# 5

# Simple Problems in One Dimension

Now that the postulates have been stated and explained, it is all over but for the applications. We begin with the simplest class of problems—concerning a single particle in one dimension. Although these one-dimensional problems are somewhat artificial, they contain most of the features of three-dimensional quantum mechanics but little of its complexity. One problem we will not discuss in this chapter is that of the harmonic oscillator. This problem is so important that a separate chapter has been devoted to its study.

## 5.1. The Free Particle

The simplest problem in this family is of course that of the free particle. The Schrödinger equation is

$$i\hbar|\dot{\psi}\rangle = H|\psi\rangle = \frac{P^2}{2m}|\psi\rangle \tag{5.1.1}$$

The normal modes or stationary states are solutions of the form

$$|\psi\rangle = |E\rangle\, e^{-iEt/\hbar} \tag{5.1.2}$$

Feeding this into Eq. (5.1.1), we get the time-independent Schrödinger equation for $|E\rangle$:

$$H|E\rangle = \frac{P^2}{2m}|E\rangle = E|E\rangle \tag{5.1.3}$$

This problem can be solved without going to any basis. First note that any eigenstate of $P$ is also an eigenstate of $P^2$. So we feed the trial solution $|p\rangle$ into Eq. (5.1.3) and find

$$\frac{P^2}{2m}|p\rangle = E|p\rangle$$

or

$$\left(\frac{p^2}{2m} - E\right)|p\rangle = 0 \tag{5.1.4}$$

Since $|p\rangle$ is not a null vector, we find that the allowed values of $p$ are

$$p = \pm(2mE)^{1/2} \tag{5.1.5}$$

In other words, there are two orthogonal eigenstates for each eigenvalue $E$:

$$|E, +\rangle = |p = (2mE)^{1/2}\rangle \tag{5.1.6}$$

$$|E, -\rangle = |p = -(2mE)^{1/2}\rangle \tag{5.1.7}$$

Thus, we find that to the eigenvalue $E$ there corresponds a degenerate two-dimensional eigenspace, spanned by the above vectors. Physically this means that a particle of energy $E$ can be moving to the right or to the left with momentum $|p| = (2mE)^{1/2}$. Now, you might say, "This is exactly what happens in classical mechanics. So what's new?" What is new is the fact that the state

$$|E\rangle = \beta|p = (2mE)^{1/2}\rangle + \gamma|p = -(2mE)^{1/2}\rangle \tag{5.1.8}$$

is also an eigenstate of energy $E$ and represents a *single* particle of energy $E$ that can be caught moving either to the right or to the left with momentum $(2mE)^{1/2}$!

To construct the complete orthonormal eigenbasis of $H$, we must pick from each degenerate eigenspace any two orthonormal vectors. The obvious choice is given by the kets $|E, +\rangle$ and $|E, -\rangle$ themselves. In terms of the ideas discussed in the past, we are using the eigenvalue of a compatible variable $P$ as an extra label within the space degenerate with respect to energy. Since $P$ is a nondegenerate operator, the label $p$ by itself is adequate. In other words, there is no need to call the state $|p, E = P^2/2m\rangle$, since the value of $E = E(p)$ follows, given $p$. We shall therefore drop this redundant label.

The propagator is then

$$\begin{aligned} U(t) &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar}\, dp \\ &= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-ip^2t/2m\hbar}\, dp \end{aligned} \tag{5.1.9}$$

*Exercise 5.1.1.* Show that Eq. (5.1.9) may be rewritten as an integral over $E$ and a sum over the $\pm$ index as

$$U(t)=\sum_{\alpha=\pm}\int_0^\infty\left[\frac{m}{(2mE)^{1/2}}\right]|E,\alpha\rangle\langle E,\alpha|\,e^{-iEt/\hbar}\,dE$$

*Exercise 5.1.2.** By solving the eigenvalue equation (5.1.3) in the $X$ basis, regain Eq. (5.1.8), i.e., show that the general solution of energy $E$ is

$$\psi_E(x)=\beta\frac{\exp[i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}+\gamma\frac{\exp[-i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}$$

[The factor $(2\pi\hbar)^{-1/2}$ is arbitrary and may be absorbed into $\beta$ and $\gamma$.] Though $\psi_E(x)$ will satisfy the equation even if $E<0$, are these functions in the Hilbert space?

The propagator $U(t)$ can be evaluated explicitly in the $X$ basis. We start with the matrix element

$$\begin{aligned}U(x,t;x')\equiv\langle x|U(t)|x'\rangle&=\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|x'\rangle\,e^{-ip^2t/2m\hbar}\,dp\\&=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{ip(x-x')/\hbar}\cdot e^{-ip^2t/2m\hbar}\,dp\\&=\left(\frac{m}{2\pi\hbar it}\right)^{1/2}e^{im(x-x')^2/2\hbar t}\end{aligned}\tag{5.1.10}$$

using the result from Appendix A.2 on Gaussian integrals. In terms of this propagator, any initial-value problem can be solved, since

$$\psi(x,t)=\int U(x,t;x')\psi(x',0)\,dx'\tag{5.1.11}$$

Had we chosen the initial time to be $t'$ rather than zero, we would have gotten

$$\psi(x,t)=\int U(x,t;x',t')\psi(x',t')dx'\tag{5.1.12}$$

where $U(x,t;x',t')=\langle x|U(t-t')|x'\rangle$, since $U$ depends only on the time interval $t-t'$ and not the absolute values of $t$ and $t'$. [Had there been a time-dependent potential such as $V(t)=V_0\,e^{-\alpha t^2}$ in $H$, we could have told what absolute time it was by looking at $V(t)$. In the absence of anything defining an absolute time in the problem, only time differences have physical significance.] Whenever we set $t'=0$, we will resort to our old convention and write $U(x,t;x',0)$ as simply $U(x,t;x')$.

A nice physical interpretation may be given to $U(x,t;x',t')$ by considering a special case of Eq. (5.1.12). Suppose we started off with a particle localized at

$x'=x_0'$, that is, with $\psi(x', t')=\delta(x'-x_0')$. Then

$$\psi(x, t)=U(x, t; x_0', t') \tag{5.1.13}$$

In other words, the propagator (in the $X$ basis) is the amplitude that a particle starting out at the space-time point $(x_0', t')$ ends with at the space–time point $(x, t)$. [It can obviously be given such an interpretation in any basis: $\langle\omega|U(t, t')|\omega'\rangle$ is the amplitude that a particle in the state $|\omega'\rangle$ at $t'$ ends up with in the state $|\omega\rangle$ at $t$.] Equation (5.1.12) then tells us that the total amplitude for the particle's arrival at $(x, t)$ is the sum of the contributions from all points $x'$ with a weight proportional to the initial amplitude $\psi(x', t')$ that the particle was at $x'$ at time $t'$. One also refers to $U(x, t; x_0', t')$ as the "fate" of the delta function $\psi(x', t')=\delta(x'-x_0')$.

### Time Evolution of the Gaussian Packet

There is an unwritten law which says that the derivation of the free-particle propagator be followed by its application to the Gaussian packet. Let us follow this tradition.

Consider as the initial wave function the wave packet

$$\psi(x', 0)=e^{ip_0x'/\hbar}\frac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} \tag{5.1.14}$$

This packet has mean position $\langle X\rangle=0$, with an uncertainty $\Delta X=\Delta/2^{1/2}$, and mean momentum $p_0$ with uncertainty $\hbar/2^{1/2}\Delta$. By combining Eqs. (5.1.10) and (5.1.12) we get

$$\psi(x, t)=\left[\pi^{1/2}\left(\Delta+\frac{i\hbar t}{m\Delta}\right)\right]^{-1/2}\cdot\exp\left[\frac{-(x-p_0t/m)^2}{2\Delta^2(1+i\hbar t/m\Delta^2)}\right]$$
$$\times\exp\left[\frac{ip_0}{\hbar}\left(x-\frac{p_0t}{2m}\right)\right] \tag{5.1.15}$$

The corresponding probability density is

$$P(x, t)=\frac{1}{\pi^{1/2}(\Delta^2+\hbar^2t^2/m^2\Delta^2)^{1/2}}\cdot\exp\left\{\frac{-[x-(p_0/m)t]^2}{\Delta^2+\hbar^2t^2/m^2\Delta^2}\right\} \tag{5.1.16}$$

The main features of this result are as follows:

(1) The mean position of the particles is

$$\langle X\rangle=\frac{p_0t}{m}=\frac{\langle P\rangle t}{m}$$

In other words, the classical relation $x=(p/m)t$ now holds between average quantities. This is just one of the consequences of the *Ehrenfest theorem* which states that the classical equations obeyed by dynamical variables will have counterparts in quantum mechanics as relations among expectation values. The theorem will be proved in the next chapter.

