[redacted]

## 8.3 THE CONNECTION FORMULAS

In the discussion so far I have assumed that the "walls" of the potential well (or the barrier) are *vertical*, so that the "exterior" solution is simple, and the boundary conditions trivial. As it turns out, our main results (Equations 8.16 and 8.22) are reasonably accurate even when the edges are not so abrupt (indeed, in Gamow's theory they were applied to just such a case). Nevertheless, it is of some interest to study more closely what happens to the wave function at a turning point ($E = V$), where the "classical" region joins the "nonclassical" region, and the WKB

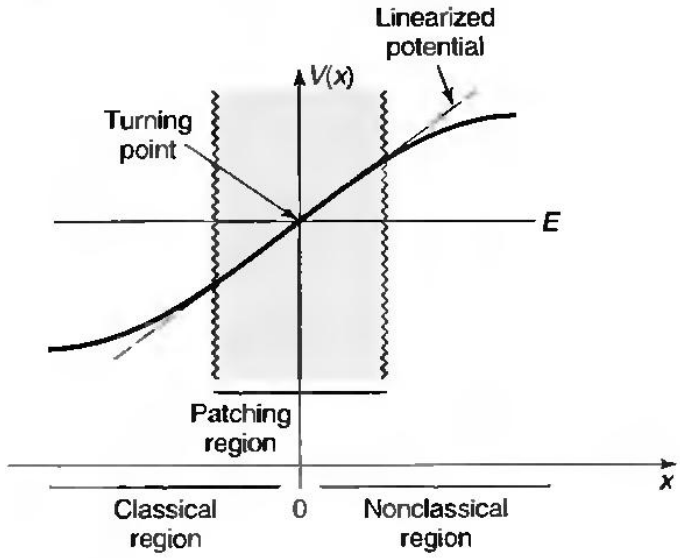


**FIGURE 8.7:** Enlarged view of the right-hand turning point.

approximation itself breaks down. In this section I'll treat the bound state problem (Figure 8.1); you get to do the scattering problem for yourself (Problem 8.10).[8]

For simplicity, let's shift the axes over so that the right-hand turning point occurs at $x = 0$ (Figure 8.7). In the WKB approximation, we have

$$\psi(x) \cong \begin{cases} \dfrac{1}{\sqrt{p(x)}}\left[Be^{\frac{i}{\hbar}\int_x^0 p(x')\,dx'} + Ce^{-\frac{i}{\hbar}\int_x^0 p(x')\,dx'}\right], & \text{if } x < 0, \\ \dfrac{1}{\sqrt{|p(x)|}}De^{-\frac{1}{\hbar}\int_0^x |p(x')|\,dx'}, & \text{if } x > 0. \end{cases} \qquad [8.31]$$

(Assuming $V(x)$ remains greater than $E$ for *all* $x > 0$, we can exclude the positive exponent in this region, because it blows up as $x \to \infty$.) Our task is to join the two solutions at the boundary. But there is a serious difficulty here: In the WKB approximation, $\psi$ goes to *infinity* at the turning point (where $p(x) \to 0$). The *true* wave function, of course, has no such wild behavior—as anticipated, the WKB method simply fails in the vicinity of a turning point. And yet, it is precisely the boundary conditions at the turning points that determine the allowed energies. What we need to do, then, is *splice* the two WKB solutions together, using a "patching" wave function that straddles the turning point.

