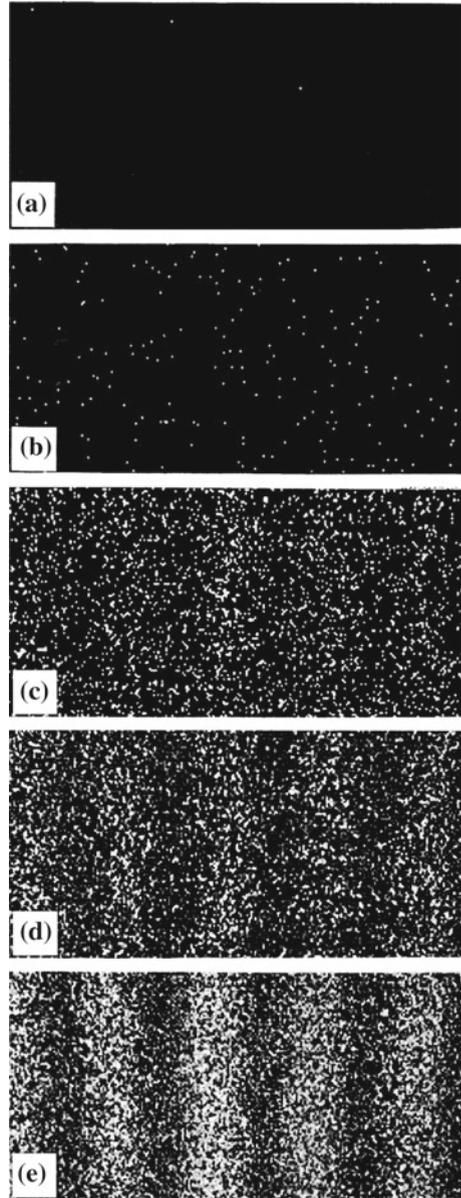
Of course, one should remember that such images of smoothly-distributed waves only tell half the story according to quantum mechanics. When an individual particle is looked for, it is not observed to be spread out like in these pictures; instead, it is found at some one particular spot, with the smooth  $|\Psi|^2$  functions providing the probability distribution for the discrete sharp “hit”. See, for example, in Fig. 2.8, the beautiful results of Tonomura *et al.* for a two-slit experiment with individual electrons and, in Fig. 2.9, the equally beautiful results of Dimitrova and Weis for a similar experiment using individual photons.

## 2.5 Spin

We will have occasion later to discuss measurements of the spin of (spin 1/2) particles. For such measurements, there are only two possible outcomes – “spin up” along the axis in question, or “spin down”. This makes spin a very simple and elegant system to treat using the quantum formalism.

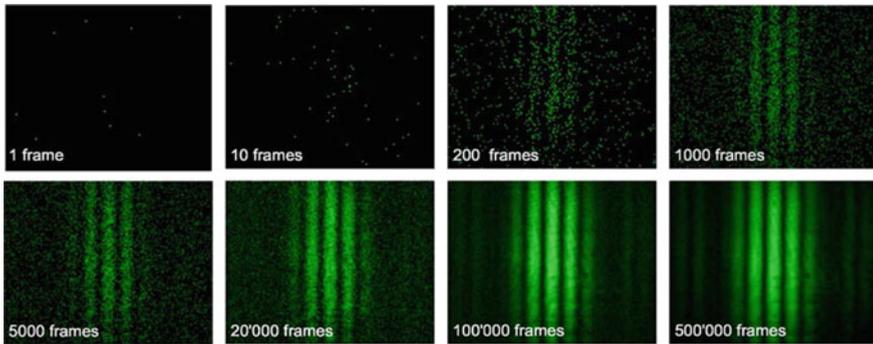
We can represent the “spin up along the  $z$ -axis” state this way:

**Fig. 2.8** Data from a double-slit experiment with electrons, in which electrons are sent through the apparatus one at a time. Each electron is found at a particular spot on the detection screen. The statistical pattern of spots – that is, the probability distribution for electron detection – builds up the classic two-slit interference pattern. (Reproduced from Tonomura et al., “Demonstration of single-electron buildup of an interference pattern” *American Journal of Physics* **57** (2), February 1989, pp. 117–120, our Ref. [1], with the permission of the American Association of Physics Teachers. <http://aapt.scitation.org/doi/abs/10.1119/1.16104>) See also Ref. [2]



$$\psi_{+z} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (2.59)$$

and the “spin down along the  $z$ -axis” state this way:



