

2.5 THE DELTA-FUNCTION POTENTIAL

2.5.1 Bound States and Scattering States

We have encountered two very different kinds of solutions to the time-independent Schrödinger equation: For the infinite square well and the harmonic oscillator they are *normalizable*, and labeled by a *discrete index* n ; for the free particle they are *non-normalizable*, and labeled by a *continuous variable* k . The former represent physically realizable states in their own right, the latter do not; but in both cases the general solution to the time-dependent Schrödinger equation is a linear combination of stationary states—for the first type this combination takes the form of a *sum* (over n), whereas for the second it is an *integral* (over k). What is the physical significance of this distinction?

In *classical* mechanics a one-dimensional time-independent potential can give rise to two rather different kinds of motion. If $V(x)$ rises higher than the particle's total energy (E) on either side (Figure 2.12(a)), then the particle is “stuck” in the potential well—it rocks back and forth between the **turning points**, but it cannot escape (unless, of course, you provide it with a source of extra energy, such as a motor, but we're not talking about that). We call this a **bound state**. If, on the other hand, E exceeds $V(x)$ on one side (or both), then the particle comes in from “infinity,” slows down or speeds up under the influence of the potential, and returns to infinity (Figure 2.12(b)). (It can't get trapped in the potential unless there is some mechanism, such as friction, to *dissipate* energy, but again, we're not talking about that.) We call this a **scattering state**. Some potentials admit only bound states (for instance, the harmonic oscillator); some allow only scattering states (a potential hill with no dips in it, for example); some permit both kinds, depending on the energy of the particle.

The two kinds of solutions to the Schrödinger equation correspond precisely to bound and scattering states. The distinction is even cleaner in the quantum domain, because the phenomenon of **tunneling** (which we'll come to shortly) allows the particle to “leak” through any finite potential barrier, so the only thing that matters is the potential at infinity (Figure 2.12(c)):

$$\begin{cases} E < [V(-\infty) \text{ and } V(+\infty)] \Rightarrow \text{bound state,} \\ E > [V(-\infty) \text{ or } V(+\infty)] \Rightarrow \text{scattering state.} \end{cases} \quad [2.109]$$

In “real life” most potentials go to *zero* at infinity, in which case the criterion simplifies even further:

$$\begin{cases} E < 0 \Rightarrow \text{bound state,} \\ E > 0 \Rightarrow \text{scattering state.} \end{cases} \quad [2.110]$$

Because the infinite square well and harmonic oscillator potentials go to infinity as $x \rightarrow \pm\infty$, they admit bound states only; because the free particle potential is zero

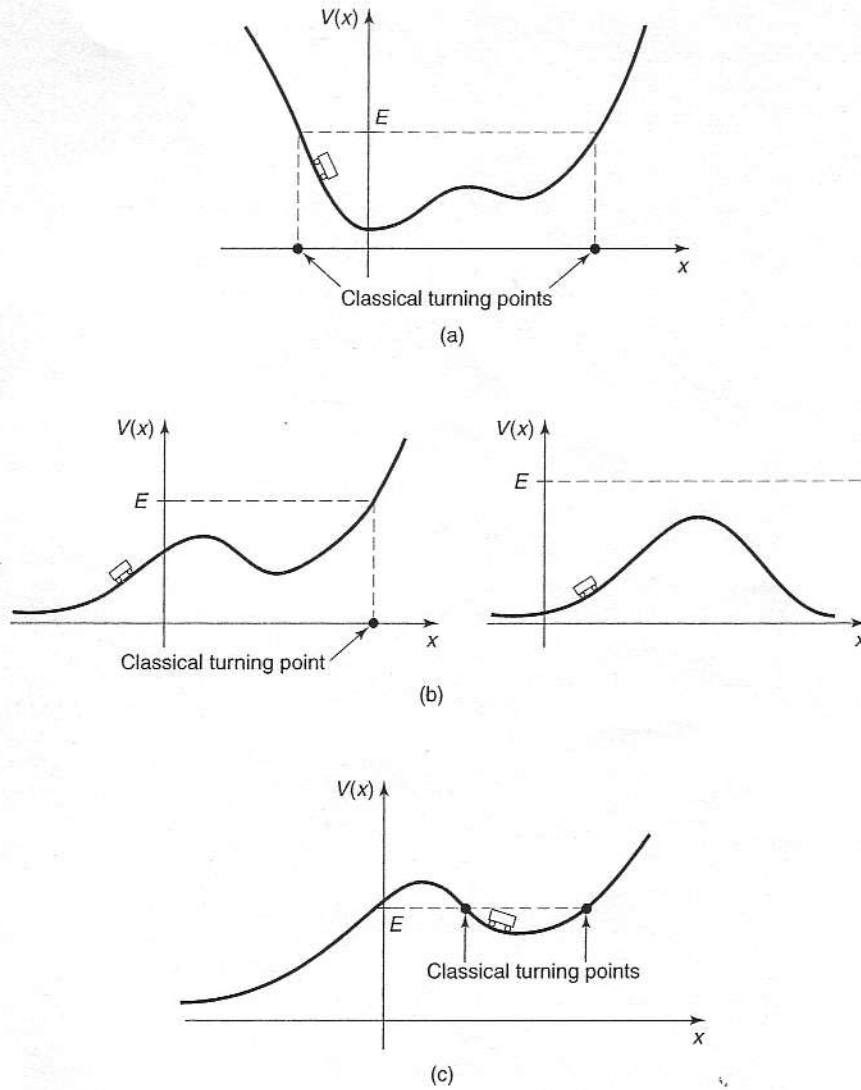


FIGURE 2.12: (a) A bound state. (b) Scattering states. (c) A *classical* bound state, but a quantum scattering state.

everywhere, it only allows scattering states.³⁴ In this section (and the following one) we shall explore potentials that give rise to both kinds of states.

³⁴If you are irritatingly observant, you may have noticed that the general theorem requiring $E > V_{\min}$ (Problem 2.2) does not really apply to scattering states, since they are not normalizable anyway. If this bothers you, try solving the Schrödinger equation with $E \leq 0$, for the free particle, and

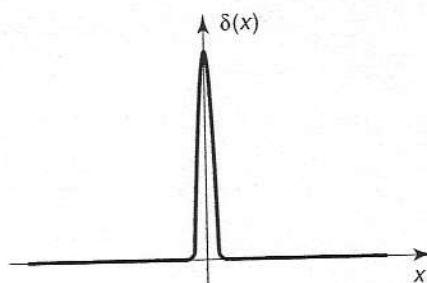


FIGURE 2.13: The Dirac delta function (Equation 2.111).