(2) The width of the packet grows as follows:

$$\Delta X(t)=\frac{\Delta(t)}{2^{1/2}}=\frac{\Delta}{2^{1/2}}\left(1+\frac{\hbar^2t^2}{m^2\Delta^4}\right)^{1/2} \tag{5.1.17}$$

The increasing uncertainty in position is a reflection of the fact that any uncertainty in the initial velocity (that is to say, the momentum) will be reflected with passing time as a growing uncertainty in position. In the present case, since $\Delta V(0)=\Delta P(0)/m=\hbar/2^{1/2}m\Delta$, the uncertainty in $X$ grows approximately as $\Delta X\simeq\hbar t/2^{1/2}m\Delta$ which agrees with Eq. (5.1.17) for large times. Although we are able to understand the spreading of the wave packet in classical terms, the fact that the initial spread $\Delta V(0)$ is *unavoidable* (given that we wish to specify the position to an accuracy $\Delta$) is a purely quantum mechanical feature.

If the particle in question were macroscopic, say of mass 1 g, and we wished to fix its initial position to within a proton width, which is approximately $10^{-13}$ cm, the uncertainty in velocity would be

$$\Delta V(0)\simeq\frac{\hbar}{2^{1/2}m\Delta}\simeq 10^{-14}\text{ cm/sec}$$

It would be over 300,000 years before the uncertainty $\Delta(t)$ grew to 1 millimeter! We may therefore treat a macroscopic particle classically for any reasonable length of time. This and similar questions will be taken up in greater detail in the next chapter.

*Exercise 5.1.3* (*Another Way to Do the Gaussian Problem*). We have seen that there exists another formula for $U(t)$, namely, $U(t)=e^{-iHt/\hbar}$. For a free particle this becomes

$$U(t)=\exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2t}{2m}\frac{d^2}{dx^2}\right)\right]=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n\frac{d^{2n}}{dx^{2n}} \tag{5.1.18}$$

Consider the initial state in Eq. (5.1.14) with $p_0=0$, and set $\Delta=1$, $t'=0$:

$$\psi(x,0)=\frac{e^{-x^2/2}}{(\pi)^{1/4}}$$

Find $\psi(x,t)$ using Eq. (5.1.18) above and compare with Eq. (5.1.15).

Hints: (1) Write $\psi(x,0)$ as a power series:

$$\psi(x,0)=(\pi)^{-1/4}\sum_{n=0}^{\infty}\frac{(-1)^nx^{2n}}{n!(2)^n}$$

(2) Find the action of a few terms

$$1, \quad \left(\frac{i\hbar t}{2m}\right)\frac{d^2}{dx^2}, \quad \frac{1}{2!}\left(\frac{i\hbar t}{2m}\frac{d^2}{dx^2}\right)^2$$

etc., on this power series.

(3) Collect terms with the same power of $x$.

(4) Look for the following series expansion in the coefficient of $x^{2n}$:

$$\left(1+\frac{it\hbar}{m}\right)^{-n-1/2} = 1-(n+1/2)\left(\frac{i\hbar t}{m}\right)+\frac{(n+1/2)(n+3/2)}{2!}\left(\frac{it\hbar}{m}\right)^2+\cdots$$

(5) Juggle around till you get the answer.

*Exercise 5.1.4: A Famous Counterexample.* Consider the wave function

$$\psi(x, 0) = \sin\left(\frac{\pi x}{L}\right), \qquad |x| \leq L/2$$
$$= 0, \qquad |x| > L/2$$

It is clear that when this function is differentiated any number of times we get another function confined to the interval $|x| \leq L/2$. Consequently the action of

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\right)\frac{d^2}{dx^2}\right]$$

on this function is to give a function confined to $|x| \leq L/2$. What about the spreading of the wave packet?

[Answer: Consider the derivatives at the boundary. We have here an example where the (exponential) operator power series doesn't converge. Notice that the convergence of an operator power series depends not just on the operator but also on the operand. So there is no paradox: if the function dies abruptly as above, so that there seems to be a paradox, the derivatives are singular at the boundary, while if it falls off continuously, the function will definitely leak out given enough time, no matter how rapid the falloff.]

## Some General Features of Energy Eigenfunctions

Consider now the energy eigenfunctions in some potential $V(x)$. These obey

$$\psi'' = -\frac{2m(E-V)}{\hbar^2}\psi$$

where each prime denotes a spatial derivative. Let us ask what the continuity of $V(x)$ implies. Let us start at some point $x_0$ where $\psi$ and $\psi'$ have the values $\psi(x_0)$ and $\psi'(x_0)$. If we pretend that $x$ is a time variable and that $\psi$ is a particle coordinate, the problem of finding $\psi$ everywhere else is like finding the trajectory of a particle (for all times past and future) given its position and velocity at some time and its acceleration as a function of its position and time. It is clear that if we integrate

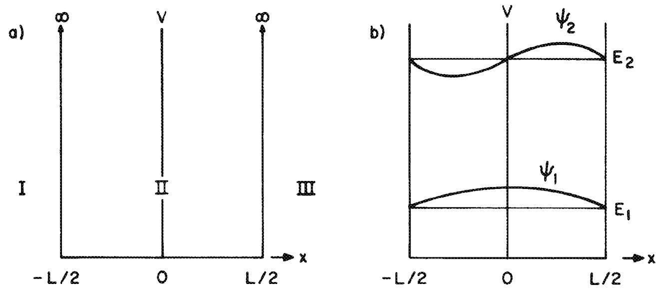


**Figure 5.1.** (a) The box potential. (b) The first two levels and wave functions in the box.

these equations we will get continuous $\psi'(x)$ and $\psi(x)$. This is the typical situation. There are, however, some problems where, for mathematical simplicity, we consider potentials that change abruptly at some point. This means that $\psi''$ jumps abruptly there. However, $\psi'$ will still be continuous, for the area under a function is continuous even if the function jumps a bit. What if the change in $V$ is infinitely large? It means that $\psi''$ is also infinitely large. This in turn means that $\psi'$ *can* change abruptly as we cross this point, for the area under $\psi''$ can be finite over an infinitesimal region that surrounds this point. But whether or not $\psi'$ is continuous, $\psi$, which is the area under it, will be continuous.‡

Let us turn our attention to some specific cases.

## 5.2. The Particle in a Box

We now consider our first problem with a potential, albeit a rather artificial one:

$$\begin{aligned} V(x) &= 0, \qquad |x| < L/2 \\ &= \infty, \qquad |x| \geq L/2 \end{aligned} \tag{5.2.1}$$

This potential (Fig. 5.1a) is called the box since there is an infinite potential barrier in the way of a particle that tries to leave the region $|x| < L/2$. The eigenvalue equation in the $X$ basis (which is the only viable choice) is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \tag{5.2.2}$$

We begin by partitioning space into three regions I, II, and III (Fig. 5.1a). The solution $\psi$ is called $\psi_{\text{I}}$, $\psi_{\text{II}}$, and $\psi_{\text{III}}$ in regions I, II, and III, respectively.

Consider first region III, in which $V = \infty$. It is convenient to first consider the case where $V$ is not infinite but equal to some $V_0$ which is greater than $E$. Now

‡ We are assuming that the jump in $\psi'$ is finite. This will be true even in the artificial potentials we will encounter. But can you think of a potential for which this is not true? (Think delta.)

Eq. (5.2.2) becomes

$$\frac{d^2\psi_{\rm III}}{dx^2}-\frac{2m(V_0-E)}{\hbar^2}\psi_{\rm III}=0 \tag{5.2.3}$$

which is solved by

$$\psi_{\rm III}=A\,e^{-\kappa x}+B\,e^{\kappa x} \tag{5.2.4}$$

where $\kappa=[2m(V_0-E)/\hbar^2]^{1/2}$.