**Fig. 2.9** Results of a similar experiment with “feeble light”, i.e., individual photons. Just as with Tonomura’s electrons, the measurement (here, using a CCD array) of the position of the photon always yields a definite, sharp location. The interference pattern is then realized in the statistical distribution of such individual sharp locations, after many photons are detected. (Reproduced from T.L. Dimitrova and A. Weis, “The Wave-Particle Duality of Light: A Demonstration Experiment,” *American Journal of Physics* **76** (2008), pp. 137–142, our Ref. [3], with the permission of the American Association of Physics Teachers. <http://aapt.scitation.org/doi/abs/10.1119/1.2815364>)

$$\psi_{-z} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.60)$$

Note that these two-component vectors (technically “spinors”) are the eigenvectors (with eigenvalues  $+1$  and  $-1$  respectively) of the spin-along- $z$  operator, which can be represented as a two-by-two matrix:

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.61)$$

Of course, this is quantum mechanics, so the two eigenstates of  $\hat{\sigma}_z$  are not the only possible states – instead they merely form a *basis* for the space of possible states. (Think of the spin up and spin down states here,  $\psi_{+z}$  and  $\psi_{-z}$ , as being like the energy eigenstates for the particle-in-a-box potential. These are not the only possible states! Instead, the general state is an arbitrary properly-normalized linear combination of them.) Here, a general state can be written as

$$\psi = c_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}. \quad (2.62)$$

The expansion coefficients  $c_+$  and  $c_-$  should of course be understood to have their usual, generalized Born rule meanings: if a particle is in the spin state  $\psi$  and its spin along the  $z$ -axis is measured, the probability for the measurement to have outcome “spin up along  $z$ ” is  $P_+ = |c_+|^2$  whereas the probability for the measurement to have outcome “spin down along  $z$ ” is  $P_- = |c_-|^2$ . And note that, since these are

the only two possible outcomes, the probabilities should sum to one. That is, proper normalization for the general spin state  $\psi$  requires  $|c_+|^2 + |c_-|^2 = 1$ .

Things get a little more interesting when we consider the possibility of measuring the spin of a particle along some axis other than the  $z$ -axis. We will only ever have occasion to care about measurements along axes in (say) the  $x-z$ -plane. The operator corresponding to spin measurements along the  $x$ -axis can be written

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (2.63)$$

whose eigenvectors are

$$\psi_{+x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (2.64)$$

(with eigenvalue  $+1$  corresponding to “spin up” along the  $x$ -direction) and

$$\psi_{-x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (2.65)$$

(with eigenvalue  $-1$  corresponding to “spin down” along the  $x$ -direction).

The operator corresponding to spin measurements along an arbitrary direction  $\hat{n}$  in the  $x$ - $z$ -plane is

$$\hat{\sigma}_n = \hat{n} \cdot \hat{\sigma} = \cos(\theta)\hat{\sigma}_z + \sin(\theta)\hat{\sigma}_x = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{pmatrix} \quad (2.66)$$

where  $\theta$  is the angle between  $\hat{n}$  and  $\hat{z}$  (toward  $\hat{x}$ ). It is a simple exercise in linear algebra to show that the eigenvectors of this matrix can be written

$$\psi_{+n} = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \quad (2.67)$$

(with eigenvalue  $+1$ , corresponding to “spin up along  $n$ ”) and

$$\psi_{-n} = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix} \quad (2.68)$$

(with eigenvalue  $-1$ , corresponding to “spin down along  $n$ ”). Notice that, for  $\theta = 0$ , these states correspond to  $\psi_{+z}$  and  $\psi_{-z}$ , as they should, and similarly for  $\theta = 90^\circ$ , they correspond to  $\psi_{+x}$  and  $\psi_{-x}$ .

Let’s consider a concrete example to illustrate these ideas. Suppose a particle is prepared in the “spin up along  $n$ ” state where  $n$  is a direction  $60^\circ$  down from the  $z$ -axis (toward the  $x$ -axis). That is, suppose

$$\psi_0 = \begin{pmatrix} \cos(30^\circ) \\ \sin(30^\circ) \end{pmatrix}. \quad (2.69)$$

Then, we are going to measure the spin of this particle along the  $z$ -axis. What is the probability that this  $z$ -spin measurement comes out “spin down”?