2.5.2 The Delta-Function Well

The **Dirac delta function** is an infinitely high, infinitesimally narrow spike at the origin, whose *area* is 1 (Figure 2.13):

$$\delta(x) \equiv \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}, \quad \text{with } \int_{-\infty}^{+\infty} \delta(x) dx = 1. \quad [2.111]$$

Technically, it isn't a function at all, since it is not finite at $x = 0$ (mathematicians call it a **generalized function**, or **distribution**).³⁵ Nevertheless, it is an extremely useful construct in theoretical physics. (For example, in electrodynamics the charge *density* of a point charge is a delta function.) Notice that $\delta(x - a)$ would be a spike of area 1 at the point a . If you multiply $\delta(x - a)$ by an *ordinary* function $f(x)$, it's the same as multiplying by $f(a)$,

$$f(x)\delta(x - a) = f(a)\delta(x - a), \quad [2.112]$$

because the product is *zero* anyway except at the point a . In particular,

$$\int_{-\infty}^{+\infty} f(x)\delta(x - a) dx = f(a) \int_{-\infty}^{+\infty} \delta(x - a) dx = f(a). \quad [2.113]$$

That's the most important property of the delta function: Under the integral sign it serves to "pick out" the value of $f(x)$ at the point a . (Of course, the integral need not go from $-\infty$ to $+\infty$; all that matters is that the domain of integration include the point a , so $a - \epsilon$ to $a + \epsilon$ would do, for any $\epsilon > 0$.)

Let's consider a potential of the form

$$V(x) = -\alpha\delta(x), \quad [2.114]$$

note that *even linear combinations* of these solutions cannot be normalized. The positive energy solutions by themselves constitute a complete set.

³⁵The delta function can be thought of as the *limit* of a *sequence* of functions, such as rectangles (or triangles) of ever-increasing height and ever-decreasing width.

where α is some positive constant.³⁶ This is an artificial potential, to be sure (so was the infinite square well), but it's delightfully simple to work with, and illuminates the basic theory with a minimum of analytical clutter. The Schrödinger equation for the delta-function well reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi; \quad [2.115]$$

it yields both bound states ($E < 0$) and scattering states ($E > 0$).

We'll look first at the bound states. In the region $x < 0$, $V(x) = 0$, so

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi, \quad [2.116]$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}. \quad [2.117]$$

(E is negative, by assumption, so κ is real and positive.) The general solution to Equation 2.116 is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}, \quad [2.118]$$

but the first term blows up as $x \rightarrow -\infty$, so we must choose $A = 0$:

$$\psi(x) = Be^{\kappa x}, \quad (x < 0). \quad [2.119]$$

In the region $x > 0$, $V(x)$ is again zero, and the general solution is of the form $F \exp(-\kappa x) + G \exp(\kappa x)$; this time it's the second term that blows up (as $x \rightarrow +\infty$), so

$$\psi(x) = Fe^{-\kappa x}, \quad (x > 0). \quad [2.120]$$

It remains only to stitch these two functions together, using the appropriate boundary conditions at $x = 0$. I quoted earlier the standard boundary conditions for ψ :

$$\left\{ \begin{array}{l} 1. \psi \quad \text{is always continuous;} \\ 2. d\psi/dx \quad \text{is continuous except at points where the potential is infinite.} \end{array} \right. \quad [2.121]$$

In this case the first boundary condition tells us that $F = B$, so

$$\psi(x) = \begin{cases} Be^{\kappa x}, & (x \leq 0), \\ Be^{-\kappa x}, & (x \geq 0); \end{cases} \quad [2.122]$$

³⁶The delta function itself carries units of $1/\text{length}$ (see Equation 2.111), so α has the dimensions $\text{energy} \times \text{length}$.

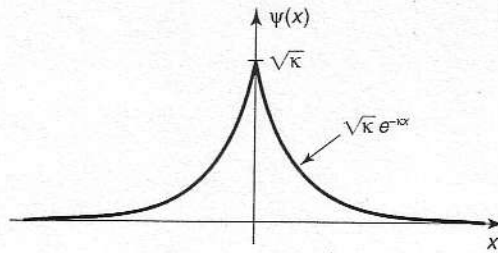


FIGURE 2.14: Bound state wave function for the delta-function potential (Equation 2.122).

$\psi(x)$ is plotted in Figure 2.14. The second boundary condition tells us nothing; this is (like the infinite square well) the exceptional case where V is infinite at the join, and it's clear from the graph that this function has a kink at $x = 0$. Moreover, up to this point the delta function has not come into the story at all. Evidently the delta function must determine the discontinuity in the derivative of ψ , at $x = 0$. I'll show you now how this works, and as a by-product we'll see why $d\psi/dx$ is ordinarily continuous.

The idea is to *integrate* the Schrödinger equation, from $-\epsilon$ to $+\epsilon$, and then take the limit as $\epsilon \rightarrow 0$:

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{+\epsilon} \frac{d^2\psi}{dx^2} dx + \int_{-\epsilon}^{+\epsilon} V(x)\psi(x) dx = E \int_{-\epsilon}^{+\epsilon} \psi(x) dx. \quad [2.123]$$

The first integral is nothing but $d\psi/dx$, evaluated at the two end points; the last integral is *zero*, in the limit $\epsilon \rightarrow 0$, since it's the area of a sliver with vanishing width and finite height. Thus

$$\Delta \left(\frac{d\psi}{dx} \right) \equiv \frac{\partial\psi}{\partial x} \Big|_{+\epsilon} - \frac{\partial\psi}{\partial x} \Big|_{-\epsilon} = \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{+\epsilon} V(x)\psi(x) dx. \quad [2.124]$$

Typically, the limit on the right is again zero, and that's why $d\psi/dx$ is ordinarily continuous. But when $V(x)$ is *infinite* at the boundary, this argument fails. In particular, if $V(x) = -\alpha\delta(x)$, Equation 2.113 yields

$$\Delta \left(\frac{d\psi}{dx} \right) = -\frac{2m\alpha}{\hbar^2} \psi(0). \quad [2.125]$$

For the case at hand (Equation 2.122),

$$\begin{cases} d\psi/dx = -B\kappa e^{-\kappa x}, & \text{for } (x > 0), & \text{so } d\psi/dx|_+ = -B\kappa, \\ d\psi/dx = +B\kappa e^{+\kappa x}, & \text{for } (x < 0), & \text{so } d\psi/dx|_- = +B\kappa, \end{cases}$$

and hence $\Delta(d\psi/dx) = -2B\kappa$. And $\psi(0) = B$. So Equation 2.125 says

$$\kappa = \frac{m\alpha}{\hbar^2}, \quad [2.126]$$

and the allowed energy (Equation 2.117) is

$$E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}. \quad [2.127]$$

Finally, we normalize ψ :

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2|B|^2 \int_0^{\infty} e^{-2\kappa x} dx = \frac{|B|^2}{\kappa} = 1,$$

so (choosing, for convenience, the positive real root):

$$B = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar}. \quad [2.128]$$

Evidently the delta-function well, regardless of its "strength" α , has *exactly one* bound state:

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2}; \quad E = -\frac{m\alpha^2}{2\hbar^2}. \quad [2.129]$$

What about *scattering* states, with $E > 0$? For $x < 0$ the Schrödinger equation reads

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi,$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad [2.130]$$

is real and positive. The general solution is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad [2.131]$$

and this time we cannot rule out either term, since neither of them blows up. Similarly, for $x > 0$,