Although $A$ and $B$ are arbitrary coefficients from a mathematical standpoint, we must set $B=0$ on physical grounds since $B\,e^{\kappa x}$ blows up exponentially as $x\to\infty$ and such functions are not members of our Hilbert space. If we now let $V\to\infty$, we see that

$$\psi_{\rm III}\equiv 0$$

It can similarly be shown that $\psi_{\rm I}\equiv 0$. In region II, since $V=0$, the solutions are exactly those of a free particle:

$$\psi_{\rm II}=A\exp[i(2mE/\hbar^2)^{1/2}x]+B\exp[-i(2mE/\hbar^2)^{1/2}x] \tag{5.2.5}$$

$$=A\,e^{ikx}+B\,e^{-ikx},\qquad k=(2mE/\hbar^2)^{1/2} \tag{5.2.6}$$

It therefore appears that the energy eigenvalues are once again continuous as in the free-particle case. This is not so, for $\psi_{\rm II}(x)=\psi$ only in region II and not in all of space. We must require that $\psi_{\rm II}$ goes continuously into its counterparts $\psi_{\rm I}$ and $\psi_{\rm III}$ as we cross over to regions I and III, respectively. In other words we require that

$$\psi_{\rm I}(-L/2)=\psi_{\rm II}(-L/2)=0 \tag{5.2.7}$$

$$\psi_{\rm III}(+L/2)=\psi_{\rm II}(+L/2)=0 \tag{5.2.8}$$

(We make no such continuity demands on $\psi'$ at the walls of the box since $V$ jumps to infinity there.) These constraints applied to Eq. (5.2.6) take the form

$$A\,e^{-ikL/2}+B\,e^{ikL/2}=0 \tag{5.2.9a}$$

$$A\,e^{ikL/2}+B\,e^{-ikL/2}=0 \tag{5.2.9b}$$

or in matrix form

$$\begin{bmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{5.2.10}$$

Such an equation has nontrivial solutions only if the determinant vanishes:

$$e^{-ikL}-e^{ikL}=-2i\sin(kL)=0 \tag{5.2.11}$$

that is, only if

$$k=\frac{n\pi}{L}, \qquad n=0,\ \pm 1,\ \pm 2, \ldots \tag{5.2.12}$$

To find the corresponding eigenfunctions, we go to Eqs. (5.2.9a) and (5.2.9b). Since only one of them is independent, we study just Eq. (5.2.9a), which says

$$A\,e^{-in\pi/2}+B\,e^{in\pi/2}=0 \tag{5.2.13}$$

Multiplying by $e^{i\pi n/2}$, we get

$$A=-e^{in\pi}B \tag{5.2.14}$$

Since $e^{in\pi}=(-1)^n$, Eq. (5.2.6) generates two families of solutions (normalized to unity):

$$\psi_n(x)=\left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{n\pi x}{L}\right), \qquad n \text{ even} \tag{5.2.15}$$

$$=\left(\frac{2}{L}\right)^{1/2}\cos\left(\frac{n\pi x}{L}\right), \qquad n \text{ odd} \tag{5.2.16}$$

Notice that the case $n=0$ is uninteresting since $\psi_0\equiv 0$. Further, since $\psi_n=\psi_{-n}$ for $n$ odd and $\psi_n=-\psi_{-n}$ for $n$ even, and since eigenfunctions differing by an overall factor are not considered distinct, we may restrict ourselves to positive nonzero $n$. In summary, we have

$$\psi_n=\left(\frac{2}{L}\right)^{1/2}\cos\left(\frac{n\pi x}{L}\right), \qquad n=1, 3, 5, 7, \ldots \tag{5.2.17a}$$

$$=\left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{n\pi x}{L}\right), \qquad n=2, 4, 6, \ldots \tag{5.2.17b}$$

and from Eqs. (5.2.6) and (5.2.12),

$$E_n=\frac{\hbar^2k_n^2}{2m}=\frac{\hbar^2\pi^2n^2}{2mL^2} \tag{5.2.17c}$$

[It is tacitly understood in Eqs. (5.2.17a) and (5.2.17b) that $|x|<L/2$.]

We have here our first encounter with the quantization of a dynamical variable. Both the variables considered so far, $X$ and $P$, had a continuous spectrum of eigenvalues from $-\infty$ to $+\infty$, which coincided with the allowed values in classical mechanics. In fact, so did the spectrum of the Hamiltonian in the free-particle case. The particle in the box is the simplest example of a situation that will be encountered again and again, wherein Schrödinger's equation, combined with appropriate boundary conditions, leads to the quantization of energy. These solutions are also examples of *bound states*, namely, states in which a potential prevents a particle from escaping to infinity. Bound states are thus characterized by

$$\psi(x) \xrightarrow[|x|\to\infty]{} 0$$

Bound states appear in quantum mechanics exactly where we expect them classically, namely, in situations where $V(\pm\infty)$ is greater than $E$.

The energy levels of bound states are always quantized. Let us gain some insight into how this happens. In the problem of the particle in a box, quantization resulted from the requirement that $\psi_{\rm II}$ completed an integral number of half-cycles within the box so that it smoothly joined its counterparts $\psi_{\rm I}$ and $\psi_{\rm III}$ which vanished identically. Consider next a particle bound by a finite well, i.e., by a potential that jumps from 0 to $V_0$ at $|x|=L/2$. We have already seen [Eq. (5.2.4)] that in the classically forbidden region ($E<V_0$, $|x|\geq L/2$) $\psi$ is a sum of rising and falling exponentials (as $|x|\to\infty$) and that we must choose the coefficient of the rising exponential to be zero to get an admissible solution. In the classically allowed region ($|x|\leq L/2$) $\psi$ is a sum of a sine and cosine. Since $V$ is everywhere finite, we demand that $\psi$ and $\psi'$ be continuous at $x=\pm L/2$. Thus we impose four conditions on $\psi$, which has only three free parameters. (It may seem that there are four—the coefficients of the two falling exponentials, the sine, and the cosine. However, the overall scale of $\psi$ is irrelevant both in the eigenvalue equation and the continuity conditions, these being *linear* in $\psi$ and $\psi'$. Thus if say, $\psi'$ does not satisfy the continuity condition at $x=L/2$, an overall rescaling of $\psi$ and $\psi'$ will not help.) Clearly, the continuity conditions cannot be fulfilled except possibly at certain special energies. (See Exercise 5.2.6 for details). This is the origin of energy quantization here.

Consider now a general potential $V(x)$ which tends to limits $V_\pm$ as $x\to\pm\infty$ and which binds a particle of energy $E$ (less than both $V_\pm$). We argue once again that we have one more constraint than we have parameters, as follows. Let us divide space into tiny intervals such that in each interval $V(x)$ is essentially constant. As $x\to\pm\infty$, these intervals can be made longer and longer since $V$ is stabilizing at its asymptotic values $V_\pm$. The right- and leftmost intervals can be made infinitely wide, since by assumption $V$ has a definite limit as $x\to\pm\infty$. Now in all the finite intervals, $\psi$ has two parameters: these will be the coefficients of the sine/cosine if $E>V$ or growing/falling exponential if $E<V$. (The rising exponential is not disallowed, since it doesn't blow up within the finite intervals.) Only in the left- and rightmost intervals does $\psi$ have just one parameter, for in these infinite intervals, the growing exponential can blow up. All these parameters are constrained by the continuity of $\psi$ and $\psi'$ at each interface between adjacent regions. To see that we have one more constraint than we have parameters, observe that every extra interval brings with it two free parameters and one new interface, i.e., two new constraints. Thus as we go from

three intervals in the finite well to the infinite number of intervals in the arbitrary potential, the constraints are always one more than the free parameters. Thus only at special energies can we expect an allowed solution.

[Later we will study the oscillator *potential*, $V=\frac{1}{2}m\omega^2x^2$, which grows without limit as $|x|\to\infty$. How do we understand energy quantization here? Clearly, any *allowed* $\psi$ will vanish even more rapidly than before as $|x|\to\infty$, since $V-E$, instead of being a constant, grows quadratically, so that the particle is "even more forbidden than before" from escaping to infinity. If $E$ is an allowed energy,‡ we expect $\psi$ to fall off rapidly as we cross the classical turning points $x_0=\pm(2E/m\omega^2)^{1/2}$. To a particle in such a state, it shouldn't matter if we flatten out the potential to some constant at distances much greater than $|x_0|$, i.e., the *allowed* levels and eigenfunctions must be the same in the two potentials which differ only in a region that the particle is so strongly inhibited from going to. Since the flattened-out potential has the asymptotic behavior we discussed earlier, we can understand energy quantization as we did before.]