To answer this, as always, we have to write the given state as a linear combination of the eigenstates of the operator corresponding to the measurement that is to be performed. Here that means writing  $\psi_0$  as a linear combination of  $\psi_{+z}$  and  $\psi_{-z}$ . But that is easy:

$$\psi_0 = \begin{pmatrix} \cos(30^\circ) \\ \sin(30^\circ) \end{pmatrix} = \cos(30^\circ) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sin(30^\circ) \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.70)$$

So then we can read off that the probability of the measurement having outcome “spin down along  $z$ ” is the square of the expansion coefficient on the “spin down along  $z$ ” term, i.e.,

$$P_{-z} = \sin^2(30^\circ) = \frac{1}{4}. \quad (2.71)$$

So if a whole beam of particles (all identically prepared in the state  $\psi_0$ ) is sent into a Stern Gerlach device (with its axis aligned along the  $z$  direction), 25% of the particles will emerge having been deflected “down” and the remaining 75% will emerge having been deflected “up”.

## 2.6 Several Particles

So far all of the examples we’ve considered involve only a single particle (and in particular its spatial or spin degrees of freedom). In situations involving two or more particles, the principles are the same, but there are some important new possibilities that will become important in subsequent chapters. Let us lay some of the groundwork here.

A crucial point is that, for an  $N$ -particle system, it is not the case that each of the  $N$  particles has its own wave function. Instead, there is a single wave function for the whole  $N$ -particle system. This wave function obeys the  $N$ -particle Schrödinger equation

$$i\hbar \frac{\partial \Psi(x_1, x_2, \dots, x_N, t)}{\partial t} = \sum_{i=1}^N \frac{-\hbar^2}{2m_i} \nabla_i^2 \Psi(x_1, x_2, \dots, x_N, t) + V(x_1, x_2, \dots, x_N) \Psi(x_1, x_2, \dots, x_N, t). \quad (2.72)$$

Note that the wave function  $\Psi(x_1, x_2, \dots, x_N, t)$  is a (time-dependent) function on the *configuration space* of the  $N$ -particle system:  $x_1$  is the spatial coordinate of particle 1,  $x_2$  is the spatial coordinate of particle 2, etc.

As an example, consider the case of two particles (which have identical  $m$  and which do not interact with each other) trapped in the box from Sect. 2.2. The time-dependent Schrödinger equation reads

$$i\hbar \frac{\partial \Psi(x_1, x_2, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x_1, x_2, t)}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x_1, x_2, t)}{\partial x_2^2} + V(x_1)\Psi(x_1, x_2, t) + V(x_2)\Psi(x_1, x_2, t) \quad (2.73)$$

where  $V$  is just the “particle-in-a-box” potential, Eq. (2.20).

It is easy to show, by separation of variables, that there are solutions of the form

$$\Psi_{m,n}(x_1, x_2, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi x_1}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x_2}{L}\right) e^{-i(E_m + E_n)t/\hbar} \quad (2.74)$$

which are *products*: one of the one-particle energy eigenfunctions for particle 1, times one of the one-particle energy eigenfunctions for particle 2, and then with the usual time-dependent phase factor involving the energy, which is just the sum of the two one-particle energies.

If the two-particle quantum state is one of these product states, the wave function  $\Psi$  is formally a function on the two-particle configuration space, but there is an obvious sense in which each particle has its own definite state.

But, as usual in quantum mechanics, these states do not exhaust the possibilities – instead, they merely form a *basis* for the space of all possible wave functions. And that gives rise to the crucially-important concept of “entanglement”. An “entangled” wave function (or quantum state) for several particles is simply one that is *not a product*. An entangled state of two particles, that is, *cannot* be written as “some wave function for particle 1” times “some wave function for particle 2”. In entangled states, the individual particles really fail to have their own, individual, states.

Here is an example. Consider the two particles in the “box” potential, and suppose we are only interested in the situation at  $t = 0$  (so we ignore time-dependence). One possible state for the two particles to be in is

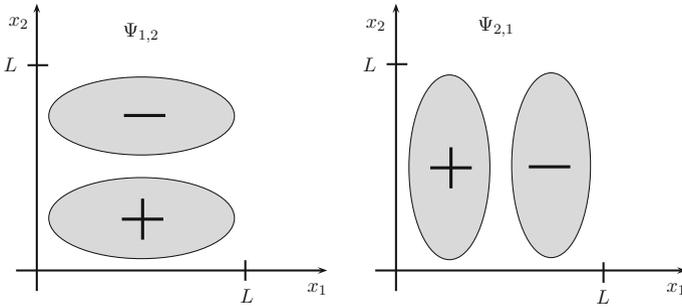
$$\Psi_{1,2} = \psi_1(x_1)\psi_2(x_2) \quad (2.75)$$

corresponding to particle 1 being in the ground state and particle 2 being in the first excited state. Another possible state is

$$\Psi_{2,1} = \psi_2(x_1)\psi_1(x_2) \quad (2.76)$$

corresponding to particle 1 being in the first excited state and particle 2 being in the ground state. Neither of these states is particularly interesting or troubling since, for each of them, each particle has its own definite state (with a definite energy).