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}. \quad [2.132]$$

The continuity of $\psi(x)$ at $x = 0$ requires that

$$F + G = A + B. \quad [2.133]$$

The derivatives are

$$\begin{cases} d\psi/dx = ik(Fe^{ikx} - Ge^{-ikx}), & \text{for } (x > 0), & \text{so } d\psi/dx|_+ = ik(F - G), \\ d\psi/dx = ik(Ae^{ikx} - Be^{-ikx}), & \text{for } (x < 0), & \text{so } d\psi/dx|_- = ik(A - B), \end{cases}$$

and hence $\Delta(d\psi/dx) = ik(F - G - A + B)$. Meanwhile, $\psi(0) = (A + B)$, so the second boundary condition (Equation 2.125) says

$$ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B), \quad [2.134]$$

or, more compactly,

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \text{where } \beta \equiv \frac{m\alpha}{\hbar^2 k}. \quad [2.135]$$

Having imposed both boundary conditions, we are left with two equations (Equations 2.133 and 2.135) in four unknowns (A , B , F , and G)—*five*, if you count k . Normalization won't help—this isn't a normalizable state. Perhaps we'd better pause, then, and examine the physical significance of these various constants. Recall that $\exp(ikx)$ gives rise (when coupled with the time-dependent factor $\exp(-iEt/\hbar)$) to a wave function propagating to the *right*, and $\exp(-ikx)$ leads to a wave propagating to the *left*. It follows that A (in Equation 2.131) is the amplitude of a wave coming in from the left, B is the amplitude of a wave returning to the left, F (Equation 2.132) is the amplitude of a wave traveling off to the right, and G is the amplitude of a wave coming in from the right (see Figure 2.15). In a typical scattering experiment particles are fired in from one direction—let's say, from the left. In that case the amplitude of the wave coming in from the *right* will be *zero*:

$$G = 0, \quad (\text{for scattering from the left}); \quad [2.136]$$

A is the amplitude of the **incident wave**, B is the amplitude of the **reflected wave**, and F is the amplitude of the **transmitted wave**. Solving Equations 2.133 and 2.135 for B and F , we find

$$B = \frac{i\beta}{1 - i\beta} A, \quad F = \frac{1}{1 - i\beta} A. \quad [2.137]$$

(If you want to study scattering from the *right*, set $A = 0$; then G is the incident amplitude, F is the reflected amplitude, and B is the transmitted amplitude.)

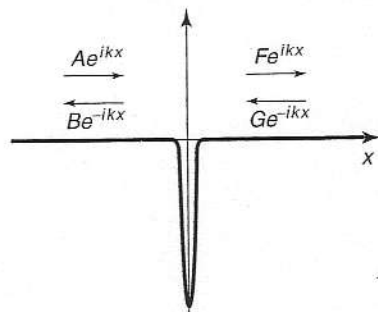


FIGURE 2.15: Scattering from a delta function well.

Now, the probability of finding the particle at a specified location is given by $|\Psi|^2$, so the *relative*³⁷ probability that an incident particle will be reflected back is

$$R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}. \quad [2.138]$$

R is called the **reflection coefficient**. (If you have a *beam* of particles, it tells you the *fraction* of the incoming number that will bounce back.) Meanwhile, the probability of transmission is given by the **transmission coefficient**

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}. \quad [2.139]$$

Of course, the *sum* of these probabilities should be 1—and it is:

$$R + T = 1. \quad [2.140]$$

Notice that R and T are functions of β , and hence (Equations 2.130 and 2.135) of E :

$$R = \frac{1}{1 + (2\hbar^2 E / m\alpha^2)}, \quad T = \frac{1}{1 + (m\alpha^2 / 2\hbar^2 E)}. \quad [2.141]$$

The higher the energy, the greater the probability of transmission (which certainly seems reasonable).

This is all very tidy, but there is a sticky matter of principle that we cannot altogether ignore: These scattering wave functions are not normalizable, so they don't actually represent possible particle states. But we know what the resolution to this problem is: We must form normalizable linear combinations of the stationary states, just as we did for the free particle—true physical particles are represented by the resulting wave packets. Though straightforward in principle, this is a messy business in practice, and at this point it is best to turn the problem over to a computer.³⁸ Meanwhile, since it is impossible to create a normalizable free-particle wave function without involving a *range* of energies, R and T should be interpreted as the *approximate* reflection and transmission probabilities for particles in the *vicinity* of E .

Incidentally, it might strike you as peculiar that we were able to analyze a quintessentially time-dependent problem (particle comes in, scatters off a potential,

³⁷This is not a normalizable wave function, so the *absolute* probability of finding the particle at a particular location is not well defined; nevertheless, the *ratio* of probabilities for the incident and reflected waves *is* meaningful. More on this in the next paragraph.

³⁸Numerical studies of wave packets scattering off wells and barriers reveal extraordinarily rich structure. The classic analysis is A. Goldberg, H. M. Schey, and J. L. Schwartz, *Am. J. Phys.* **35**, 177 (1967); more recent work can be found on the Web.

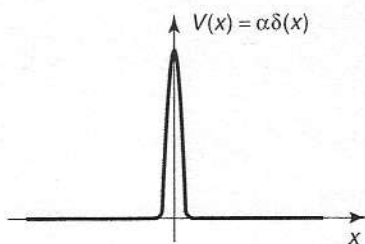


FIGURE 2.16: The delta-function barrier.

and flies off to infinity) using *stationary* states. After all, ψ (in Equations 2.131 and 2.132) is simply a complex, time-independent, sinusoidal function, extending (with constant amplitude) to infinity in both directions. And yet, by imposing appropriate boundary conditions on this function we were able to determine the probability that a particle (represented by a *localized* wave packet) would bounce off, or pass through, the potential. The mathematical miracle behind this is, I suppose, the fact that by taking linear combinations of states spread over all space, and with essentially trivial time dependence, we can *construct* wave functions that are concentrated about a (moving) point, with quite elaborate behavior in time (see Problem 2.43).

As long as we've got the relevant equations on the table, let's look briefly at the case of a delta-function *barrier* (Figure 2.16). Formally, all we have to do is change the sign of α . This kills the bound state, of course (Problem 2.2). On the other hand, the reflection and transmission coefficients, which depend only on α^2 , are unchanged. Strange to say, the particle is just as likely to pass through the barrier as to cross over the well! *Classically*, of course, a particle cannot make it over an infinitely high barrier, regardless of its energy. In fact, classical scattering problems are pretty dull: If $E > V_{\max}$, then $T = 1$ and $R = 0$ —the particle certainly makes it over; if $E < V_{\max}$ then $T = 0$ and $R = 1$ —it rides up the hill until it runs out of steam, and then returns the same way it came. *Quantum* scattering problems are much richer: The particle has some nonzero probability of passing through the potential even if $E < V_{\max}$. We call this phenomenon **tunneling**; it is the mechanism that makes possible much of modern electronics—not to mention spectacular advances in microscopy. Conversely, even if $E > V_{\max}$ there is a possibility that the particle will bounce back—though I wouldn't advise driving off a cliff in the hope that quantum mechanics will save you (see Problem 2.35).

