15
The WKB Approximation

15.1 Introduction

The WKB method, named for Gregor Wentzel, Hendrik Kramers, and Léon Brillouin, gives an approximation to the eigenfunctions and eigenvalues of the Hamiltonian operator $\hat{H}$ in one dimension. The approximation is best understood as applying to a fixed range of energies as $\hbar$ tends to zero. (It is also reasonable in many cases to think of the approximation as applying to a fixed value of $\hbar$ as the energy tends to infinity.)

The idea of the WKB approximation is that the potential function $V(x)$ can be thought of as being "slowly varying," with the result that solutions to the time-independent Schrödinger equation will look locally like the solutions in the case of a constant potential. In the classically allowed region, this line of thinking will yield an approximation consisting of a rapidly oscillating complex exponential multiplied by a slowly varying amplitude. We make the "local frequency" of the exponential equal to what it would be if V were constant. Having made this choice, there is a unique choice for the amplitude that yields an error that is of order $\hbar^2$. This amplitude, however, tends to infinity as we approach the "turning points," that is, the points where the classical particle changes directions. Similarly, in the classically forbidden region, we obtain approximate solutions that are rapidly growing or decaying exponentials, multiplied by a slowly varying factor. Again, there is a unique choice for the slowly varying factor that gives errors of order $\hbar^2$, and again, this factor blows up at the turning points.

B.C. Hall, *Quantum Theory for Mathematicians*, Graduate Texts in Mathematics 267, DOI 10.1007/978-1-4614-7116-5_15,

The difficulty near the turning points means that we cannot directly "match" the approximate solutions in different regimes the way we did in Chap. 5. Instead, we will use the Airy function to approximate the solution to the Schrödinger equation near the turning points. Asymptotics of the Airy function will then yield the appropriate matching condition, which turns out to be a corrected form of the Bohr–Sommerfeld rule that appears in the "old" quantum theory.

15.2 The Old Quantum Theory and the Bohr–Sommerfeld Condition

The old quantum theory, developed by Bohr, Sommerfeld, and de Broglie, among others, may be pictured as follows. Consider, for simplicity, a particle with one degree of freedom, and let C be a level set in phase space of the Hamiltonian,

$$C = \left\{ (x,p) \in \mathbb{R}^2 \middle| \, H(x,p) = E \right\}, \tag{15.1}$$

which we assume to be a closed curve. We now imagine drawing a "wave" on C, that is, some oscillatory function defined over C. Following the *de Broglie hypothesis* (Sect. 1.2.2), we postulate that the local frequency k of the wave as a function of x is $p/\hbar$. This means that the phase of our wave should be obtained by integrating the 1-form

$$\frac{1}{\hbar} p \, dx \tag{15.2}$$

along the curve. Thus, the wave itself can be pictured as a function on C of the form

$$\cos\left(\frac{1}{\hbar} \int_{x_0}^{x} p \, dx - \delta \right), \tag{15.3}$$

where x_0 is some arbitrary starting point on the curve C and where δ is an arbitrary phase. Note that the old quantum theory did not offer a physical interpretation of this wave; it was simply a crude attempt to introduce waves into the picture.

The *Bohr–Sommerfeld condition* is simply the requirement that the function in (15.3) should match up with itself when we go all the way around the curve. This will happen precisely if

$$\frac{1}{\hbar} \int_C p \, dx = 2\pi n, \tag{15.4}$$

for some integer n. The energy levels in the old quantum theory were taken to be those numbers E for which the corresponding level curve C satisfies the Bohr–Sommerfeld condition (15.4). Although Bohr–Sommerfeld

quantization had some successes, notably explaining the energy levels of the hydrogen atom, it ultimately failed to correctly predict the energies of complex systems.

For systems with one degree of freedom, a vestige of the Bohr–Sommerfeld approach survives in modern quantum theory, with two modifications. First, the condition (15.4) has to be corrected by replacing the n by $n+1/2$ on the right-hand side of (15.4). (The replacement of n by $n+1/2$ is known as the *Maslov correction*.) Second, this condition does not (in most cases) give the exact energy levels, but only the leading-order semiclassical approximation to the energy levels. The preceding discussion leads to the following definition.