Let us restate the origin of energy quantization in another way. Consider the search for acceptable energy eigenfunctions, taking the finite well as an example. If we start with some arbitrary values $\psi(x_0)$ and $\psi'(x_0)$, at some point $x_0$ to the right of the well, we can integrate Schrödinger's equation numerically. (Recall the analogy with the problem of finding the trajectory of a particle given its initial position and velocity and the force on it.) As we integrate out to $x\to\infty$, $\psi$ will surely blow up since $\psi_{\text{III}}$ contains a growing exponential. Since $\psi(x_0)$ merely fixes the overall scale, we vary $\psi'(x_0)$ until the growing exponential is killed. [Since we can solve the problem analytically in region III, we can even say what the desired value of $\psi'(x_0)$ is: it is given by $\psi'(x_0)=-\kappa\psi(x_0)$. Verify, starting with Eq. (5.2.4), that this implies $B=0$.] We are now out of the fix as $x\to\infty$, but we are committed to whatever comes out as we integrate to the left of $x_0$. We wiil find that $\psi$ grows exponentially till we reach the well, whereupon it will oscillate. When we cross the well, $\psi$ will again start to grow exponentially, for $\psi_{\text{I}}$ also contains a growing exponential in general. Thus there will be no acceptable solution at some randomly chosen energy. It can, however, happen that for certain values of energy, $\psi$ will be exponentially damped in both regions I *and* III. [At any point $x_0'$ in region I, there is a ratio $\psi'(x_0')/\psi(x_0')$ for which only the damped exponential survives. The $\psi$ we get integrating from region III will not generally have this feature. At special energies, however, this can happen.] These are the allowed energies and the corresponding functions are the allowed eigenfunctions. Having found them, we can choose $\psi(x_0)$ such that they are normalized to unity. For a nice numerical analysis of this problem see the book by Eisberg and Resnick.§

It is clear how these arguments generalize to a particle bound by some arbitrary potential: if we try to keep $\psi$ exponentially damped as $x\to-\infty$, it blows up as $x\to\infty$ (and vice versa), except at some special energies. It is also clear why there is no quantization of energy for unbound states: since the particle is classically allowed at infinity, $\psi$ *oscillates* there and so we have two more parameters, one from each end (why?), and so two solutions (normalizable to $\delta(0)$) at *any* energy.

‡ We are not assuming $E$ is quantized.

§ R. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles*, Wiley, New York (1974). See Section 5.7 and Appendix F.

Let us now return to the problem of the particle in a box and discuss the fact that the lowest energy is not zero (as it would be classically, corresponding to the particle at rest inside the well) but $\hbar^2\pi^2/2mL^2$. The reason behind it is the uncertainty principle, which prevents the particle, whose position (and hence $\Delta X$) is bounded by $|x| \le L/2$, from having a well-defined momentum of zero. This in turn leads to a lower bound on the energy, which we derive as follows. We begin with‡

$$H = \frac{P^2}{2m} \tag{5.2.18}$$

so that

$$\langle H \rangle = \frac{\langle P^2 \rangle}{2m} \tag{5.2.19}$$

Now $\langle P \rangle = 0$ in any bound state for the following reason. Since a bound state is a stationary state, $\langle P \rangle$ is time independent. If this $\langle P \rangle \neq 0$, the particle must (in the average sense) drift either to the right or to the left and eventually escape to infinity, which cannot happen in a bound state.

Consequently we may rewrite Eq. (5.2.19) as

$$\langle H \rangle = \frac{\langle (P - \langle P \rangle)^2 \rangle}{2m} = \frac{(\Delta P)^2}{2m}$$

If we now use the uncertainty relation

$$\Delta P \cdot \Delta X \ge \hbar/2$$

we find

$$\langle H \rangle \ge \frac{\hbar^2}{8m(\Delta X)^2}$$

Since the variable $x$ is constrained by $-L/2 \le x \le L/2$, its standard deviation $\Delta X$ cannot exceed $L/2$. Consequently

$$\langle H \rangle \ge \hbar^2/2mL^2$$

In an energy eigenstate, $\langle H \rangle = E$ so that

$$E \ge \hbar^2/2mL^2 \tag{5.2.20}$$

The actual ground-state energy $E_1$ happens to be $\pi^2$ times as large as the lower

‡ We are suppressing the infinite potential due to the walls of the box. Instead we will restrict $x$ to the range $|x| \le L/2$.

bound. The uncertainty principle is often used in this fashion to provide a quick order-of-magnitude estimate for the ground-state energy.

If we denote by $|n\rangle$ the abstract ket corresponding to $\psi_n(x)$, we can write the propagator as

$$U(t)=\sum_{n=1}^{\infty} |n\rangle\langle n| \exp\left[-\frac{i}{\hbar}\left(\frac{\hbar^2\pi^2 n^2}{2mL^2}\right)t\right] \quad (5.2.21)$$

The matrix elements of $U(t)$ in the $X$ basis are then

$$\begin{aligned}\langle x| U(t)|x'\rangle &= U(x, t; x')\\ &=\sum_{n=1}^{\infty} \psi_n(x)\psi_n^*(x') \exp\left[-\frac{i}{\hbar}\left(\frac{\hbar^2\pi^2 n^2}{2mL^2}\right)t\right]\end{aligned} \quad (5.2.22)$$

Unlike in the free-particle case, there exists no simple closed expression for this sum.

*Exercise 5.2.1.** A particle is in the ground state of a box of length $L$. Suddenly the box expands (symmetrically) to twice its size, leaving the wave function undisturbed. Show that the probability of finding the particle in the ground state of the new box is $(8/3\pi)^2$.

*Exercise 5.2.2.** (a) Show that for any normalized $|\psi\rangle$, $\langle\psi|H|\psi\rangle \geq E_0$, where $E_0$ is the lowest-energy eigenvalue. (Hint: Expand $|\psi\rangle$ in the eigenbasis of $H$.)

(b) Prove the following theorem: Every attractive potential in one dimension has at least one bound state. Hint: Since $V$ is attractive, if we define $V(\infty)=0$, it follows that $V(x)=-|V(x)|$ for all $x$. To show that there exists a bound state with $E<0$, consider

$$\psi_\alpha(x)=\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

and calculate

$$E(\alpha)=\langle\psi_\alpha|H|\psi_\alpha\rangle, \qquad H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-|V(x)|$$

Show that $E(\alpha)$ can be made negative by a suitable choice of $\alpha$. The desired result follows from the application of the theorem proved above.

*Exercise 5.2.3.** Consider $V(x)=-aV_0\delta(x)$. Show that it admits a bound state of energy $E=-ma^2V_0^2/2\hbar^2$. Are there any other bound states? Hint: Solve Schrödinger's equation outside the potential for $E<0$, and keep only the solution that has the right behavior at infinity and is continuous at $x=0$. Draw the wave function and see how there is a cusp, or a discontinuous change of slope at $x=0$. Calculate the change in slope and equate it to

$$\int_{-\varepsilon}^{+\varepsilon}\left(\frac{d^2\psi}{dx^2}\right)dx$$

(where $\varepsilon$ is infinitesimal) determined from Schrödinger's equation.

*Exercise 5.2.4.* Consider a particle of mass $m$ in the state $|n\rangle$ of a box of length $L$. Find the force $F=-\partial E/\partial L$ encountered when the walls are slowly pushed in, assuming the particle remains in the $n$th state of the box as its size changes. Consider a classical particle of energy $E_n$ in this box. Find its velocity, the frequency of collision on a given wall, the momentum transfer per collision, and hence the average force. Compare it to $-\partial E/\partial L$ computed above.

*Exercise 5.2.5.** If the box extends from $x=0$ to $L$ (instead of $-L/2$ to $L/2$) show that $\psi_n(x)=(2/L)^{1/2}\sin(n\pi x/L)$, $n=1, 2, \ldots, \infty$ and $E_n=\hbar^2\pi^2n^2/2mL^2$.

*Exercise 5.2.6.** *Square Well Potential.* Consider a particle in a square well potential:

$$V(x)=\begin{cases}0, & |x|\leq a\\ V_0, & |x|\geq a\end{cases}$$

Since when $V_0\to\infty$, we have a box, let us guess what the lowering of the walls does to the states. First of all, all the bound states (which alone we are interested in), will have $E\leq V_0$. Second, the wave functions of the low-lying levels will look like those of the particle in a box, with the obvious difference that $\psi$ will not vanish at the walls but instead spill out with an exponential tail. The eigenfunctions will still be even, odd, even, etc.

(1) Show that the even solutions have energies that satisfy the transcendental equation

$$k\tan ka=\kappa \tag{5.2.23}$$

while the odd ones will have energies that satisfy

$$k\cot ka=-\kappa \tag{5.2.24}$$

where $k$ and $i\kappa$ are the real and complex wave numbers inside and outside the well, respectively. Note that $k$ and $\kappa$ are related by

$$k^2+\kappa^2=2mV_0/\hbar^2 \tag{5.2.25}$$

Verify that as $V_0$ tends to $\infty$, we regain the levels in the box.