*Problem 2.23 Evaluate the following integrals:

(a) $\int_{-3}^{+1} (x^3 - 3x^2 + 2x - 1)\delta(x + 2) dx.$

(b) $\int_0^{\infty} [\cos(3x) + 2]\delta(x - \pi) dx.$

(c) $\int_{-1}^{+1} \exp(|x| + 3)\delta(x - 2) dx.$

Problem 2.24 Delta functions live under integral signs, and two expressions ($D_1(x)$ and $D_2(x)$) involving delta functions are said to be equal if

$$\int_{-\infty}^{+\infty} f(x) D_1(x) dx = \int_{-\infty}^{+\infty} f(x) D_2(x) dx,$$

for every (ordinary) function $f(x)$.

(a) Show that

$$\delta(cx) = \frac{1}{|c|} \delta(x), \quad [2.142]$$

where c is a real constant. (Be sure to check the case where c is negative.)

(b) Let $\theta(x)$ be the **step function**:

$$\theta(x) \equiv \begin{cases} 1, & \text{if } x > 0, \\ 0, & \text{if } x < 0. \end{cases} \quad [2.143]$$

(In the rare case where it actually matters, we define $\theta(0)$ to be $1/2$.) Show that $d\theta/dx = \delta(x)$.

***Problem 2.25** Check the uncertainty principle for the wave function in Equation 2.129. *Hint:* Calculating $\langle p^2 \rangle$ is tricky, because the derivative of ψ has a step discontinuity at $x = 0$. Use the result in Problem 2.24(b). *Partial answer:* $\langle p^2 \rangle = (m\alpha/\hbar)^2$.

***Problem 2.26** What is the Fourier transform of $\delta(x)$? Using Plancherel's theorem, show that

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk. \quad [2.144]$$

Comment: This formula gives any respectable mathematician apoplexy. Although the integral is clearly infinite when $x = 0$, it doesn't converge (to zero or anything else) when $x \neq 0$, since the integrand oscillates forever. There are ways to patch it up (for instance, you can integrate from $-L$ to $+L$, and interpret Equation 2.144 to mean the *average* value of the finite integral, as $L \rightarrow \infty$). The source of the problem is that the delta function doesn't meet the requirement (square-integrability) for Plancherel's theorem (see footnote 33). In spite of this, Equation 2.144 can be extremely useful, if handled with care.

***Problem 2.27** Consider the *double* delta-function potential

$$V(x) = -\alpha[\delta(x+a) + \delta(x-a)],$$

where α and a are positive constants.

- (a) Sketch this potential.
- (b) How many bound states does it possess? Find the allowed energies, for $\alpha = \hbar^2/ma$ and for $\alpha = \hbar^2/4ma$, and sketch the wave functions.

**Problem 2.28 Find the transmission coefficient for the potential in Problem 2.27.

2.6 THE FINITE SQUARE WELL

As a last example, consider the *finite* square well potential

$$V(x) = \begin{cases} -V_0, & \text{for } -a < x < a, \\ 0, & \text{for } |x| > a, \end{cases} \quad [2.145]$$

where V_0 is a (positive) constant (Figure 2.17). Like the delta-function well, this potential admits both bound states (with $E < 0$) and scattering states (with $E > 0$). We'll look first at the bound states.

In the region $x < -a$ the potential is zero, so the Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi,$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad [2.146]$$

is real and positive. The general solution is $\psi(x) = A \exp(-\kappa x) + B \exp(\kappa x)$, but the first term blows up (as $x \rightarrow -\infty$), so the physically admissible solution (as before—see Equation 2.119) is

$$\psi(x) = B e^{\kappa x}, \quad \text{for } x < -a. \quad [2.147]$$

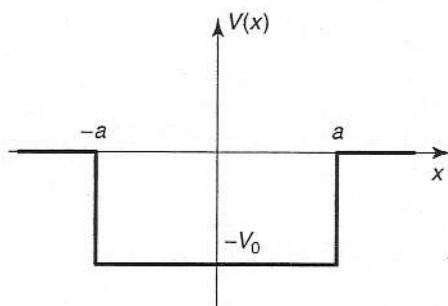


FIGURE 2.17: The finite square well (Equation 2.145).

In the region $-a < x < a$, $V(x) = -V_0$, and the Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\psi = E\psi, \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -l^2\psi,$$

where

$$l \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar}. \quad [2.148]$$

Although E is negative, for bound states, it must be greater than $-V_0$, by the old theorem $E > V_{\min}$ (Problem 2.2); so l is also real and positive. The general solution is³⁹

$$\psi(x) = C \sin(lx) + D \cos(lx), \quad \text{for } -a < x < a, \quad [2.149]$$

where C and D are arbitrary constants. Finally, in the region $x > a$ the potential is again zero; the general solution is $\psi(x) = F \exp(-\kappa x) + G \exp(\kappa x)$, but the second term blows up (as $x \rightarrow \infty$), so we are left with

$$\psi(x) = F e^{-\kappa x}, \quad \text{for } x > a. \quad [2.150]$$

The next step is to impose boundary conditions: ψ and $d\psi/dx$ continuous at $-a$ and $+a$. But we can save a little time by noting that this potential is an even function, so we can assume with no loss of generality that the solutions are either even or odd (Problem 2.1(c)). The advantage of this is that we need only impose the boundary conditions on one side (say, at $+a$); the other side is then automatic, since $\psi(-x) = \pm \psi(x)$. I'll work out the even solutions; you get to do the odd ones in Problem 2.29. The cosine is even (and the sine is odd), so I'm looking for solutions of the form

$$\psi(x) = \begin{cases} F e^{-\kappa x}, & \text{for } x > a, \\ D \cos(lx), & \text{for } 0 < x < a, \\ \psi(-x), & \text{for } x < 0. \end{cases} \quad [2.151]$$

The continuity of $\psi(x)$, at $x = a$, says

$$F e^{-\kappa a} = D \cos(la), \quad [2.152]$$

and the continuity of $d\psi/dx$, says

$$-\kappa F e^{-\kappa a} = -l D \sin(la). \quad [2.153]$$

Dividing Equation 2.153 by Equation 2.152, we find that

$$\kappa = l \tan(la). \quad [2.154]$$

³⁹You can, if you like, write the general solution in exponential form ($C'e^{ilx} + D'e^{-ilx}$). This leads to the same final result, but since the potential is symmetric we know the solutions will be either even or odd, and the sine/cosine notation allows us to exploit this directly.

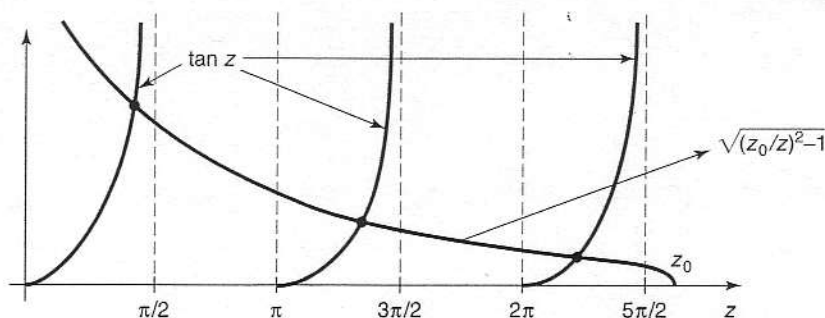


FIGURE 2.18: Graphical solution to Equation 2.156, for $z_0 = 8$ (even states).