Condition 15.1 *A number E is said to satisfy the Maslov-corrected Bohr–Sommerfeld condition if*

$$\frac{1}{\hbar}\int_C p\, dx = 2\pi(n+1/2) \tag{15.5}$$

for some integer n, where C is the classical energy curve in (15.1). In light of Green's theorem, this condition may be rewritten as

$$\frac{1}{2\pi\hbar}(\textit{Area enclosed by } C) = n + \frac{1}{2}.$$

When the Maslov correction is included, the Bohr–Sommerfeld condition can be stated as saying that the wave with phase given by integrating the 1-form in (15.2) should be 180° out of phase with itself after one trip around the energy curve. Figure 15.1 shows an example, which should be contrasted with Fig. 1.3. (Note also that Fig. 1.3 is drawn in the configuration space, whereas Fig. 15.1 is in the phase space.)

In our analysis in the subsequent sections, we will see that the Maslov correction—that is, the extra 1/2 in (15.5), as compared to (15.4)—actually consists of a contribution of 1/4 from each of the two "turning points" of the classical particle. (The turning points are the points where the classical particle changes directions.) Specifically, in the WKB approximation, the phase of the wave function will be computed as the integral of $(p\, dx)/\hbar$ along one "branch" of the classical energy curve C. Using the Airy function to approximate the wave function near the turning points, we will obtain an "extra" $\pi/4$ of phase between each turning point and the last local maximum or minimum of the wave function. Because of the two branches of C, the extra $\pi/4$ of phase near each of the two turning points actually contributes an extra π to the integral on the left-hand side of (15.5).

The reader may wonder why there is no comparable correction term in our discussion of the Bohr–de Broglie model of the hydrogen atom in Sect. 1.2.2. One way to answer this question is as follows. As we will see in Sect. 18.1, the Schrödinger operator for the hydrogen atom can be reduced

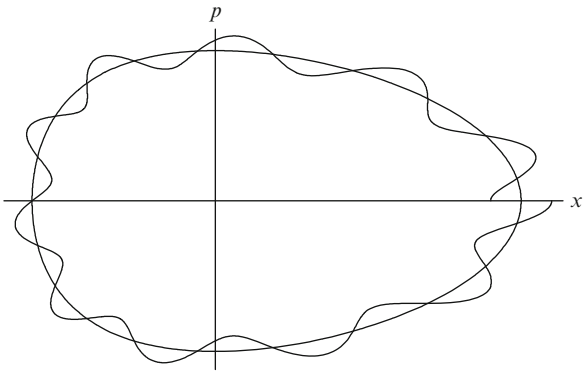

FIGURE 15.1. A trajectory satisfying the corrected Bohr–Sommerfeld condition with $n = 10$.

to a one-dimensional Schrödinger operator with an *effective potential* of the form

$$V_{\text{eff}}(r) = -\frac{Q^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2}.$$

Here l is a non-negative integer that labels the "total angular momentum" of the wave function. At least when $l > 0$, one can analyze this Schrödinger operator using a WKB-type analysis very similar to the one in the current chapter, with one important modification: The radial wave function [the quantity $h(r)$ in (18.5)] must be zero at $r = 0$ in order for the wave function to be in the domain of the Hamiltonian.

If one analyzes the situation carefully, it turns out that the zero boundary condition at $r = 0$ introduces *another* correction into the Bohr–Sommerfeld condition in the amount of $1/2$. There is still also a correction of $1/4$ for each of the two turning points, leading to the condition

$$\frac{1}{\hbar}\int_C p\, dx = 2\pi\left(n + \frac{1}{4} + \frac{1}{4} + \frac{1}{2}\right) = 2\pi(n+1).$$

Since $n + 1$ is again an integer, we are effectively back to the uncorrected Bohr–Sommerfeld condition. See Chap. 11 of [8] for a discussion of different approaches to the WKB approximation for radial potentials.