(2) Equations (5.2.23) and (5.2.24) must be solved graphically. In the $(\alpha=ka,\ \beta=\kappa a)$ plane, imagine a circle that obeys Eq. (5.2.25). The bound states are then given by the intersection of the curve $\alpha\tan\alpha=\beta$ or $\alpha\cot\alpha=-\beta$ with the circle. (Remember $\alpha$ and $\beta$ are positive.)

(3) Show that there is always one even solution and that there is no odd solution unless $V_0\geq\hbar^2\pi^2/8ma^2$. What is $E$ when $V_0$ just meets this requirement? Note that the general result from Exercise 5.2.2b holds.

## 5.3. The Continuity Equation for Probability

We interrupt our discussion of one-dimensional problems to get acquainted with two concepts that will be used in the subsequent discussions, namely, those of the *probability current density* and the *continuity equation* it satisfies. Since the probability current concept will also be used in three-dimensional problems, we discuss here a particle in three dimensions.

As a prelude to our study of the continuity equation in quantum mechanics, let us recall the analogous equation from electromagnetism. We know in this case that the total charge in the universe is a constant, that is

$$Q(t) = \text{const, independent of time } t \tag{5.3.1}$$

This is an example of a global conservation law, for it refers to the total charge in the universe. But charge is also conserved locally, a fact usually expressed in the form of the continuity equation

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{j} \tag{5.3.2}$$

where $\rho$ and $\mathbf{j}$ are the charge and current densities, respectively. By integrating this equation over a volume $V$ bounded by a surface $S_V$ we get, upon invoking Gauss's law,

$$\frac{d}{dt}\int_V \rho(\mathbf{r}, t)\, d^3\mathbf{r} = -\int_V \boldsymbol{\nabla}\cdot\mathbf{j}\, d^3\mathbf{r} = -\int_{S_V} \mathbf{j}\cdot d\mathbf{S} \tag{5.3.3}$$

This equation states that any decrease in charge in the volume $V$ is accounted for by the flow of charge out of it, that is to say, charge is not created or destroyed in any volume.

The continuity equation forbids certain processes that obey global conservation, such as the sudden disappearance of charge from one region of space and its immediate reappearance in another.

In quantum mechanics the quantity that is globally conserved is the total probability for finding the particle anywhere in the universe. We get this result by expressing the invariance of the norm in the coordinate basis: since

$$\langle \psi(t) | \psi(t)\rangle = \langle \psi(0) | U^\dagger(t) U(t) | \psi(0)\rangle = \langle \psi(0) | \psi(0)\rangle$$

then

$$\begin{aligned} \text{const} = \langle \psi(t) | \psi(t)\rangle &= \iiint \langle \psi(t) | x, y, z\rangle\langle x, y, z | \psi(t)\rangle \, dx\, dy\, dz\ddagger \\ &= \iiint \langle \psi(t) | \mathbf{r}\rangle\langle \mathbf{r} | \psi(t)\rangle \, d^3\mathbf{r} \\ &= \iiint \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)\, d^3\mathbf{r} \\ &= \iiint P(\mathbf{r}, t)\, d^3\mathbf{r} \end{aligned} \tag{5.3.4}$$

‡ The range of integration will frequently be suppressed when obvious.

This global conservation law is the analog of Eq. (5.3.1). To get the analog of Eq. (5.3.2), we turn to the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi \tag{5.3.5}$$

and its conjugate

$$-i\hbar\frac{\partial\psi^*}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi^*+V\psi^* \tag{5.3.6}$$

Note that $V$ has to be real if $H$ is to be Hermitian. Multiplying the first of these equations by $\psi^*$, the second by $\psi$, and taking the difference, we get

$$i\hbar\frac{\partial}{\partial t}(\psi^*\psi)=-\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi-\psi\nabla^2\psi^*)$$

$$\frac{\partial P}{\partial t}=-\frac{\hbar}{2mi}\mathbf{\nabla}\cdot(\psi^*\mathbf{\nabla}\psi-\psi\mathbf{\nabla}\psi^*)$$

$$\frac{\partial P}{\partial t}=-\mathbf{\nabla}\cdot\mathbf{j} \tag{5.3.7}$$

where

$$\mathbf{j}=\frac{\hbar}{2mi}(\psi^*\mathbf{\nabla}\psi-\psi\mathbf{\nabla}\psi^*) \tag{5.3.8}$$

is the *probability current density*, that is to say, the probability flow per unit time per unit area perpendicular to $\mathbf{j}$. To regain the global conservation law, we integrate Eq. (5.3.7) over all space:

$$\frac{d}{dt}\int P(\mathbf{r},t)\,d^3\mathbf{r}=-\int_{S_\infty}\mathbf{j}\cdot d\mathbf{S} \tag{5.3.9}$$

where $S_\infty$ is the sphere at infinity. For (typical) wave functions which are normalizable to unity, $r^{3/2}\psi\to 0$ as $r\to\infty$ in order that $\int\psi^*\psi r^2\,dr\,d\Omega$ is bounded, and the surface integral of $\mathbf{j}$ on $S_\infty$ vanishes. The case of momentum eigenfunctions that do not vanish on $S_\infty$ is considered in one of the following exercises.

*Exercise 5.3.1.* Consider the case where $V=V_r-iV_i$, where the imaginary part $V_i$ is a constant. Is the Hamiltonian Hermitian? Go through the derivation of the continuity equation and show that the total probability for finding the particle decreases exponentially as $e^{-2V_it/\hbar}$. Such complex potentials are used to describe processes in which particles are absorbed by a sink.

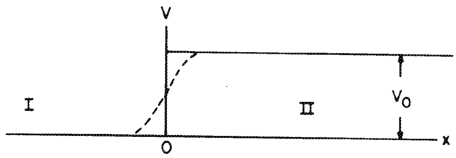


**Figure 5.2.** The single-step potential. The dotted line shows a more realistic potential idealized by the step, which is mathematically convenient. The total energy $E$ and potential energy $V$ are measured along the $y$ axis.

*Exercise 5.3.2.* Convince yourself that if $\psi = c\tilde{\psi}$, where $c$ is constant (real or complex) and $\tilde{\psi}$ is real, the corresponding $\mathbf{j}$ vanishes.

*Exercise 5.3.3.* Consider

$$\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar}$$

Find $\mathbf{j}$ and $P$ and compare the relation between them to the electromagnetic equation $\mathbf{j} = \rho\mathbf{v}$, $\mathbf{v}$ being the velocity. Since $\rho$ and $\mathbf{j}$ are constant, note that the continuity Eq. (5.3.7) is trivially satisfied.

*Exercise 5.3.4.** Consider $\psi = A\, e^{ipx/\hbar} + B\, e^{-ipx/\hbar}$ in one dimension. Show that $j = (|A|^2 - |B|^2)p/m$. The absence of cross terms between the right- and left-moving pieces in $\psi$ allows us to associate the two parts of $j$ with corresponding parts of $\psi$.

### Ensemble Interpretation of j

Recall that $\mathbf{j}\cdot d\mathbf{S}$ is the rate at which probability flows past the area $d\mathbf{S}$. If we consider an ensemble of $N$ particles all in some state $\psi(\mathbf{r}, t)$, then $N\mathbf{j}\cdot d\mathbf{S}$ particles will trigger a particle detector of area $d\mathbf{S}$ per second, assuming that $N$ tends to infinity and that $\mathbf{j}$ is the current associated with $\psi(\mathbf{r}, t)$.

## 5.4. The Single-Step Potential: A Problem in Scattering‡

Consider the step potential (Fig. 5.2)

$$\begin{aligned} V(x) &= 0 \qquad x<0 \quad \text{(region I)} \\ &= V_0 \qquad x>0 \quad \text{(region II)} \end{aligned} \tag{5.4.1}$$

Such an abrupt change in potential is rather unrealistic but mathematically convenient. A more realistic transition is shown by dotted lines in the figure.

Imagine now that a classical particle of energy $E$ is shot in from the left (region I) toward the step. One expects that if $E > V_0$, the particle would climb the barrier and travel on to region II, while if $E < V_0$, it would get reflected. We now compare this classical situation with its quantum counterpart.

‡ This rather difficult section may be postponed till the reader has gone through Chapter 7 and gained more experience with the subject. It is for the reader or the instructor to decide which way to go.