This is a formula for the allowed energies, since κ and l are both functions of E . To solve for E , we first adopt some nicer notation: Let

$$z \equiv la, \quad \text{and} \quad z_0 \equiv \frac{a}{\hbar} \sqrt{2mV_0}. \quad [2.155]$$

According to Equations 2.146 and 2.148, $(\kappa^2 + l^2) = 2mV_0/\hbar^2$, so $\kappa a = \sqrt{z_0^2 - z^2}$, and Equation 2.154 reads

$$\tan z = \sqrt{(z_0/z)^2 - 1}. \quad [2.156]$$

This is a transcendental equation for z (and hence for E) as a function of z_0 (which is a measure of the “size” of the well). It can be solved numerically, using a computer, or graphically, by plotting $\tan z$ and $\sqrt{(z_0/z)^2 - 1}$ on the same grid, and looking for points of intersection (see Figure 2.18). Two limiting cases are of special interest:

1. Wide, deep well. If z_0 is very large, the intersections occur just slightly below $z_n = n\pi/2$, with n odd; it follows that

$$E_n + V_0 \cong \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}. \quad [2.157]$$

But $E + V_0$ is the energy *above the bottom of the well*, and on the right side we have precisely the infinite square well energies, for a well of width $2a$ (see Equation 2.27)—or rather, *half* of them, since this n is odd. (The other ones, of course, come from the *odd* wave functions, as you’ll discover in Problem 2.29.) So the finite square well goes over to the infinite square well, as $V_0 \rightarrow \infty$; however, for any *finite* V_0 there are only a finite number of bound states.

2. Shallow, narrow well. As z_0 decreases, there are fewer and fewer bound states, until finally (for $z_0 < \pi/2$, where the lowest *odd* state disappears) only one remains. It is interesting to note, however, that there is always *one* bound state, no matter *how* “weak” the well becomes.

You're welcome to normalize ψ (Equation 2.151), if you're interested (Problem 2.30), but I'm going to move on now to the scattering states ($E > 0$). To the left, where $V(x) = 0$, we have

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } (x < -a), \quad [2.158]$$

where (as usual)

$$k \equiv \frac{\sqrt{2mE}}{\hbar}. \quad [2.159]$$

Inside the well, where $V(x) = -V_0$,

$$\psi(x) = C \sin(lx) + D \cos(lx), \quad \text{for } (-a < x < a), \quad [2.160]$$

where, as before,

$$l \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar}. \quad [2.161]$$

To the right, assuming there is no incoming wave in this region, we have

$$\psi(x) = Fe^{ikx}. \quad [2.162]$$

Here A is the incident amplitude, B is the reflected amplitude, and F is the transmitted amplitude.⁴⁰

There are four boundary conditions: Continuity of $\psi(x)$ at $-a$ says

$$Ae^{-ika} + Be^{ika} = -C \sin(la) + D \cos(la), \quad [2.163]$$

continuity of $d\psi/dx$ at $-a$ gives

$$ik[Ae^{-ika} - Be^{ika}] = l[C \cos(la) + D \sin(la)] \quad [2.164]$$

continuity of $\psi(x)$ at $+a$ yields

$$C \sin(la) + D \cos(la) = Fe^{ika}, \quad [2.165]$$

and continuity of $d\psi/dx$ at $+a$ requires

$$l[C \cos(la) - D \sin(la)] = ikFe^{ika}. \quad [2.166]$$

⁴⁰We *could* look for even and odd functions, as we did in the case of bound states, but the scattering problem is inherently asymmetric, since the waves come in from one side only, and the exponential notation (representing traveling waves) is more natural in this context.

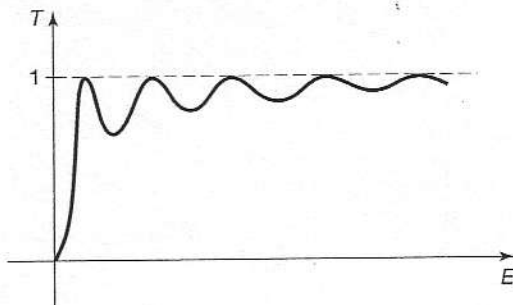


FIGURE 2.19: Transmission coefficient as a function of energy (Equation 2.169).

We can use two of these to eliminate C and D , and solve the remaining two for B and F (see Problem 2.32):

$$B = i \frac{\sin(2la)}{2kl} (l^2 - k^2) F, \quad [2.167]$$

$$F = \frac{e^{-2ika} A}{\cos(2la) - i \frac{(k^2 + l^2)}{2kl} \sin(2la)}. \quad [2.168]$$

The transmission coefficient ($T = |F|^2/|A|^2$), expressed in terms of the original variables, is given by

$$T^{-1} = 1 + \frac{V_0^2}{4E(E + V_0)} \sin^2 \left(\frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right). \quad [2.169]$$

Notice that $T = 1$ (the well becomes “transparent”) whenever the sine is zero, which is to say, when

$$\frac{2a}{\hbar} \sqrt{2m(E_n + V_0)} = n\pi, \quad [2.170]$$

where n is any integer. The energies for perfect transmission, then, are given by

$$E_n + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}, \quad [2.171]$$

which happen to be precisely the allowed energies for the *infinite* square well. T is plotted in Figure 2.19, as a function of energy.⁴¹

***Problem 2.29** Analyze the *odd* bound state wave functions for the finite square well. Derive the transcendental equation for the allowed energies, and solve it graphically. Examine the two limiting cases. Is there always an odd bound state?

⁴¹This remarkable phenomenon has been observed in the laboratory, in the form of the **Ramsauer-Townsend effect**. For an illuminating discussion see Richard W. Robinett, *Quantum Mechanics*, Oxford U.P., 1997, Section 12.4.1.

Problem 2.30 Normalize $\psi(x)$ in Equation 2.151, to determine the constants D and F .

Problem 2.31 The Dirac delta function can be thought of as the limiting case of a rectangle of area 1, as the height goes to infinity and the width goes to zero. Show that the delta-function well (Equation 2.114) is a “weak” potential (even though it is infinitely deep), in the sense that $z_0 \rightarrow 0$. Determine the bound state energy for the delta-function potential, by treating it as the limit of a finite square well. Check that your answer is consistent with Equation 2.129. Also show that Equation 2.169 reduces to Equation 2.141 in the appropriate limit.

Problem 2.32 Derive Equations 2.167 and 2.168. *Hint:* Use Equations 2.165 and 2.166 to solve for C and D in terms of F :

$$C = \left[\sin(la) + i \frac{k}{l} \cos(la) \right] e^{ika} F; \quad D = \left[\cos(la) - i \frac{k}{l} \sin(la) \right] e^{ika} F.$$

Plug these back into Equations 2.163 and 2.164. Obtain the transmission coefficient, and confirm Equation 2.169.