15.3 Classical and Semiclassical Approximations

We are interested in finding approximate solutions to the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V(x) - E)\psi(x) = 0 \tag{15.6}$$

for small values of $\hbar$. Ultimately, we will need to analyze the behavior of solutions in three different regions, the classically allowed region [points where $V(x) < E$], the classically forbidden region (points where $V(x) > E$), and the region near the "turning points," that is, the points where $V(x) = E$.

Let us consider at first the classically allowed region. Given a potential V and an energy level E, we can solve (up to a choice of sign) for the momentum of a classical particle as a function of position as

$$p(x) = \sqrt{2m(E - V(x))}.$$

We look for approximate solutions ψ to (15.6) of the form

$$\psi(x) = A(x)e^{\pm iS(x)/\hbar}, \tag{15.7}$$

where S satisfies $S'(x) = p(x)$. Note that we are taking the phase of our wave function to be

$$\text{phase} = \pm\frac{1}{\hbar}\int p(x)\ dx,$$

as in the old quantum theory in Sect. 15.2. The "amplitude function" $A(x)$ will be chosen to be independent of $\hbar$ and thus "slowly varying" (for small $\hbar$) compared to the exponent $S(x)/\hbar$.

Our first, elementary, result is that for *any* number E for which there is a classically allowed region and for *any* reasonable choice of the amplitude $A(x)$ in (15.7), we obtain an approximate eigenvector solution to the time-independent Schrödinger equation, with an error term of order $\hbar$.

Proposition 15.2 *For any two numbers E_1 and E_2 with $E_1 > \inf_{x\in\mathbb{R}} V(x)$, there exists a constant C and a nonzero function $A \in C_c^\infty(\mathbb{R})$ with the following property. For every $E \in [E_1, E_2]$, the support of A is contained in the classically allowed region at energy E and the function ψ given by*

$$\psi(x) = A(x)\exp\left\{\pm\frac{i}{\hbar}\int p(x)\ dx\right\}$$

satisfies

$$\|\hat{H}\psi - E\psi\| \leq C\hbar\,\|\psi\|\,. \tag{15.8}$$

Proof. For any $E \in [E_1, E_2]$, the classically allowed region for energy E contains the classically allowed region for energy E_1. We choose, then, A to be any nonzero element of $C_c^\infty(\mathbb{R})$ with support in the classically allowed region for energy E_1. If we evaluate $\hat{H}\psi - E\psi$ by direct calculation, there will a term in which two derivatives fall on the exponential factor, bringing down a factor involving $p(x)^2$. The definition of $p(x)$ is such that the term

involving $p(x)^2$ will cancel the term involving $V(x) - E$, leaving us with

$$\hat{H}\psi - E\psi = -\frac{\hbar^2}{2m}\left(A''(x) \pm \frac{i}{\hbar}2A'(x)p(x) \pm \frac{i}{\hbar}p'(x)A(x)\right) \times \exp\left\{\pm\frac{i}{\hbar}\int p(x)\, dx\right\}. \tag{15.9}$$

(Here, each occurrence of the symbol $\pm$ has the same value, either all pluses or all minuses.) Thus,

$$\|\hat{H}\psi - E\psi\| \leq \frac{\hbar^2}{2m}\|A''\| + \frac{\hbar}{2m}\|2A'p + Ap'\|. \tag{15.10}$$

Since $\|\psi\|$ is independent of $\hbar$, the right-hand side of (15.10) is of order $\hbar\,\|\psi\|$. It is easy to check that $\|2A'p + Ap'\|$ is bounded as a function of E for any E in the range $[E_1, E_2]$ and the result follows. ■

Proposition 15.2, along with elementary spectral theory, tells us that for any E larger than the minimum of V, there is a point $\tilde{E}$ in the spectrum of $\hat{H}$ such that

$$|E - \tilde{E}| \leq c\hbar. \tag{15.11}$$

(See Exercise 4 in Chap. 10.) If we assume that $V(x)$ tends to $+\infty$ as $x \to \pm\infty$, then $\hat{H}$ will have discrete spectrum and we can say that $\tilde{E}$ is an eigenvalue for $\hat{H}$. The conclusion, for such potentials, is this: Given *any* number $E \in [E_1, E_2]$, there is an eigenvalue of $\hat{H}$ within $C\hbar$ of E. Thus, as $\hbar$ tends to zero, the eigenvalues of $\hat{H}$ "fill up" the entire range of values of the classical energy function.