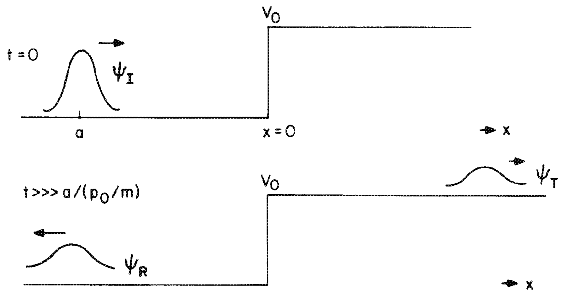


**Figure 5.3.** A schematic description of the wave function long before and long after it hits the step. The area under $|\psi_I|^2$ is unity. The areas under $|\psi_R|^2$ and $|\psi_T|^2$, respectively, are the probabilities for reflection and transmission.

First of all, we must consider an initial state that is compatible with quantum principles. We replace the incident particle possessing a well-defined trajectory with a wave packet.‡ Though the detailed wave function will be seen to be irrelevant in the limit we will consider, we start with a Gaussian, which is easy to handle analytically§:

$$\psi_I(x, 0) = \psi_I(x) = (\pi\Delta^2)^{-1/4} e^{ik_0(x+a)} e^{-(x+a)^2/2\Delta^2} \tag{5.4.2}$$

This packet has a mean momentum $p_0 = \hbar k_0$, a mean position $\langle X \rangle = -a$ (which we take to be far away from the step), with uncertainties

$$\Delta X = \frac{\Delta}{2^{1/2}}, \qquad \Delta P = \frac{\hbar}{2^{1/2}\Delta}$$

We shall be interested in the case of large $\Delta$, where the particle has essentially well-defined momentum $\hbar k_0$ and energy $E_0 \simeq \hbar^2 k_0^2/2m$. *We first consider the case* $E_0 > V_0$.

After a time $t \simeq a[p_0/m]^{-1}$, the packet will hit the step and in general break into two packets: $\psi_R$, the reflected packet, and $\psi_T$, the transmitted packet (Fig. 5.3). The area under $|\psi_R|^2$ at large $t$ is the probability of finding the particle in region I in the distant future, that is to say, the probability of reflection. Likewise the area under $|\psi_T|^2$ at large $t$ is the probability of transmission. Our problem is to calculate the *reflection coefficient*

$$R = \int |\psi_R|^2 \, dx, \qquad t \to \infty \tag{5.4.3}$$

and *transmission coefficient*

$$T = \int |\psi_T|^2 \, dx, \qquad t \to \infty \tag{5.4.4}$$

Generally $R$ and $T$ will depend on the detailed shape of the initial wave function. If, however, we go to the limit in which the initial momentum is well defined (i.e.,

‡ A wave packet is any wave function with reasonably well-defined position and momentum.
§ This is just the wave packet in Eq. (5.1.14), displaced by an amount $-a$.

when the Gaussian in $x$ space has infinite width), we expect the answer to depend only on the initial energy, it being the only characteristic of the state. In the following analysis we will assume that $\Delta X = \Delta/2^{1/2}$ is large and that the wave function in $k$ space is very sharply peaked near $k_0$.

We follow the standard procedure for finding the fate of the incident wave packet, $\psi_I$:

Step 1: Solve for the *normalized* eigenfunction of the step potential Hamiltonian, $\psi_E(x)$.
Step 2: Find the projection $a(E) = \langle \psi_E | \psi_I \rangle$.
Step 3: Append to each coefficient $a(E)$ a time dependence $e^{-iEt/\hbar}$ and get $\psi(x, t)$ at any future time.
Step 4: Identify $\psi_R$ and $\psi_T$ in $\psi(x, t \to \infty)$ and determine $R$ and $T$ using Eqs. (5.4.3) and (5.4.4).

*Step 1.* In region I, as $V=0$, the (*unnormalized*) solution is the familiar one:

$$\psi_E(x) = A\, e^{ik_1 x} + B\, e^{-ik_1 x}, \qquad k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2} \tag{5.4.5}$$

In region II, we simply replace $E$ by $E - V_0$ [see Eq. (5.2.2)],

$$\psi_E(x) = C\, e^{ik_2 x} + D\, e^{-ik_2 x}, \qquad k_2 = \left[\frac{2m(E-V_0)}{\hbar^2}\right]^{1/2} \tag{5.4.6}$$

(We consider only $E > V_0$; the eigenfunction with $E < V_0$ will be orthogonal to $\psi_I$ as will be shown on the next two pages.) Of interest to us are eigenfunctions with $D = 0$, since we want only a transmitted (right-going) wave in region II, and incident plus reflected waves in region I. If we now impose the continuity of $\psi$ and its derivative at $x=0$; we get

$$A + B = C \tag{5.4.7}$$

$$ik_1(A - B) = ik_2 C \tag{5.4.8}$$

In anticipation of future use, we solve these equations to express $B$ and $C$ in terms of $A$:

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A = \left(\frac{E^{1/2} - (E - V_0)^{1/2}}{E^{1/2} + (E - V_0)^{1/2}}\right) A \tag{5.4.9}$$

$$C = \left(\frac{2k_1}{k_1 + k_2}\right) A = \left(\frac{2E^{1/2}}{E^{1/2} + (E - V_0)^{1/2}}\right) A \tag{5.4.10}$$

Note that if $V_0=0$, $B=0$ and $C=A$ as expected. The solution with energy $E$ is then

$$\psi_E(x)=A\left[\left(e^{ik_1x}+\frac{B}{A}e^{-ik_1x}\right)\theta(-x)+\frac{C}{A}e^{ik_2x}\,\theta(x)\right] \tag{5.4.11}$$

where

$$\begin{aligned}\theta(x)&=1 \qquad \text{if } x>0\\ &=0 \qquad \text{if } x<0\end{aligned}$$

Since to each $E$ there is a unique $k_1=+(2mE/\hbar^2)^{1/2}$, we can label the eigenstates by $k_1$ instead of $E$. Eliminating $k_2$ in favor of $k_1$, we get

$$\begin{aligned}\psi_{k_1}(x)=A\Bigg[&\left(\exp(ik_1x)+\frac{B}{A}\exp(-ik_1x)\right)\theta(-x)\\ &+\frac{C}{A}\exp[i(k_1^2-2mV_0/\hbar^2)^{1/2}x]\theta(x)\Bigg]\end{aligned} \tag{5.4.12}$$

Although the overall scale factor $A$ is generally arbitrary (and the physics depends only on $B/A$ and $C/A$), here we must choose $A=(2\pi)^{-1/2}$ because $\psi_k$ has to be properly normalized in the four-step procedure outlined above. We shall verify shortly that $A=(2\pi)^{-1/2}$ is the correct normalization factor.

*Step 2.* Consider next

$$\begin{aligned}a(k_1)&=\langle\psi_{k_1}|\psi_I\rangle\\ &=\frac{1}{(2\pi)^{1/2}}\left\{\int_{-\infty}^{\infty}\left[e^{-ik_1x}+\left(\frac{B}{A}\right)^* e^{ik_1x}\right]\theta(-x)\psi_I(x)\,dx\right.\\ &\quad\left.+\int_{-\infty}^{\infty}\left(\frac{C}{A}\right)^* e^{-ik_2x}\theta(x)\psi_I(x)\,dx\right\}\end{aligned} \tag{5.4.13}$$

The second integral vanishes (to an excellent approximation) since $\psi_I(x)$ is nonvanishing far to the left of $x=0$, while $\theta(x)$ is nonvanishing only for $x>0$. Similarly the second piece of the first integral also vanishes since $\psi_I$ in $k$ space is peaked around $k=+k_0$ and is orthogonal to (left-going) negative momentum states. [We can ignore the $\theta(-x)$ factor in Eq. (5.4.13) since it equals 1 where $\psi_I(x)\neq 0$.] So

$$\begin{aligned}a(k_1)&=\left(\frac{1}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}e^{-ik_1x}\psi_I(x)\,dx\\ &=\left(\frac{\Delta^2}{\pi}\right)^{1/4}e^{-(k_1-k_0)^2\Delta^2/2}\,e^{ik_1a}\end{aligned} \tag{5.4.14}$$

*is just the Fourier transform of* $\psi_I$. Notice that for large $\Delta$, $a(k_1)$ is very *sharply peaked at* $k_1 = k_0$. This justifies our neglect of eigenfunctions with $E < V_0$, for these correspond to $k_1$ not near $k_0$.