****Problem 2.33** Determine the transmission coefficient for a rectangular barrier (same as Equation 2.145, only with $V(x) = +V_0 > 0$ in the region $-a < x < a$). Treat separately the three cases $E < V_0$, $E = V_0$, and $E > V_0$ (note that the wave function inside the barrier is different in the three cases). *Partial answer:* For $E < V_0$,⁴²

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left(\frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right).$$

***Problem 2.34** Consider the “step” potential:

$$V(x) = \begin{cases} 0, & \text{if } x \leq 0, \\ V_0, & \text{if } x > 0. \end{cases}$$

- Calculate the reflection coefficient, for the case $E < V_0$, and comment on the answer.
- Calculate the reflection coefficient for the case $E > V_0$.
- For a potential such as this, which does not go back to zero to the right of the barrier, the transmission coefficient is *not* simply $|F|^2/|A|^2$ (with A the

⁴²This is a good example of tunneling—classically the particle would bounce back.

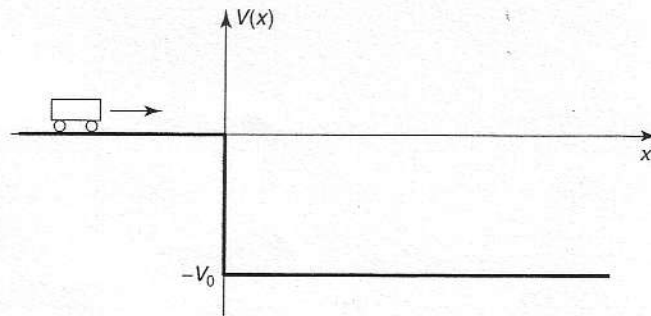


FIGURE 2.20: Scattering from a “cliff” (Problem 2.35).

incident amplitude and F the transmitted amplitude), because the transmitted wave travels at a different *speed*. Show that

$$T = \sqrt{\frac{E - V_0}{E}} \frac{|F|^2}{|A|^2}, \quad [2.172]$$

for $E > V_0$. *Hint*: You can figure it out using Equation 2.98, or—more elegantly, but less informatively—from the probability current (Problem 2.19). What is T , for $E < V_0$?

- (d) For $E > V_0$, calculate the transmission coefficient for the step potential, and check that $T + R = 1$.

Problem 2.35 A particle of mass m and kinetic energy $E > 0$ approaches an abrupt potential drop V_0 (Figure 2.20).

- (a) What is the probability that it will “reflect” back, if $E = V_0/3$? *Hint*: This is just like Problem 2.34, except that the step now goes *down*, instead of up.
- (b) I drew the figure so as to make you think of a car approaching a cliff, but obviously the probability of “bouncing back” from the edge of a cliff is *far* smaller than what you got in (a)—unless you’re Bugs Bunny. Explain why this potential does *not* correctly represent a cliff. *Hint*: In Figure 2.20 the potential energy of the car drops *discontinuously* to $-V_0$, as it passes $x = 0$; would this be true for a falling car?
- (c) When a free neutron enters a nucleus, it experiences a sudden drop in potential energy, from $V = 0$ outside to around -12 MeV (million electron volts) inside. Suppose a neutron, emitted with kinetic energy 4 MeV by a fission event, strikes such a nucleus. What is the probability it will be absorbed, thereby initiating another fission? *Hint*: You calculated the probability of *reflection* in part (a); use $T = 1 - R$ to get the probability of transmission through the surface.

FURTHER PROBLEMS

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FURTHER PROBLEMS FOR CHAPTER 2

Problem 2.36 Solve the time-independent Schrödinger equation with appropriate boundary conditions for the “centered” infinite square well: $V(x) = 0$ (for $-a < x < +a$), $V(x) = \infty$ (otherwise). Check that your allowed energies are consistent with mine (Equation 2.27), and confirm that your ψ 's can be obtained from mine (Equation 2.28) by the substitution $x \rightarrow (x + a)/2$ (and appropriate renormalization). Sketch your first three solutions, and compare Figure 2.2. Note that the width of the well is now $2a$.

Problem 2.37 A particle in the infinite square well (Equation 2.19) has the initial wave function

$$\Psi(x, 0) = A \sin^3(\pi x/a) \quad (0 \leq x \leq a).$$

Determine A , find $\Psi(x, t)$, and calculate $\langle x \rangle$, as a function of time. What is the expectation value of the energy? *Hint:* $\sin^n \theta$ and $\cos^n \theta$ can be reduced, by repeated application of the trigonometric sum formulas, to linear combinations of $\sin(m\theta)$ and $\cos(m\theta)$, with $m = 0, 1, 2, \dots, n$.

***Problem 2.38** A particle of mass m is in the ground state of the infinite square well (Equation 2.19). Suddenly the well expands to twice its original size—the right wall moving from a to $2a$ —leaving the wave function (momentarily) undisturbed. The energy of the particle is now measured.

- What is the most probable result? What is the probability of getting that result?
- What is the *next* most probable result, and what is its probability?
- What is the *expectation value* of the energy? *Hint:* If you find yourself confronted with an infinite series, try another method.

Problem 2.39

- Show that the wave function of a particle in the infinite square well returns to its original form after a quantum **revival time** $T = 4ma^2/\pi\hbar$. That is: $\Psi(x, T) = \Psi(x, 0)$ for any state (*not* just a stationary state).
- What is the *classical* revival time, for a particle of energy E bouncing back and forth between the walls?
- For what energy are the two revival times equal?⁴³

⁴³The fact that the classical and quantum revival times bear no obvious relation to one another (and the quantum one doesn't even depend on the energy) is a curious paradox; see Daniel Styer, *Am. J. Phys.* **69**, 56 (2001).

Problem 2.40 A particle of mass m is in the potential

$$V(x) = \begin{cases} \infty & (x < 0), \\ -32\hbar^2/ma^2 & (0 \leq x \leq a), \\ 0 & (x > a). \end{cases}$$

- (a) How many bound states are there?
 (b) In the highest-energy bound state, what is the probability that the particle would be found *outside* the well ($x > a$)? *Answer:* 0.542, so even though it is “bound” by the well, it is more likely to be found outside than inside!

Problem 2.41 A particle of mass m in the harmonic oscillator potential (Equation 2.43) starts out in the state

$$\Psi(x, 0) = A \left(1 - 2\sqrt{\frac{m\omega}{\hbar}} x \right)^2 e^{-\frac{m\omega}{2\hbar} x^2},$$

for some constant A .

- (a) What is the expectation value of the energy?
 (b) At some later time T the wave function is

$$\Psi(x, T) = B \left(1 + 2\sqrt{\frac{m\omega}{\hbar}} x \right)^2 e^{-\frac{m\omega}{2\hbar} x^2},$$

for some constant B . What is the smallest possible value of T ?

Problem 2.42 Find the allowed energies of the *half* harmonic oscillator

$$V(x) = \begin{cases} (1/2)m\omega^2 x^2, & \text{for } x > 0, \\ \infty, & \text{for } x < 0. \end{cases}$$

(This represents, for example, a spring that can be stretched, but not compressed.)
Hint: This requires some careful thought, but very little actual computation.

- **Problem 2.43** In Problem 2.22 you analyzed the *stationary* gaussian free particle wave packet. Now solve the same problem for the *traveling* gaussian wave packet, starting with the initial wave function

$$\Psi(x, 0) = A e^{-ax^2} e^{ilx},$$

where l is a real constant.