Proposition 15.2 is one manifestation of the "classical limit" of quantum mechanics: the quantum energy spectrum is, in a certain sense, approximating the classical energy spectrum as $\hbar$ gets small. Notice, however, that this result tells us only that the eigenvalues are at most order $\hbar$ apart and nothing further about the location of the individual eigenvalues.

In this chapter, we will show that if E satisfies the corrected Bohr–Sommerfeld condition, then there exists an eigenvalue $\tilde{E}$ of $\hat{H}$ such that

$$|E - \tilde{E}| \leq C\hbar^{9/8}. \tag{15.12}$$

An estimate of the form (15.12) locates eigenvalues with an error bound that is small compared to the expected average spacing between the eigenvalues, which is of order $\hbar$. On the other hand, the approximate energy levels E are determined by Condition 15.1, which is a condition on the *classical* energy curve. Thus, (15.12) can be described as a *semiclassical* estimate: It is estimating quantum mechanical quantities (the individual energy levels) in classical terms (the level curves of the classical Hamiltonian).

15.4 The WKB Approximation Away from the Turning Points

We consider only the simplest interesting case of the WKB approximation, in which the following assumption holds. See the book of Miller [30] for much about this sort of asymptotic analysis.

Assumption 15.3 *Consider a smooth, real-valued potential $V(x)$, with $V(x) \to +\infty$ as $x \to \pm\infty$. Assume that the functions $V'(x)/V(x)$ and $V''(x)/V(x)$ are bounded for x near $\pm\infty$.*

Consider also a range of energies of the form $E_1 \leq E \leq E_2$. Assume that for each E in this range, there are exactly two points, $a(E)$ and $b(E)$, with $a(E) < b(E)$, for which $V(x) = E$. Further assume that the derivative of V is nonzero at $a(E)$ and $b(E)$, for all $E \in [E_1, E_2]$.

See Fig. 15.2 for a typical example. Since V is locally bounded and tends to $+\infty$ at infinity, $\hat{H}$ is essentially self-adjoint on $C_c^\infty(\mathbb{R})$ (Theorem 9.39) and has purely discrete spectrum (Theorem XIII.16 in Volume IV of [34]). The assumption that V'/V and V''/V be bounded near infinity is stronger than necessary, but still applies to most of the interesting cases.

We refer to $a(E)$ and $b(E)$ as the *turning points*, since these are the points where a classical particle with energy E changes direction. When the energy E is understood as being fixed, we will write the turning points simply as a and b.

15.4.1 The Classically Allowed Region

As in Sect. 15.3, we seek approximate solutions to the time-independent Schrödinger equation having the following form in the classically allowed region:

$$\psi = A(x) \exp\left\{ \pm \frac{i}{\hbar} \int p(x)\, dx \right\}, \tag{15.13}$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the momentum of a classical particle with energy E and position x. According to (15.9), this form for ψ gives

$$\begin{aligned} \hat{H}\psi - E\psi = -\frac{\hbar^2}{2m} \left(A''(x) \pm \frac{i}{\hbar} 2A'(x)p(x) \pm \frac{i}{\hbar} p'(x)A(x) \right) \\ \times \exp\left\{ \pm \frac{i}{\hbar} \int p(x)\, dx \right\}. \end{aligned} \tag{15.14}$$