But here is another possible state that the two-particle system could be in:



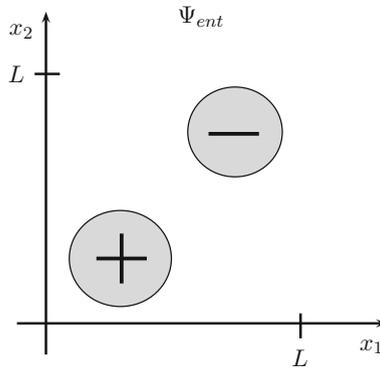
**Fig. 2.10** The cartoon graph on the *left* indicates (in a very rough way) the structure (in the two-dimensional configuration space) of  $\Psi_{1,2} \sim \sin(\pi x_1/L) \sin(2\pi x_2/L)$ . This is the product of a function that is positive for all  $x_1$  between 0 and  $L$ , but then switches from being positive for  $0 < x_2 < L/2$  to being negative for  $L/2 < x_2 < L$ . So the product has a reasonably large magnitude in roughly the *grey-shaded* areas and is positive and negative in the regions indicated. The graph on the *right* indicates the structure of  $\Psi_{2,1} \sim \sin(2\pi x_1/L) \sin(\pi x_2/L)$  in a similar way

$$\Psi_{ent} = \frac{1}{\sqrt{2}} (\Psi_{1,2} + \Psi_{2,1}) = \frac{1}{\sqrt{2}} [\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)]. \quad (2.77)$$

This is a *superposition* of (on the one hand) a state in which particle 1 is in the ground state and particle 2 is in the first excited state and (on the other hand) a state in which particle 2 is in the first excited state and particle 2 is in the ground state. So neither particle 1 nor particle 2 is in a state of definite energy at all. (Interestingly, though, this entangled two-particle state *is* an eigenstate of the total energy: the two particles definitely have a total energy of  $E_1 + E_2 \dots$  there’s just no particular fact of the matter about how this total energy is distributed between the two particles!)

It is perhaps helpful to practice visualizing these states in the two-particle configuration space. Figure 2.10 shows sketchy cartoon versions of the two states  $\Psi_{1,2}$  and  $\Psi_{2,1}$ . Each wave function is positive in one part, negative in another, and zero between them.

The sum of these two states – the *entangled superposition* state in Eq. (2.77) – is shown in this same sketchy cartoon style in Fig. 2.11. There is (approximate) destructive interference in the upper-left and lower-right corners of the configuration space, and instead constructive interference in the lower-left and upper-right corners. So the state  $\Psi_{ent}$  has a large positive value in the lower-left corner, a large negative value in the upper-right corner, and is approximately zero elsewhere. Note that, since the probability of finding the particles at positions  $x_1$  and  $x_2$  is  $|\Psi|^2$ , this means that, if the two particles are in the state  $\Psi_{ent}$ , they are unlikely to be found at different locations: the upper-left and lower-right corners of the configuration space here correspond, respectively, to “particle 1 is on the left and particle 2 is on the right” and “particle 1 is on the right and particle 2 is on the left”. These are precisely the regions of configuration space where  $\Psi$  has a small amplitude and hence the corresponding probability is small. On the other hand, the probabilities for finding



**Fig. 2.11** The structure of the entangled state  $\Psi_{ent} = \frac{1}{\sqrt{2}} (\Psi_{1,2} + \Psi_{2,1})$  in configuration space. In the *upper-left corner* (i.e.,  $0 < x_1 < L/2$  and  $L/2 < x_2 < L$ ) the two superposed terms have opposite sign and (partially) cancel out. The same thing happens in the *lower-right corner*. But in the *lower left corner* (i.e.,  $0 < x_1 < L/2$  and  $0 < x_2 < L/2$ ) the two superposed terms have the same (positive) sign and hence add up to a function with a large (positive) value. The same thing happens in the *upper-right corner*, but with “positive” replaced by “negative”

both particles “on the left” and finding both particles “on the right” are high. So in some sense this particular entangled state is one in which neither particle has a definite energy, and of course neither particle has a definite position either, and yet there are certain *correlations* between them, i.e., certain *joint properties* that are more well-defined: the *total* energy of the two particles, for example, is perfectly definite, and it is extremely likely that the particles will be found to be near one another if their positions are measured.