Since we only need the patching wave function ($\psi_p$) in the neighborhood of the origin, we'll *approximate the potential by a straight line*:

$$V(x) \cong E + V'(0)x. \qquad [8.32]$$

[8] *Warning:* The following argument is quite technical, and you may wish to skip it on a first reading.

and solve the Schrödinger for this linearized $V$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_p}{dx^2} + [E + V'(0)x]\psi_p = E\psi_p,$$

or

$$\frac{d^2\psi_p}{dx^2} = \alpha^3 x\psi_p, \qquad [8.33]$$

where

$$\alpha \equiv \left[\frac{2m}{\hbar^2}V'(0)\right]^{1/3}. \qquad [8.34]$$

The $\alpha$'s can be absorbed into the independent variable by defining

$$z \equiv \alpha x, \qquad [8.35]$$

so that

$$\frac{d^2\psi_p}{dz^2} = z\psi_p. \qquad [8.36]$$

This is **Airy's equation**, and the solutions are called **Airy functions**.[9] Since the Airy equation is a second-order differential equation, there are two linearly independent Airy functions, $Ai(z)$ and $Bi(z)$.

**TABLE 8.1:** Some properties of the Airy functions.

| | |
|---|---|
| *Differential Equation:* | $\frac{d^2y}{dz^2} = zy.$ |
| *Solutions:* | Linear combinations of Airy Functions, $Ai(z)$ and $Bi(z)$. |
| *Integral Representation:* | $Ai(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{s^3}{3} + sz\right)ds.$ |
| | $Bi(z) = \frac{1}{\pi}\int_0^\infty \left[e^{-\frac{s^3}{3}+sz} + \sin\left(\frac{s^3}{3} + sz\right)\right]ds.$ |
| *Asymptotic Forms:* | |
| $Ai(z) \sim \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-\frac{2}{3}z^{3/2}}$, $Bi(z) \sim \frac{1}{\sqrt{\pi}z^{1/4}}e^{\frac{2}{3}z^{3/2}}$; $z \gg 0$; | $Ai(z) \sim \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right]$, $Bi(z) \sim \frac{1}{\sqrt{\pi}(-z)^{1/4}}\cos\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right]$; $z \ll 0$. |

[9] *Classically*, a linear potential means a constant force, and hence a constant acceleration—the simplest nontrivial motion possible, and the *starting* point for elementary mechanics. It is ironic that the same potential in *quantum* mechanics gives rise to unfamiliar transcendental functions, and plays only a peripheral role in the theory.

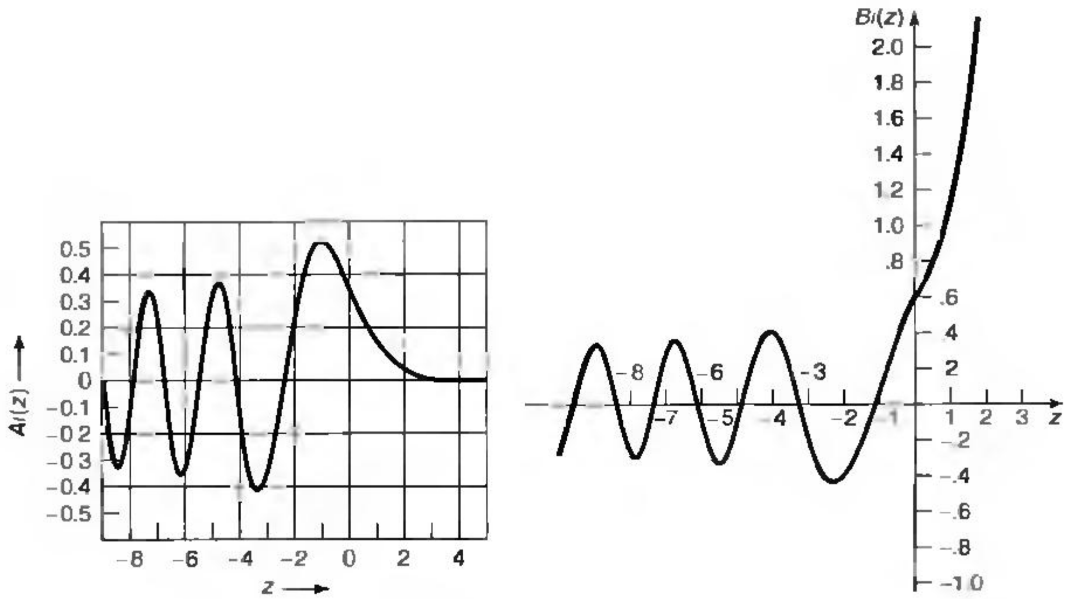


**FIGURE 8.8:** Graph of the Airy functions.

They are related to Bessel functions of order 1/3; some of their properties are listed in Table 8.1 and they are plotted in Figure 8.8. Evidently the patching wave function is a linear combination of $Ai(z)$ and $Bi(z)$:

$$\psi_p(x) = aAi(\alpha x) + bBi(\alpha x), \tag{8.37}$$

for appropriate constants $a$ and $b$.

Now $\psi_p$ is the (approximate) wave function in the neighborhood of the origin; our job is to match it to the WKB solutions in the overlap regions on either side (see Figure 8.9). These overlap zones are close enough to the turning point that the linearized potential is reasonably accurate (so that $\psi_p$ is a good approximation to the true wave function), and yet far enough away from the turning point that the WKB approximation is reliable.[10] In the overlap regions Equation 8.32 holds, and therefore (in the notation of Equation 8.34)

$$p(x) \cong \sqrt{2m(E - E - V'(0)x)} = \hbar\alpha^{3/2}\sqrt{-x}. \tag{8.38}$$

In particular, in overlap region 2,

$$\int_0^x |p(x')|\,dx' \cong \hbar\alpha^{3/2}\int_0^x \sqrt{x'}\,dx' = \frac{2}{3}\hbar(\alpha x)^{3/2}.$$

[10] This is a delicate double constraint, and it is possible to concoct potentials so pathological that no such overlap region exists. However, in practical applications this seldom occurs. See Problem 8.8.

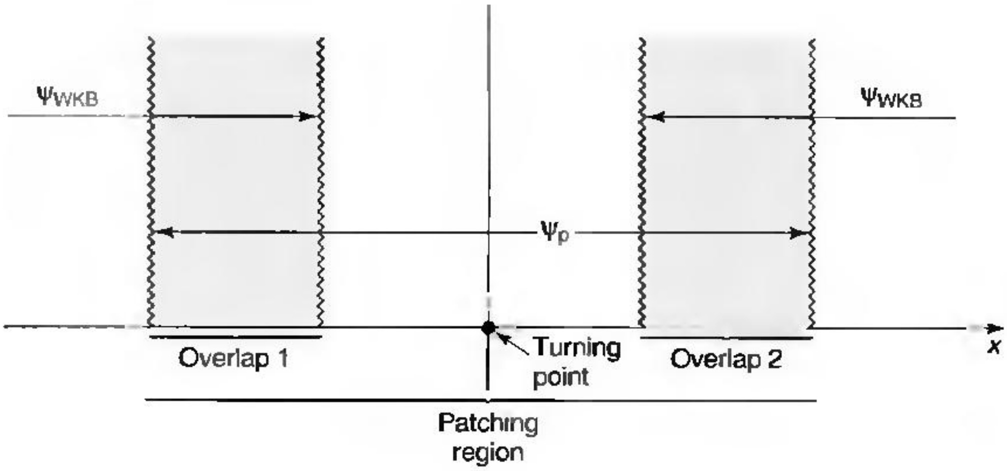


**FIGURE 8.9:** Patching region and the two overlap zones.

and therefore the WKB wave function (Equation 8.31) can be written as

$$\psi(x) \cong \frac{D}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}}e^{-\frac{2}{3}(\alpha x)^{3/2}}. \quad [8.39]$$

Meanwhile, using the large-$z$ asymptotic forms[11] of the Airy functions (from Table 8.1), the patching wave function (Equation 8.37) in overlap region 2 becomes

$$\psi_p(x) \cong \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}}e^{-\frac{2}{3}(\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}}e^{\frac{2}{3}(\alpha x)^{3/2}}. \quad [8.40]$$