Since we want to obtain an approximate solution with an error smaller than $\hbar$, we require that the second and third terms in parentheses in (15.14) cancel. This cancellation will occur if A satisfies

$$2A'(x)p(x) = -p'(x)A(x)$$

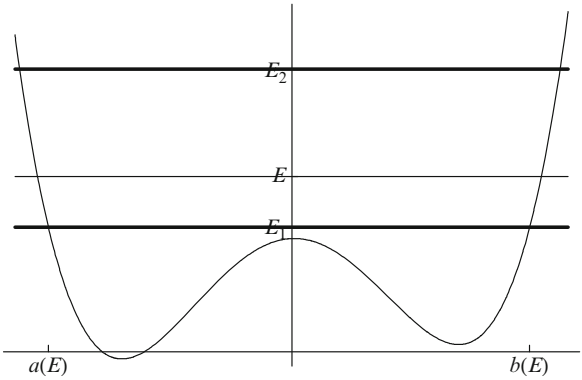

FIGURE 15.2. A potential satisfying Assumption 15.3.

or

$$\frac{A'(x)}{A(x)} = -\frac{1}{2}\frac{p'(x)}{p(x)}, \tag{15.15}$$

which we can easily solve (Exercise 3) as

$$A(x) = C(p(x))^{-1/2}. \tag{15.16}$$

If A is given by (15.16), we will have

$$\hat{H}\psi - E\psi = -\frac{\hbar^2}{2m}\frac{A''(x)}{A(x)}\psi(x), \tag{15.17}$$

indicating that our error is of order $\hbar^2$. This expression, however, is only local, in that it applies only in the classically allowed region. Furthermore, $p(x)$ tends to zero at the turning points, which means that $A(x)$ becomes unbounded at these points. This blow-up of the amplitude is a substantial complicating factor in the analysis.

We can get an approximate solution to the Schrödinger equation by taking a linear combination of the function in (15.13) with two different choices for the sign in the exponent, with constants c_1 and c_2. It is convenient to take the basepoint of our integration to be the left-hand turning point $a = a(E)$. Furthermore, since the Schrödinger operator $\hat{H}$ commutes with complex conjugation, the real and imaginary parts of any solution to the time-independent Schrödinger equation is again a solution. We will therefore consider only real-valued approximate solutions, i.e., those in which $c_2 = \overline{c_1}$. Using Exercise 1, we can then write our approximate solution as follows.

Summary 15.4 *Suppose ψ is a real-valued solution to the time-independent Schrödinger equation. Then in the classically allowed region but away from the turning points, we expect that ψ is well approximated by an expression of the form*

$$\frac{R}{\sqrt{p(x)}} \cos\left\{\frac{1}{\hbar}\int_a^x p(y)\ dy - \delta\right\}, \tag{15.18}$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the momentum of a classical particle with energy E and position x. Here R and δ are real constants, referred to as the amplitude and the phase of the approximate solution.

We refer to the function in (15.18) as the *oscillatory WKB function*. In integrating the square of the oscillatory WKB function over some interval, we may apply the identity $\cos^2\theta = (1 + \cos(2\theta))/2$ to the cosine factor. The rapidly oscillating $\cos(2\theta)$ term will be small for small $\hbar$ because of cancellation between positive and negative values. Thus, the integral of $\psi^2(x)$ over an interval will be, to leading order, just a constant times the integral of $1/p(x)$, or, equivalently, a constant times $1/v(x)$, where v is the velocity of the classical particle. But the integral of $1/v(x) = dt/dx$ with respect to x is just the time t that the classical particle spends in the interval. We obtain, then, the following result.

Conclusion 15.5 *If the amplitude R in (15.18) is chosen so that ψ has L^2 norm 1 over $[a, b]$, then the probability of finding the quantum particle in an interval $[c, d] \subset [a, b]$ is approximately the* fraction of time *the classical particle spends in $[c, d]$ over one period of classical motion.*

15.4.2 The Classically Forbidden Region

In the classically forbidden region, let us introduce the quantity

$$q(x) := \sqrt{2m(V(x) - E)}.$$

We look for approximate solutions to the Schrödinger equation (15.6) of the form

$$\psi(x) = A(x) \exp\left\{\pm\frac{1}{\hbar}\int_{x_0}^x q(y)\ dy\right\}.$$

If we analyze approximate solutions of this form precisely as in the classically allowed region, we again find that there is a unique choice for A (up to multiplication by a constant) that causes the order-$\hbar$ terms in $\hat{H}\psi - E\psi$ to cancel, namely $A(x) = C(q(x))^{-1/2}$. If we are hoping to approximate a *square-integrable* solution of the Schrödinger equation, we want to take a minus sign in the exponent on the interval (b, ∞), and it is convenient to the basepoint of our integration to be b. In the region $(-\infty, a)$, we want to take a plus sign in the exponent; it is then convenient to take the basepoint of our integration to be a and to reverse the direction of integration, which changes the sign in the exponent back to being negative.