*Step 3.* The wave function at any future time $t$ is

$$\psi(x, t) = \int_{-\infty}^{\infty} a(k_1)\, e^{-iE(k_1)t/\hbar}\, \psi_{k_1}(x)\, dk_1 \tag{5.4.15}$$

$$= \left(\frac{\Delta^2}{4\pi^3}\right)^{1/4} \int_{-\infty}^{\infty} \exp\left(\frac{-i\hbar k_1^2 t}{2m}\right) \cdot \exp\left[\frac{-(k_1 - k_0)^2 \Delta^2}{2}\right] \exp(ik_1 a)$$
$$\times \left\{ e^{ik_1 x}\theta(-x) + \left(\frac{B}{A}\right) e^{-ik_1 x}\theta(-x) \right.$$
$$\left. + \left(\frac{C}{A}\right) \exp[i(k_1^2 - 2mV_0/\hbar^2)^{1/2} x]\theta(x) \right\} dk_1 \tag{5.4.16}$$

You can convince yourself that if we set $t = 0$ above we regain $\psi_I(x)$, which corroborates our choice $A = (2\pi)^{-1/2}$.

*Step 4.* Consider the first of the three terms. If $\theta(-x)$ were absent, we would be propagating the original Gaussian. After replacing $x$ by $x + a$ in Eq. (5.1.15), and inserting the $\theta(-x)$ factor, the first term of $\psi(x, t)$ is

$$\theta(-x)\pi^{-1/4}\left(\Delta + \frac{i\hbar t}{m}\right)^{-1/2} \exp\left[\frac{-(x + a - \hbar k_0 t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\right]$$
$$\times \exp\left[ik_0\left(x + a - \frac{\hbar k_0 t}{2m}\right)\right] \equiv \theta(-x)G(-a, k_0, t) \tag{5.4.17}$$

Since the Gaussian $G(-a, k_2, t)$ is centered at $x = -a + \hbar k_0 t/m \simeq \hbar k_0 t/m$ as $t \to \infty$, and $\theta(-x)$ vanishes for $x > 0$, the product $\theta G$ vanishes. Thus the initial packet has disappeared and in its place are the reflected and transmitted packets given by the next two terms. In the middle term if we replace $B/A$, which is a function of $k_1$, by its value $(B/A)_0$ at $k_1 = k_0$ (because $a(k_1)$ is very sharply peaked at $k_1 = k_0$) and pull it out of the integral, changing the dummy variable from $k_1$ to $-k_1$, it is easy to see that apart from the factor $(B/A)_0\theta(-x)$ up front, the middle term represents the free propagation of a normalized Gaussian packet that was originally peaked at $x = +a$ and began drifting to the *left* with mean momentum $-\hbar k_0$. Thus

$$\psi_R = \theta(-x)G(a, -k_0, t)(B/A)_0 \tag{5.4.18}$$

As $t\to\infty$, we can set $\theta(-x)$ equal to 1, since $G$ is centered at $x=a-\hbar k_0 t/m\simeq -\hbar k_0 t/m$. Since the Gaussian $G$ has unit norm, we get from Eqs. (5.4.3) and (5.4.9),

$$R=\int |\psi_R|^2\,dx=\left|\frac{B}{A}\right|_0^2=\left|\frac{E_0^{1/2}-(E_0-V_0)^{1/2}}{E_0^{1/2}+(E_0-V_0)^{1/2}}\right|^2$$

where

$$E_0=\frac{\hbar^2 k_0^2}{2m} \tag{5.4.19}$$

This formula is exact only when the incident packet has a well-defined energy $E_0$, that is to say, when the width of the incident Gaussian tends to infinity. But it is an excellent approximation for *any* wave packet that is narrowly peaked in momentum space.

To find $T$, we can try to evaluate the third piece. But there is no need to do so, since we know that

$$R+T=1 \tag{5.4.20}$$

which follows from the global conservation of probability. It then follows that

$$T=1-R=\frac{4E_0^{1/2}(E_0-V_0)^{1/2}}{[E_0^{1/2}+(E_0-V_0)^{1/2}]^2}=\left|\frac{C}{A}\right|_0^2\frac{(E_0-V_0)^{1/2}}{E_0^{1/2}} \tag{5.4.21}$$

By inspecting Eqs. (5.4.19) and (5.4.21) we see that both $R$ and $T$ are readily expressed in terms of the ratios $(B/A)_0$ and $(C/A)_0$ and a kinematical factor, $(E_0-V_0)^{1/2}/E_0^{1/2}$. Is there some way by which we can directly get to Eqs. (5.4.19) and (5.4.21), which describe the dynamic phenomenon of scattering, from Eqs. (5.4.9) and (5.4.10), which describe the static solution to Schrödinger's equation? Yes.

Consider the unnormalized eigenstate

$$\psi_{k_0}(x)=[A_0\exp(ik_0x)+B_0\exp(-ik_0x)]\theta(-x)$$
$$+C_0\exp\left[i\left(k_0^2-\frac{2mV_0}{\hbar^2}\right)^{1/2}x\right]\theta(x) \tag{5.4.22}$$

The incoming plane wave $A\,e^{ik_0x}$ has a probability current associated with it equal to

$$j_I=|A_0|^2\frac{\hbar k_0}{m} \tag{5.4.23}$$

while the currents associated with the reflected and transmitted pieces are

$$j_R = |B_0|^2 \frac{\hbar k_0}{m} \tag{5.4.24}$$

and

$$j_T = |C_0|^2 \frac{\hbar(k_0^2 - 2mV_0/\hbar^2)^{1/2}}{m} \tag{5.4.25}$$

(Recall Exercise 5.3.4, which provides the justification for viewing the two parts of the $j$ in region I as being due to the incident and reflected wave functions.) In terms of these currents

$$R = \frac{j_R}{j_I} = \left|\frac{B_0}{A_0}\right|^2 \tag{5.4.26}$$

and

$$T = \frac{j_T}{j_I} = \left|\frac{C_0}{A_0}\right|^2 \frac{(k_0^2 - 2mV_0/\hbar^2)^{1/2}}{k_0} = \left|\frac{C_0}{A_0}\right|^2 \frac{(E_0 - V_0)^{1/2}}{E_0^{1/2}} \tag{5.4.27}$$

Let us now enquire as to why it is that $R$ and $T$ are calculable in these two ways. Recall that $R$ and $T$ were exact only for the incident packet whose momentum was well defined and equal to $\hbar k_0$. From Eq. (5.4.2) we see that this involves taking the width of the Gaussian to infinity. As the incident Gaussian gets wider and wider (we ignore now the $\Delta^{-1/2}$ factor up front and the normalization) the following things happen:

(1) It becomes impossible to say when it hits the step, for it has spread out to be a right-going plane wave in region I.
(2) The reflected packet also gets infinitely wide and coexists with the incident one, as a left-going plane wave.
(3) The transmitted packet becomes a plane wave with wave number $(k_0^2 - 2mV_0/\hbar^2)^{1/2}$ in region II.

In other words, the dynamic picture of an incident packet hitting the step and disintegrating into two becomes the steady-state process described by the eigenfunction Eq. (5.4.22). We cannot, however, find $R$ and $T$ by calculating areas under $|\psi_T|^2$ and $|\psi_R|^2$ since all the areas are infinite, the wave packets having been transformed into plane waves. We find instead that the ratios of the probability currents associated with the incident, reflected, and transmitted waves give us $R$ and $T$. The equivalence between the wave packet and static descriptions that we were able to demonstrate in this simple case happens to be valid for any potential. When we come to scattering in three dimensions, we will assume that the equivalence of the two approaches holds.

*Exercise 5.4.1* (*Quite Hard*). Evaluate the third piece in Eq. (5.4 16) and compare the resulting $T$ with Eq. (5.4.21). [Hint: Expand the factor $(k_1^2-2mV_0/\hbar^2)^{1/2}$ near $k_1=k_0$, keeping just the first derivative in the Taylor series.]

Before we go on to examine some of the novel features of the reflection and transmission coefficients, let us ask how they are used in practice. Consider a general problem with some $V(x)$, which tends to constants $V_+$ and $V_-$ as $x\to\pm\infty$. For simplicity we take $V_\pm=0$. Imagine an accelerator located to the far left ($x\to-\infty$) which shoots out a beam of nearly monoenergetic particles with $\langle P\rangle=\hbar k_0$ toward the potential. The question one asks in practice is what fraction of the particles will get transmitted and what fraction will get reflected to $x=-\infty$, respectively. In general, the question cannot be answered because we know only the mean momenta of the particles and not their individual wave functions. But the preceding analysis shows that *as long as the wave packets are localized sharply in momentum space, the reflection and transmission probabilities* (*R and T*) *depend only on the mean momentum and not the detailed shape of the wave functions.* So the answer to the question raised above is that a fraction $R(k_0)$ will get reflected and a fraction $T(k_0)=1-R(k_0)$ will get transmitted. To find $R$ and $T$ we solve for the time-independent eigenfunctions of $H=T+V$ with energy eigenvalue $E_0=\hbar^2k_0^2/2m$, and asymptotic behavior

$$\psi_{k_0}(x)\begin{cases}\xrightarrow[x\to-\infty]{} A\,e^{ik_0x}+B\,e^{-ik_0x}\\ \xrightarrow[x\to\infty]{} C\,e^{ik_0x}\end{cases}$$

and obtain from it $R=|B/A|^2$ and $T=|C/A|^2$. Solutions with this asymptotic behavior (namely, free-pa ːcle behavior) will always exist provided $V$ vanishes rapidly enough as $|x|\to\infty$. [Later we will see that this means $|xV(x)|\to 0$ as $|x|\to\infty$.] The general solution will also contain a piece $D\exp(-ik_0x)$ as $x\to\infty$, but we set $D=0$ here, for if $a\exp(ik_0x)$ is to be identified with the incident wave, it must only produce a right-moving transmitted wave $C\,e^{ik_0x}$ as $x\to\infty$.