Comparing the two solutions, we see that

$$a = \sqrt{\frac{4\pi}{\alpha\hbar}}D, \quad \text{and} \quad b = 0. \quad [8.41]$$

Now we go back and repeat the procedure for overlap region 1. Once again, $p(x)$ is given by Equation 8.38, but this time $x$ is *negative*, so

$$\int_x^0 p(x')\,dx' \cong \frac{2}{3}\hbar(-\alpha x)^{3/2} \quad [8.42]$$

and the WKB wave function (Equation 8.31) is

$$\psi(x) \cong \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}}\left[Be^{i\frac{2}{3}(-\alpha x)^{3/2}} + Ce^{-i\frac{2}{3}(-\alpha x)^{3/2}}\right]. \quad [8.43]$$

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[11] At first glance it seems absurd to use a *large-z* approximation in this region, which after all is supposed to be reasonably close to the turning point at $z = 0$ (so that the linear approximation to the potential is valid). But notice that the argument here is $\alpha x$, and if you study the matter carefully (see Problem 8.8) you will find that there *is* (typically) a region in which $\alpha x$ is large, but at the same time it is reasonable to approximate $V(x)$ by a straight line.

Meanwhile, using the asymptotic form of the Airy function for large *negative* $z$ (Table 8.1), the patching function (Equation 8.37, with $b = 0$) reads

$$\psi_p(x) \cong \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}} \sin\left[\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right]$$

$$= \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}} \frac{1}{2i}\left[e^{i\pi/4}e^{i\frac{2}{3}(-\alpha x)^{3/2}} - e^{-i\pi/4}e^{-i\frac{2}{3}(-\alpha x)^{3/2}}\right]. \quad [8.44]$$

Comparing the WKB and patching wave functions in overlap region 1, we find

$$\frac{a}{2i\sqrt{\pi}}e^{i\pi/4} = \frac{B}{\sqrt{\hbar\alpha}} \quad \text{and} \quad \frac{-a}{2i\sqrt{\pi}}e^{-i\pi/4} = \frac{C}{\sqrt{\hbar\alpha}},$$

or, putting in Equation 8.41 for $a$:

$$B = -ie^{i\pi/4}D, \quad \text{and} \quad C = ie^{-i\pi/4}D. \quad [8.45]$$

These are the so-called **connection formulas**, joining the WKB solutions at either side of the turning point. We're done with the patching wave function now—its only purpose was to bridge the gap. Expressing everything in terms of the one normalization constant $D$, and shifting the turning point back from the origin to an arbitrary point $x_2$, the WKB wave function (Equation 8.31) becomes

$$\psi(x) \cong \begin{cases} \dfrac{2D}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar}\displaystyle\int_x^{x_2} p(x')\,dx' + \dfrac{\pi}{4}\right], & \text{if } x < x_2; \\ \dfrac{D}{\sqrt{|p(x)|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{x_2}^{x} |p(x')|\,dx'\right], & \text{if } x > x_2. \end{cases} \quad [8.46]$$

---

**Example 8.3 Potential well with one vertical wall.** Imagine a potential well that has one vertical side (at $x = 0$) and one sloping side (Figure 8.10). In this case $\psi(0) = 0$, so Equation 8.46 says

$$\frac{1}{\hbar}\int_0^{x_2} p(x)\,dx + \frac{\pi}{4} = n\pi, \quad (n = 1, 2, 3, \ldots),$$

or

$$\boxed{\int_0^{x_2} p(x)\,dx = \left(n - \frac{1}{4}\right)\pi\hbar.} \quad [8.47]$$