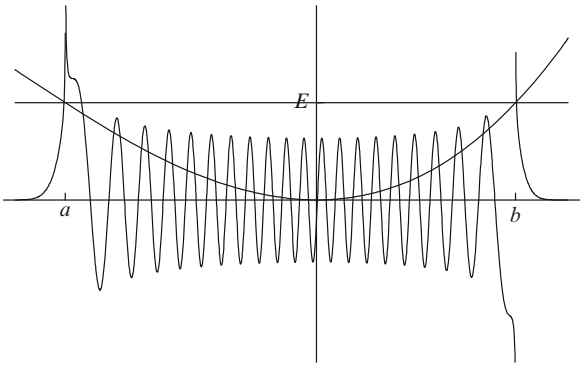

FIGURE 15.3. The WKB functions, extended all the way to the turning points.

Summary 15.6 *If $\psi_1(x)$ is a solution to the time-independent Schrödinger equation that tends to zero as x approaches $-\infty$, we expect that ψ_1 will be well approximated on $(-\infty, a)$, but away from the turning point, by the expression*

$$\frac{c_1}{\sqrt{q(x)}} \exp\left\{-\frac{1}{\hbar}\int_x^a q(y)\ dy\right\}, \tag{15.19}$$

where $q(x) = \sqrt{2m(V(x) - E)}$. Meanwhile, if $\psi_2(x)$ is a solution to the time-independent Schrödinger equation that tends to zero as x approaches $+\infty$, we expect that ψ will be well approximated on $(b, +\infty)$, but away from the turning point, by the expression

$$\frac{c_2}{\sqrt{q(x)}} \exp\left\{-\frac{1}{\hbar}\int_b^x q(y)\ dy\right\}. \tag{15.20}$$

We refer to the functions in (15.19) and (15.20) as the *exponential WKB functions*. The general theory of ordinary differential equations tells us that any solution to the time-independent Schrödinger equation for a smooth potential is smooth. Thus, the singularity at the turning points is an artifact of our approximation method. Nevertheless, for small values of $\hbar$, the true solution will "track" the WKB approximation until x gets very close to the turning point, with the result that the true solution will be large, but finite, near the turning points.

Figure 15.3 plots a potential function $V(x)$, an energy level E, and the WKB functions in both the classically allowed and classically forbidden regions. In the figure, the WKB functions have been (improperly) used all the way up to the turning points.

15.5 The Airy Function and the Connection Formulas

For any constant c_1 and any energy level E, we expect that there is a unique solution ψ_1 of the Schrödinger equation (15.6) that is well approximated for x tending to $-\infty$ by a function of the form (15.19). We expect that this solution will be well approximated in the classically allowed region (but not too close to the turning points) by a function of the form (15.18) for a unique pair of constants R and δ. In this section, we will see that the correct choices for R and δ are

$$R = 2c_1, \quad \delta = \frac{\pi}{4}. \tag{15.21}$$

The formula (15.21) for R and δ is called a *connection formula*; there is a similar formula connecting an approximate solution that tends to zero as x tends to $+\infty$ to an approximate solution in the classically allowed region. By comparing the two connection formulas, we will obtain conditions on the energy E under which the two approximate solutions (one that decays near $-\infty$ and one that decays near $+\infty$) agree up to a constant in the classically allowed region. The condition on E will turn out to be precisely Condition 15.1.

The discussion in the previous paragraph should be compared to the analysis in Chap. 5, where we determined the constants for the solution inside the well in terms of the energy level and the constant in front of the exponentially decaying solution outside the well. Here, of course, the analysis is more complicated because neither of the approximations (15.19) or (15.18) is valid near the turning point. The connection formula will be obtained, then, by using the Airy equation to approximate the Schrödinger equation near the turning points.