That last sentence, by the way, should kind of blow your mind. So slow down and let it percolate for a while if you didn’t already!

This example of two particles in a box has dealt exclusively with the spatial degrees of freedom of two particles. Note that it is also possible for the spin degrees of freedom of two particles to be entangled. For example, we might have two particles in the joint spin state:

$$\Psi_{singlet} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \right]. \quad (2.78)$$

This can be understood as a superposition (with, for variety, a minus sign this time) of (on the one hand) a state in which particle 1 is “spin up along z” and particle 2 is “spin down along z”, and then (on the other hand) a state in which particle 1 is “spin down along z” and particle 2 is “spin up along z”. As in the previous example, neither particle individually has a definite spin state, but there are certain correlations between the particles’ spins; for example, here, if the z-spins of both particles are measured, one cannot predict in advance whether it will be “particle 1 is spin up” and “particle 2 is spin down” (which joint outcome has probability 50%) or instead

“particle 1 is spin down” and “particle 2 is spin up” (which also has probability 50%)... but one can predict in advance, with 100% certainty, that the outcomes of the two spin measurements will be *opposite* – one “up” and one “down”.

You can play around a little bit more with this entangled spin state in the Projects if you so choose. And then we will encounter it again soon when we discuss the famous argument of Einstein, Podolsky, and Rosen in Chap. 4.

### Projects:

- (2.1) For the example from the Particle-in-a-box section – with  $\Psi(x, 0)$  given by Eq. (2.27) – calculate the probability that a measurement of the particle’s position  $x$  at time  $t$  finds the particle on the left-hand-side of the box:  $0 < x < L/2$ .
- (2.2) Use Mathematica or a similar software package to make nice movies of the exact evolution of the real and imaginary parts of  $\Psi(x, t)$  given by Eq. (2.29).
- (2.3) A particle in a box starts in the state  $\Psi(x, 0) = 1/\sqrt{L}$ . What is  $\Psi(x, t)$ ? What is the probability that an energy measurement at time  $t$  yields the ground state energy?
- (2.4) Show explicitly that Eq. (2.26) satisfies the time-dependent Schrödinger Equation.
- (2.5) The uncertainty of some quantity  $A$  is defined as:  $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$ . Use this definition to calculate the exact uncertainty  $\Delta x$  of the position for the Gaussian wave packet given by Eq. (2.33). Note that, for example,  $\langle x^2 \rangle = \int x^2 |\Psi(x)|^2 dx$ . (Here’s a clever way to do integrals of this form:  $\int x^2 e^{-ax^2} dx = -\frac{\partial}{\partial a} \int e^{-ax^2} dx$ .) Then calculate also the uncertainty  $\Delta k$  in the wave number using (2.47) and convert this into a statement about the uncertainty in the momentum. What, exactly, is the product of  $\Delta x$  and  $\Delta p$ ? As it turns out, this Gaussian is a “minimum uncertainty wave packet” – meaning that the product of  $\Delta x$  and  $\Delta p$  for this state is the smallest the product can ever be. (But it can be and usually is bigger!) Summarize this fact by writing down an exact mathematical statement of the Heisenberg uncertainty principle.
- (2.6) Work through the gory mathematical details of deriving Eq. (2.51) from Eq. (2.50). Or better, develop a general formula for Gaussian integrals of the form  $\int e^{-Ak^2} e^{Bk} dk$  in terms of  $A$  and  $B$ . Then use the general formula to show how (2.51) follows from (2.50).
- (2.7) Show explicitly that the  $\Psi(x, t)$  in Eq. (2.51) solves the time-dependent Schrödinger Equation.
- (2.8) Use Mathematica (or some similar package) to make some nice animations showing the time-evolution of  $\Psi(x, t)$  for the initially Gaussian wave packet, Eq. (2.51). For example, what does the real part look like? The imaginary part? The modulus squared?
- (2.9) Suppose the initial wave function is a position eigenstate:  $\Psi(x, 0) = \delta(x - x')$ . What is  $\Psi(x, t)$ ? Note that this is a very useful result, since *any* initial wave function can be written as a linear combination of  $\delta$  functions in a rather trivial way:  $\Psi(x, 0) = \int \Psi(x', 0) \delta(x - x') dx$ . And of

course the Schrödinger equation is linear, so  $\Psi(x, t)$  is just that same linear combination of the time-evolved versions of  $\delta(x - x')$ , i.e.,  $\Psi(x, t) = \int \Psi(x', 0)G(x, x', t) dx$ , where  $G(x, x', t)$  is just the wave function that  $\Psi(x, 0) = \delta(x - x')$  evolves into at time  $t$ . Use this alternative approach to re-derive our expression for  $\Psi(x, t)$  for the initially Gaussian wave packet.