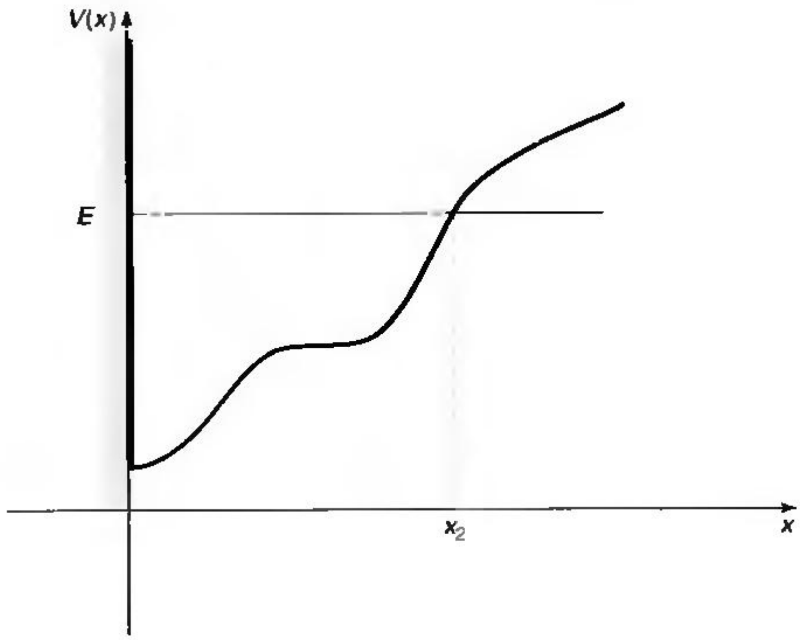


**FIGURE 8.10:** Potential well with one vertical wall.

For instance, consider the "half-harmonic oscillator."

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & \text{if } x > 0, \\ 0, & \text{otherwise.} \end{cases} \qquad [8.48]$$

In this case

$$p(x) = \sqrt{2m[E - (1/2)m\omega^2 x^2]} = m\omega\sqrt{x_2^2 - x^2},$$

where

$$x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

is the turning point. So

$$\int_0^{x_2} p(x)\,dx = m\omega \int_0^{x_2} \sqrt{x_2^2 - x^2}\,dx = \frac{\pi}{4}m\omega x_2^2 = \frac{\pi E}{2\omega},$$

and the quantization condition (Equation 8.47) yields

$$E_n = \left(2n - \frac{1}{2}\right)\hbar\omega = \left(\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots\right)\hbar\omega. \qquad [8.49]$$

In this particular case the WKB approximation actually delivers the *exact* allowed energies (which are precisely the *odd* energies of the *full* harmonic oscillator—see Problem 2.42).

**Example 8.4 Potential well with no vertical walls.** Equation 8.46 connects the WKB wave functions at a turning point where the potential slopes *upward* (Figure 8.11(a)); the same reasoning, applied to a *downward*-sloping turning point (Figure 8.11(b)), yields (Problem 8.9)

$$\psi(x) \cong \begin{cases} \dfrac{D'}{\sqrt{|p(x)|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_x^{x_1} |p(x')|\,dx'\right], & \text{if } x < x_1; \\ \dfrac{2D'}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar}\displaystyle\int_{x_1}^{x} p(x')\,dx' + \dfrac{\pi}{4}\right], & \text{if } x > x_1. \end{cases} \qquad [8.50]$$

In particular, if we're talking about a potential *well* (Figure 8.11(c)), the wave function in the "interior" region ($x_1 < x < x_2$) can be written *either* as

$$\psi(x) \cong \frac{2D}{\sqrt{p(x)}} \sin\theta_2(x), \quad \text{where } \theta_2(x) \equiv \frac{1}{\hbar}\int_x^{x_2} p(x')\,dx' + \frac{\pi}{4},$$

(Equation 8.46), *or* as

$$\psi(x) \cong \frac{-2D'}{\sqrt{p(x)}} \sin\theta_1(x), \quad \text{where } \theta_1(x) \equiv -\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' - \frac{\pi}{4},$$

(Equation 8.50). Evidently the arguments of the sine functions must be equal, modulo $\pi$:[12] $\theta_2 = \theta_1 + n\pi$, from which it follows that

$$\boxed{\int_{x_1}^{x_2} p(x)\,dx = \left(n - \frac{1}{2}\right)\pi\hbar, \quad \text{with } n = 1, 2, 3, \ldots.} \qquad [8.51]$$