To get a reasonable approximation of our wave function near the turning points, we approximate V locally by a linear function. (By contrast, in the WKB functions, we are essentially thinking of V as being locally constant.) Thus, for example, near the turning point a, we write $V(x) \approx (a-x)F_0$, where $F_0 = -V'(a)$, yielding the approximate equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (a-x)F_0\psi = 0.$$

By making the change of variable

$$u = \left(\frac{2mF_0}{\hbar^2}\right)^{1/3}(a-x) \tag{15.22}$$

we can reduce the equation to

$$\frac{d^2\psi}{du^2} - u\psi(u) = 0, \tag{15.23}$$

which is the Airy equation.

Equation (15.23) has two linearly independent solutions, denoted $\mathrm{Ai}(u)$ and $\mathrm{Bi}(u)$. We are interested in the solution $\mathrm{Ai}(u)$, since this is the one that decays for $u > 0$, that is, for $x < a$. The function $\mathrm{Ai}(u)$ is defined by the following convergent improper integral

$$\mathrm{Ai}(u) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + ut\right)\, dt. \tag{15.24}$$

Intuitively, convergence is due to the very rapid oscillation of the integrand for large t, which produces a cancellation between the positive and negative values of the cosine function. Rigorously, convergence can be proved using integration by parts, as in Exercise 6. By differentiating under the integral sign (Exercise 7), one can show that Ai indeed satisfies the Airy equation (15.23).

As $|u|$ gets large, the integrand in (15.24) becomes more and more rapidly oscillating, producing more cancellation. The only exception to this behavior is when the derivative (with respect to t) of the function $t^3/3+ut$ is zero. Near such a point, the argument of the cosine function is changing slowly and there is little oscillation. If u is negative, there is a unique critical point of $t^3/3 + ut$, at $t = \sqrt{-u}$, and we expect that the main contribution to the integral in (15.24) will come from $t \approx \sqrt{-u}$. If u is positive, $t^3/3+ut$ has no critical points, and we expect that the integral in (15.24) will become quite small as u tends to $+\infty$. This sort of reasoning can be used to determine the precise asymptotics of the Airy function as u tends to $+\infty$ and as u tends to $-\infty$; see the discussion following (15.32) and (15.33).

We now state our main result, which will be derived in the remainder of this section. The result is not rigorous, because we have not estimated any of errors involved; such error estimates will be performed in Sect. 15.6.

Claim 15.7 *If ψ_1 is a solution of the Schrödinger equation (15.6) that tends to zero near $-\infty$, then ψ_1 can be normalized so that the following approximations hold*

$$\psi_1(x) \approx \frac{1}{2\sqrt{q(x)}} \exp\left\{-\frac{1}{\hbar}\int_x^a q(y)\, dy\right\} \quad (\textit{near } -\infty) \tag{15.25}$$

$$\psi_1(x) \approx \frac{\sqrt{\pi}}{(2mF_0\hbar)^{1/6}} \mathrm{Ai}\left(\left(\frac{2mF_0}{\hbar^2}\right)^{1/3}(a-x)\right) \quad (\textit{near } x = a) \tag{15.26}$$

$$\psi_1(x) \approx \frac{1}{\sqrt{p(x)}} \cos\left\{\frac{1}{\hbar}\int_a^x p(y)\, dy - \frac{\pi}{4}\right\} \quad (a < x < b). \tag{15.27}$$

Here $F_0 = -V'(a)$ and in the case of (15.27), x should not be too close to a or to b.