Let us turn to Eqs. (5.4.19) and (5.4.21) for $R$ and $T$. These contain many nonclassical features. First of all we find that an incident particle with $E_0>V_0$ gets reflected some of the time. It can also be shown that a particle with $E_0>V_0$ *incident from the right* will also get reflected some of the time, contrary to classical expectations.

Consider next the case $E_0<V_0$. Classically one expects the particle to be reflected at $x=0$, and never to get to region II. This is not so quantum mechanically. In region II, the solution to

$$\frac{d^2\psi_{\rm II}}{dx^2}+\frac{2m}{\hbar^2}(E_0-V_0)\psi_{\rm II}=0$$

with $E_0<V_0$ is

$$\psi_{\rm II}(x)=C\,e^{-\kappa x},\qquad \kappa=\left(\frac{2m|(E_0-V_0)|}{\hbar^2}\right)^{1/2}\tag{5.4.28}$$

(The growing exponential $e^{\kappa x}$ does not belong to the physical Hilbert space.) Thus there is a finite probability for finding the particle in the region where its kinetic energy $E_0 - V_0$ is negative. There is, however, no steady flow of probability current into region II, since $\psi_{\text{II}}(x) = C\tilde{\psi}$, where $\tilde{\psi}$ is real. This is also corroborated by the fact the reflection coefficient in this case is

$$R = \left| \frac{(E_0)^{1/2} - (E_0 - V_0)^{1/2}}{(E_0)^{1/2} + (E_0 - V_0)^{1/2}} \right|^2 = \left| \frac{k_0 - i\kappa}{k_0 + i\kappa} \right|^2 = 1 \tag{5.4.29}$$

The fact that the particle can penetrate into the classically forbidden region leads to an interesting quantum phenomenon called *tunneling*. Consider a modification of Fig. 5.2, in which $V = V_0$ only between $x = 0$ and $L$ (region II) and is once again zero beyond $x = L$ (region III). If now a plane wave is incident on this barrier from the left with $E < V_0$, there is an exponentially small probability for the particle to get to region III. Once a particle gets to region III, it is free once more and described by a plane wave. An example of tunneling is that of $\alpha$ particles trapped in the nuclei by a barrier. Every once in a while an $\alpha$ particle manages to penetrate the barrier and come out. The rate for this process can be calculated given $V_0$ and $L$.

*Exercise 5.4.2.* (a)* Calculate $R$ and $T$ for scattering of a potential $V(x) = V_0 a\delta(x)$. (b) Do the same for the case $V=0$ for $|x| > a$ and $V = V_0$ for $|x| < a$. Assume that the energy is positive but less than $V_0$.

*Exercise 5.4.3.* Consider a particle subject to a constant force $f$ in one dimension. Solve for the propagator in momentum space and get

$$U(p, t; p', 0) = \delta(p - p' - ft)\, e^{i(p'^3 - p^3)/6m\hbar f} \tag{5.4.30}$$

Transform back to coordinate space and obtain

$$U(x, t; x', 0) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \exp\left\{\frac{i}{\hbar}\left[\frac{m(x-x')^2}{2t} + \frac{1}{2} ft(x+x') - \frac{f^2 t^3}{24m}\right]\right\} \tag{5.4.31}$$

[Hint: Normalize $\psi_E(p)$ such that $\langle E|E'\rangle = \delta(E - E')$. Note that $E$ is not restricted to be positive.]

## 5.5. The Double-Slit Experiment

Having learned so much quantum mechanics, it now behooves us to go back and understand the double-slit experiment (Fig. 3.1). Let us label by I and II the regions to the left and right of the screen. The incident particle, which must really be represented by a wave packet, we approximate by a plane wave of wave number $k = p/\hbar$. The impermeable screen we treat as a region with $V = \infty$, and hence the region of vanishing $\psi$. Standard wave theory (which we can borrow from classical electromagnetism) tells us what happens in region II: the two slits act as sources of radially outgoing waves of the same wavelength. These two waves interfere on the line $AB$ and produce the interference pattern. We now return to quantum mechanics and interpret the intensity $|\psi|^2$ as the probability density for finding the particle.

## 5.6. Some Theorems

*Theorem 15.* There is no degeneracy in one-dimensional bound states.

*Proof.* Let $\psi_1$ and $\psi_2$ be two solutions with the same eigenvalue $E$:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_1}{dx^2}+V\psi_1=E\psi_1 \tag{5.6.1}$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_2}{dx^2}+V\psi_2=E\psi_2 \tag{5.6.2}$$

Multiply the first by $\psi_2$, the second by $\psi_1$ and subtract, to get

$$\psi_1\frac{d^2\psi_2}{dx^2}-\psi_2\frac{d^2\psi_1}{dx^2}=0$$

or

$$\frac{d}{dx}\left(\psi_1\frac{d\psi_2}{dx}-\psi_2\frac{d\psi_1}{dx}\right)=0$$

so that

$$\psi_1\frac{d\psi_2}{dx}-\psi_2\frac{d\psi_1}{dx}=c \tag{5.6.3}$$

To find the constant $c$, go to $|x|\to\infty$, where $\psi_1$ and $\psi_2$ vanish, since they describe bound states by assumption.‡ It follows that $c=0$. So

$$\frac{1}{\psi_1}d\psi_1=\frac{1}{\psi_2}d\psi_2$$

$$\log\psi_1=\log\psi_2+d \qquad (d \text{ is a constant})$$

$$\psi_1=e^d\psi_2 \tag{5.6.4}$$

‡ The theorem holds even if $\psi$ vanishes at either $+\infty$ or $-\infty$. In a bound state it vanishes at both ends. But one can think of situations where the potential confines the wave function at one end but not the other.

Thus the two eigenfunctions differ only by a scale factor and represent the same state. Q.E.D.

What about the free-particle case, where to every energy there are two degenerate solutions with $p = \pm(2mE/\hbar^2)^{1/2}$? The theorem doesn't apply here since $\psi_p(x)$ does not vanish at spatial infinity. [Calculate $c$ in Eq. (5.6.3).]

*Theorem 16.* The eigenfunctions of $H$ can always be chosen pure real in the coordinate basis.

*Proof.* If

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_n = E_n\psi_n$$

then by conjugation

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_n^* = E_n\psi_n^*$$

Thus $\psi_n$ and $\psi_n^*$ are eigenfunctions with the same eigenvalue. It follows that the real and imaginary parts of $\psi_n$,

$$\psi_r = \frac{\psi_n + \psi_n^*}{2}$$

and

$$\psi_i = \frac{\psi_n - \psi_n^*}{2i}$$

are also eigenfunctions with energy $E$. Q.E.D.

The theorem holds in higher dimensions as well for *Hamiltonians of the above form*, which in addition to being Hermitian, are *real*. Note, however, that while Hermiticity is preserved under a unitary change of basis, reality is not.

If the problem involves a magnetic field, the Hamiltonian is no longer real in the coordinate basis, as is clear from Eq. (4.3.7). In this case the eigenfunctions cannot be generally chosen real. This question will be explored further at the end of Chapter 11.

Returning to one dimension, due to nondegeneracy of bound states, we must have

$$\psi_i = c\psi_r, \qquad c\text{, a constant}$$

Consequently,

$$\psi = \psi_r + i\psi_i = (1 + ic)\psi_r = \tilde{c}\psi_r$$

Since the overall scale $\tilde{c}$ is irrelevant, we can ignore it, i.e., work with real eigenfunctions with no loss of generality.

This brings us to the end of our study of one-dimensional problems, except for the harmonic oscillator, which is the subject of Chapter 7.