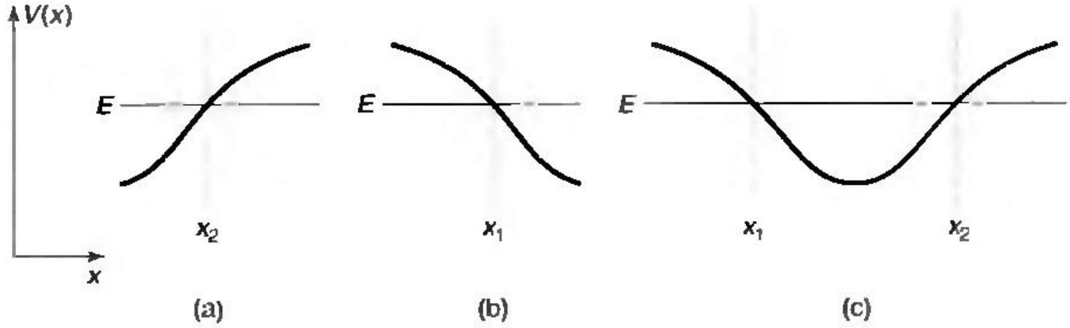


**FIGURE 8.11: Upward-sloping and downward-sloping turning points.**

[12] *Not* $2\pi$—an overall minus sign can be absorbed into the normalization factors $D$ and $D'$.

This quantization condition determines the allowed energies for the "typical" case of a potential well with two sloping sides. Notice that it differs from the formulas for two vertical walls (Equation 8.16) or one vertical wall (Equation 8.47) only in the number that is subtracted from $n$ (0, 1/4, or 1/2). Since the WKB approximation works best in the semi-classical (large $n$) regime, the distinction is more in appearance than in substance. In any event, the result is extraordinarily powerful, for it enables us to calculate (approximate) allowed energies *without ever solving the Schrödinger equation*, by simply evaluating one integral. The wave function itself has dropped out of sight.

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****Problem 8.5** Consider the quantum mechanical analog to the classical problem of a ball (mass $m$) bouncing elastically on the floor.[13]

(a) What is the potential energy, as a function of height $x$ above the floor? (For negative $x$, the potential is *infinite*—the ball can't get there at all.)

(b) Solve the Schrödinger equation for this potential, expressing your answer in terms of the appropriate Airy function (note that $Bi(z)$ blows up for large $z$, and must therefore be rejected). Don't bother to normalize $\psi(x)$.

(c) Using $g = 9.80\ \text{m/s}^2$ and $m = 0.100$ kg, find the first four allowed energies, in joules, correct to three significant digits. *Hint:* See Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions*, Dover, New York (1970), page 478; the notation is defined on page 450.

(d) What is the ground state energy, in eV, of an *electron* in this gravitational field? How high off the ground is this electron, on the average? *Hint:* Use the virial theorem to determine $\langle x \rangle$.

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***Problem 8.6** Analyze the bouncing ball (Problem 8.5) using the WKB approximation.

(a) Find the allowed energies, $E_n$, in terms of $m$, $g$, and $\hbar$.

(b) Now put in the particular values given in Problem 8.5(c), and compare the WKB approximation to the first four energies with the "exact" results.

(c) About how large would the quantum number $n$ have to be to give the ball an average height of, say, 1 meter above the ground?

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[13] For more on the quantum bouncing ball see J. Gea-Banacloche, *Am. J. Phys.* **67**, 776 (1999) and N. Wheeler, "Classical/quantum dynamics in a uniform gravitational field," unpublished Reed College report (2002). This may sound like an awfully artificial problem, but the experiment has actually been done, using neutrons (V. V. Nesvizhevsky *et al.*, Nature **415**, 297 (2002)).