- **Problem 2.44 Solve the time-independent Schrödinger equation for a centered infinite square well with a delta-function barrier in the middle:

$$V(x) = \begin{cases} \alpha\delta(x), & \text{for } -a < x < +a, \\ \infty, & \text{for } |x| \geq a. \end{cases}$$

Treat the even and odd wave functions separately. Don't bother to normalize them. Find the allowed energies (graphically, if necessary). How do they compare with the corresponding energies in the absence of the delta function? Explain why the odd solutions are not affected by the delta function. Comment on the limiting cases $\alpha \rightarrow 0$ and $\alpha \rightarrow \infty$.

Problem 2.45 If two (or more) distinct⁴⁴ solutions to the (time-independent) Schrödinger equation have the same energy E , these states are said to be **degenerate**. For example, the free particle states are doubly degenerate—one solution representing motion to the right, and the other motion to the left. But we have never encountered *normalizable* degenerate solutions, and this is no accident. Prove the following theorem: *In one dimension⁴⁵ there are no degenerate bound states.* *Hint:* Suppose there are *two* solutions, ψ_1 and ψ_2 , with the same energy E . Multiply the Schrödinger equation for ψ_1 by ψ_2 , and the Schrödinger equation for ψ_2 by ψ_1 , and subtract, to show that $(\psi_2 d\psi_1/dx - \psi_1 d\psi_2/dx)$ is a constant. Use the fact that for normalizable solutions $\psi \rightarrow 0$ at $\pm\infty$ to demonstrate that this constant is in fact zero. Conclude that ψ_2 is a multiple of ψ_1 , and hence that the two solutions are not distinct.

Problem 2.46 Imagine a bead of mass m that slides frictionlessly around a circular wire ring of circumference L . (This is just like a free particle, except that $\psi(x+L) = \psi(x)$.) Find the stationary states (with appropriate normalization) and the corresponding allowed energies. Note that there are *two* independent solutions for each energy E_n —corresponding to clockwise and counter-clockwise circulation; call them $\psi_n^+(x)$ and $\psi_n^-(x)$. How do you account for this degeneracy, in view of the theorem in Problem 2.45 (why does the theorem fail, in this case)?

- **Problem 2.47 *Attention:* This is a *strictly qualitative* problem—no calculations allowed! Consider the “double square well” potential (Figure 2.21). Suppose the

⁴⁴If two solutions differ only by a multiplicative constant (so that, once normalized, they differ only by a phase factor $e^{i\phi}$), they represent the same physical state, and in this sense they are *not* distinct solutions. Technically, by “distinct” I mean “linearly independent.”

⁴⁵In higher dimensions such degeneracy is very common, as we shall see in Chapter 4. Assume that the potential does not consist of isolated pieces separated by regions where $V = \infty$ —two isolated infinite square wells, for instance, would give rise to degenerate bound states, for which the particle is either in the one or in the other.

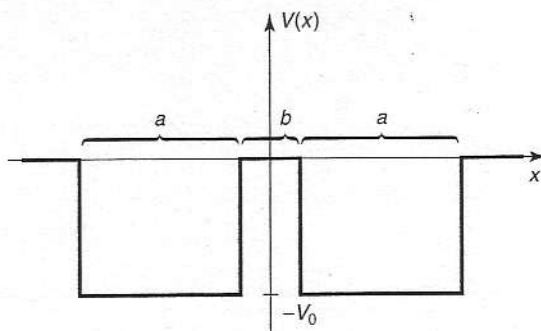


FIGURE 2.21: The double square well (Problem 2.47).

depth V_0 and the width a are fixed, and large enough so that several bound states occur.

- Sketch the ground state wave function ψ_1 and the first excited state ψ_2 , (i) for the case $b = 0$, (ii) for $b \approx a$, and (iii) for $b \gg a$.
- Qualitatively, how do the corresponding energies (E_1 and E_2) vary, as b goes from 0 to ∞ ? Sketch $E_1(b)$ and $E_2(b)$ on the same graph.
- The double well is a very primitive one-dimensional model for the potential experienced by an electron in a diatomic molecule (the two wells represent the attractive force of the nuclei). If the nuclei are free to move, they will adopt the configuration of minimum energy. In view of your conclusions in (b), does the electron tend to draw the nuclei together, or push them apart? (Of course, there is also the internuclear repulsion to consider, but that's a separate problem.)

Problem 2.48 In Problem 2.7(d) you got the expectation value of the energy by summing the series in Equation 2.39, but I warned you (in footnote 15) not to try it the "old fashioned way," $\langle H \rangle = \int \Psi(x, 0)^* H \Psi(x, 0) dx$, because the discontinuous first derivative of $\Psi(x, 0)$ renders the second derivative problematic. Actually, you *could* have done it using integration by parts, but the Dirac delta function affords a much cleaner way to handle such anomalies.

- Calculate the first derivative of $\Psi(x, 0)$ (in Problem 2.7), and express the answer in terms of the step function, $\theta(x - a/2)$, defined in Equation 2.143. (Don't worry about the end points—just the interior region $0 < x < a$.)
- Exploit the result of Problem 2.24(b) to write the second derivative of $\Psi(x, 0)$ in terms of the delta function.
- Evaluate the integral $\int \Psi(x, 0)^* H \Psi(x, 0) dx$, and check that you get the same answer as before.

***Problem 2.49

(a) Show that

$$\Psi(x, t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}\left(x^2 + \frac{a^2}{2}(1 + e^{-2i\omega t}) + \frac{i\hbar t}{m} - 2axe^{-i\omega t}\right)\right]$$

satisfies the time-dependent Schrödinger equation for the harmonic oscillator potential (Equation 2.43). Here a is any real constant with the dimensions of length.⁴⁶

(b) Find $|\Psi(x, t)|^2$, and describe the motion of the wave packet.(c) Compute $\langle x \rangle$ and $\langle p \rangle$, and check that Ehrenfest's theorem (Equation 1.38) is satisfied.

***Problem 2.50 Consider the moving delta-function well:

$$V(x, t) = -\alpha\delta(x - vt),$$

where v is the (constant) velocity of the well.

(a) Show that the time-dependent Schrödinger equation admits the exact solution

$$\Psi(x, t) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x-vt|/\hbar^2} e^{-i[(E+(1/2)mv^2)t-mvx]/\hbar},$$

where $E = -m\alpha^2/2\hbar^2$ is the bound-state energy of the stationary delta function. *Hint:* Plug it in and check it! Use the result of Problem 2.24(b).

(b) Find the expectation value of the Hamiltonian in this state, and comment on the result.

***Problem 2.51 Consider the potential

$$V(x) = -\frac{\hbar^2 a^2}{m} \operatorname{sech}^2(ax),$$

where a is a positive constant, and "sech" stands for the hyperbolic secant.

(a) Graph this potential.

(b) Check that this potential has the ground state

$$\psi_0(x) = A \operatorname{sech}(ax),$$

and find its energy. Normalize ψ_0 , and sketch its graph.

⁴⁶This rare example of an exact closed-form solution to the time-dependent Schrödinger equation was discovered by Schrödinger himself, in 1926.