- (2.10) Use the approach from Project 2.9 to write an expression for  $\Psi(x, t)$  for a  $\Psi(x, 0)$  that is constant for  $-L/2 < x < L/2$ , and zero otherwise. This expression will have some divergence issues. But you should be able to show that in the  $t \rightarrow \infty$  limit, a certain simplification allows you to derive a nice result for (what can be understood as) the probability density associated with (regular, non-Gaussian) single-slit diffraction (assuming the detection screen is far behind the slit). Make a nice graph.
- (2.11) Let's try to understand the mathematics behind the idea, from Sect. 2.4, of trading out the  $t$ -dependence of our one-dimensional  $\Psi(x, t)$ , using  $y = vt$ , for a wave function that we interpret as a solution  $\psi(x, y)$  of the two-dimensional TISE. Start with the Schrödinger Equation in two dimensions,

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{2mi}{\hbar} \frac{\partial}{\partial t} \right) \Psi(x, y, t) = 0, \quad (2.79)$$

and look for solutions of the form

$$\Psi(x, y, t) = \phi(x, y)e^{i(ky - \omega t)} \quad (2.80)$$

corresponding to a plane wave propagating in the  $y$ -direction, but with a slowly-varying  $y$ -dependent transverse profile  $\phi$ . (a) Plug Eq. (2.80) into Eq. (2.79) and show that, for  $\omega = \hbar k^2/2m$  and  $2k \frac{\partial \phi}{\partial y} \gg \frac{\partial^2 \phi}{\partial y^2}$ ,  $\phi$  should satisfy

$$\frac{\partial^2 \phi}{\partial x^2} + 2ik \frac{\partial \phi}{\partial y} = 0. \quad (2.81)$$

(b) Explain why the two conditions used in (a) are reasonable and what they mean physically. (c) Argue that, with  $y \leftrightarrow vt$  (where  $v = \hbar k/m$ ), Eq. (2.81) is just the one-dimensional time-dependent Schrödinger equation. [Note that this technique is called the “paraxial approximation”.]

- (2.12) A spin 1/2 particle is prepared in the state  $\psi_{-x}$  (spin down along  $x$ ). We then perform a measurement of its spin along the same  $\hat{n}$  direction used in the example in the text:  $60^\circ$  down from the  $z$ -axis (toward the  $x$ -axis). Find the probabilities for the two possible measurement outcomes.
- (2.13) If a spin 1/2 particle is placed in a magnetic field  $\vec{B}$ , the spin-up and spin-down states (parallel to the magnetic field direction) have different energies, which one can capture with an appropriate Hamiltonian operator. For example, if the magnetic field is in the  $y$ -direction, we can write

$$\hat{H} = \hbar\omega\hat{\sigma}_y = \hbar\omega \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

where  $\omega$  is a constant (with angular frequency units, hence the letter) that depends on the magnetic dipole moment of the particle and the strength of the field. Use this Hamiltonian operator in Eq. (2.1) to find out how the (spin) state of a particle, say initially in the state  $\psi_{+z}$ , evolves in time. (Hint: use the general method outlined in the chapter of solving the time-dependent Schrödinger equation, namely, first find the energy eigenstates, then write the initial state as a linear combination of energy eigenstates, then tack the appropriate time-dependent exponential factor onto each term in the linear combination.)

- (2.14) For the “two particles in a box” system, construct an entangled state in which even the total energy of the two particles is not well-defined. Use Mathematica to make some density plots and/or movies showing how the state looks and how it evolves in time.
- (2.15) The “two particles in a box” system is mathematically isomorphic to a “one particle in a two-dimensional box” system. Explain and contemplate.
- (2.16) Re-write the “singlet” spin state for two spin 1/2 particles – Eq. (2.78) – in terms of the spin-up and spin-down *along the x-axis* states,  $\psi_{+x}$  and  $\psi_{-x}$ .
- (2.17) Re-write the “singlet” spin state for two spin 1/2 particles – Eq. (2.78) – in terms of the spin-up and spin-down *along the n-axis* states,  $\psi_{+n}$  and  $\psi_{-n}$ .

## References

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