(c) Show that the function

$$\psi_k(x) = A \left(\frac{ik - a \tanh(ax)}{ik + a} \right) e^{ikx},$$

(where $k \equiv \sqrt{2mE}/\hbar$, as usual) solves the Schrödinger equation for any (positive) energy E . Since $\tanh z \rightarrow -1$ as $z \rightarrow -\infty$,

$$\psi_k(x) \approx Ae^{ikx}, \quad \text{for large negative } x.$$

This represents, then, a wave coming in from the left with *no accompanying reflected wave* (i.e., no term $\exp(-ikx)$). What is the asymptotic form of $\psi_k(x)$ at large *positive* x ? What are R and T , for this potential? *Comment:* This is a famous example of a **reflectionless potential**—every incident particle, regardless of its energy, passes right through.⁴⁷

Problem 2.52 The scattering matrix. The theory of scattering generalizes in a pretty obvious way to arbitrary localized potentials (Figure 2.22). To the left (Region I), $V(x) = 0$, so

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \quad [2.173]$$

To the right (Region III), $V(x)$ is again zero, so

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}. \quad [2.174]$$

In between (Region II), of course, I can't tell you what ψ is until you specify the potential, but because the Schrödinger equation is a linear, second-order differential equation, the general solution has got to be of the form

$$\psi(x) = Cf(x) + Dg(x),$$

where $f(x)$ and $g(x)$ are two linearly independent particular solutions.⁴⁸ There will be four boundary conditions (two joining Regions I and II, and two joining

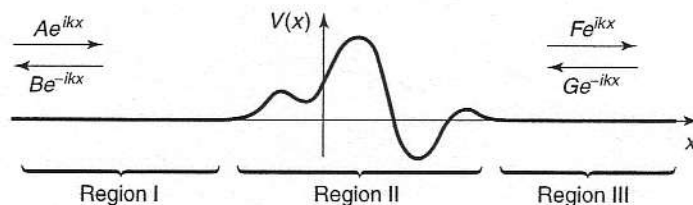


FIGURE 2.22: Scattering from an arbitrary localized potential ($V(x) = 0$ except in Region II); Problem 2.52.

⁴⁷R. E. Crandall and B. R. Litt, *Annals of Physics*, **146**, 458 (1983).

⁴⁸See any book on differential equations—for example, J. L. Van Iwaarden, *Ordinary Differential Equations with Numerical Techniques*, Harcourt Brace Jovanovich, San Diego, 1985, Chapter 3.

Regions II and III). Two of these can be used to eliminate C and D , and the other two can be "solved" for B and F in terms of A and G :

$$B = S_{11}A + S_{12}G, \quad F = S_{21}A + S_{22}G.$$

The four coefficients S_{ij} , which depend on k (and hence on E), constitute a 2×2 matrix \mathbf{S} , called the **scattering matrix** (or **S-matrix**, for short). The S -matrix tells you the outgoing amplitudes (B and F) in terms of the incoming amplitudes (A and G):

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}. \quad [2.175]$$

In the typical case of scattering from the left, $G = 0$, so the reflection and transmission coefficients are

$$R_l = \left. \frac{|B|^2}{|A|^2} \right|_{G=0} = |S_{11}|^2, \quad T_l = \left. \frac{|F|^2}{|A|^2} \right|_{G=0} = |S_{21}|^2. \quad [2.176]$$

For scattering from the right, $A = 0$, and

$$R_r = \left. \frac{|F|^2}{|G|^2} \right|_{A=0} = |S_{22}|^2, \quad T_r = \left. \frac{|B|^2}{|G|^2} \right|_{A=0} = |S_{12}|^2. \quad [2.177]$$

- (a) Construct the S -matrix for scattering from a delta-function well (Equation 2.114).
- (b) Construct the S -matrix for the finite square well (Equation 2.145). *Hint:* This requires no new work, if you carefully exploit the symmetry of the problem.

****Problem 2.53 The transfer matrix.** The S -matrix (Problem 2.52) tells you the *outgoing* amplitudes (B and F) in terms of the *incoming* amplitudes (A and G)—Equation 2.175. For some purposes it is more convenient to work with the **transfer matrix**, \mathbf{M} , which gives you the amplitudes to the *right* of the potential (F and G) in terms of those to the *left* (A and B):

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}. \quad [2.178]$$

- (a) Find the four elements of the M -matrix, in terms of the elements of the S -matrix, and vice versa. Express R_l , T_l , R_r , and T_r (Equations 2.176 and 2.177) in terms of elements of the M -matrix.
- (b) Suppose you have a potential consisting of two isolated pieces (Figure 2.23). Show that the M -matrix for the combination is the *product* of the two M -matrices for each section separately:

$$\mathbf{M} = \mathbf{M}_2 \mathbf{M}_1. \quad [2.179]$$

(This obviously generalizes to any number of pieces, and accounts for the usefulness of the M -matrix.)

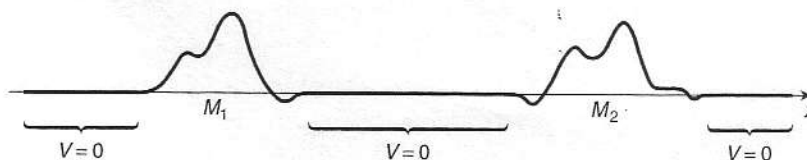


FIGURE 2.23: A potential consisting of two isolated pieces (Problem 2.53).

- (c) Construct the M -matrix for scattering from a single delta-function potential at point a :

$$V(x) = -\alpha\delta(x - a).$$

- (d) By the method of part (b), find the M -matrix for scattering from the double delta function

$$V(x) = -\alpha[\delta(x + a) + \delta(x - a)].$$

What is the transmission coefficient for this potential?

Problem 2.54 Find the ground state energy of the harmonic oscillator, to five significant digits, by the “wag-the-dog” method. That is, solve Equation 2.72 numerically, varying K until you get a wave function that goes to zero at large ξ . In Mathematica, appropriate input code would be

```
Plot[Evaluate[u[x]/.NDSolve[{u''[x] -(x^2 - K)*u[x] == 0, u[0] == 1,
u'[0] == 0}, u[x], {x, 10^-8, 10}, MaxSteps -> 10000]], {x, a, b},
PlotRange -> {c, d}];
```

(Here (a, b) is the horizontal range of the graph, and (c, d) is the vertical range—start with $a = 0$, $b = 10$, $c = -10$, $d = 10$.) We know that the correct solution is $K = 1$, so you might start with a “guess” of $K = 0.9$. Notice what the “tail” of the wave function does. Now try $K = 1.1$, and note that the tail flips over. Somewhere in between those values lies the correct solution. Zero in on it by bracketing K tighter and tighter. As you do so, you may want to adjust a , b , c , and d , to zero in on the cross-over point.

Problem 2.55 Find the first three excited state energies (to five significant digits) for the harmonic oscillator, by wagging the dog (Problem 2.54). For the first (and third) excited state you will need to set $u[0] == 0$, $u'[0] == 1$.

Problem 2.56 Find the first four allowed energies (to five significant digits) for the infinite square well, by wagging the dog. *Hint:* Refer to Problem 2.54, making appropriate changes to the differential equation. This time the condition you are looking for is $u(1) = 0$.