Similarly, if ψ_2 is a solution of the Schrödinger equation (15.6) that tends to zero near $+\infty$, then ψ_2 can be normalized so that the following approximations hold

$$\psi_2(x) \approx \frac{1}{\sqrt{p(x)}} \cos\left\{-\frac{1}{\hbar}\int_x^b p(y)\, dy + \frac{\pi}{4}\right\} \quad (a < x < b) \tag{15.28}$$

$$\psi_2(x) \approx \frac{\sqrt{\pi}}{(2mF_1\hbar)^{1/6}} \mathrm{Ai}\left(\left(\frac{2F_1 m}{\hbar^2}\right)^{1/3}(x-b)\right) \quad (\text{near } x = b) \tag{15.29}$$

$$\psi_2(x) \approx \frac{1}{2\sqrt{q(x)}} \exp\left\{-\frac{1}{\hbar}\int_b^x q(y)\, dy\right\} \quad (\text{near } +\infty). \tag{15.30}$$

Here $F_1 = V'(b)$ and in the case of (15.28), x should not be too close to a or to b.

The approximate formulas for ψ_1 and ψ_2 will agree, up to multiplication by a constant, in the classically allowed region if and only if we have

$$\frac{1}{\hbar}\int_a^b p(x)\, dx = \left(n + \frac{1}{2}\right)\pi \tag{15.31}$$

for some non-negative integer n.

More specifically, (15.27) and (15.28) are equal when the integer n in (15.31) is even and they are negatives of each other when n is odd. Note that there is a factor of 2 in the denominator in (15.25) but not in (15.27); this factor accounts for the expression $R = 2c_1$ in (15.21).

Since the classical energy curve consists of two "branches," of the form $(x, p(x))$ and $(x, -p(x))$, the compatibility condition (15.31) is equivalent to Condition 15.1. Since the phase of the approximate wave function in the classically allowed region is given by $1/\hbar$ times the integral of $p\, dx$, the condition (15.31) says that the wave function goes through *a little more than n half-cycles* between the two turning points, where a half-cycle corresponds to a change in the phase in the amount of π, or the interval between two critical points of the wave function. In particular, the wave function has exactly $n+1$ critical points inside the classically allowed region. The first and last critical points occur slightly inside the turning points, leaving a change in phase of roughly $\pi/4$ between the extreme critical point and the turning point.

Figure 15.4 considers the same potential as in Fig. 15.3. The figure shows the WKB functions (15.25) and (15.27), together with the scaled Airy function (15.26), near the turning point $x = a$. Note that there is a good match between the WKB functions and the scaled Airy function when x is close to, but not *too* close to, the turning point. Meanwhile, Fig. 15.5 then shows the full approximate wave function with $\hbar$ chosen so that (15.31) holds with $n = 39$, obtained by using the WKB functions away from the turning points and the scaled Airy functions near the turning points. Finally,

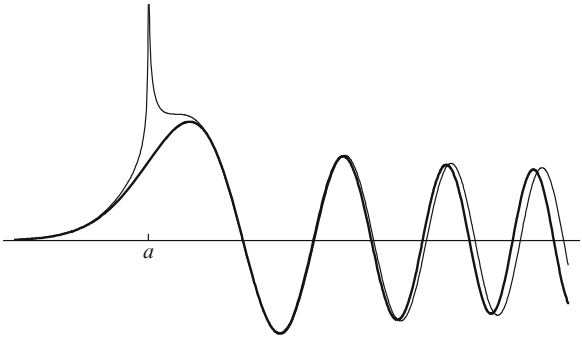

FIGURE 15.4. Plots of the scaled Airy function (*thick curve*) and the WKB functions, near the turning point $x = a$.

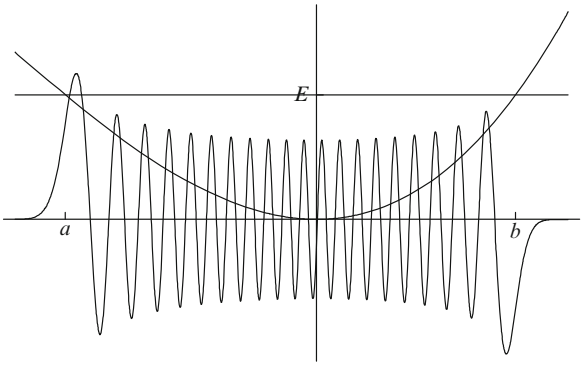

FIGURE 15.5. The approximate wave function with $n = 39$.

Fig. 15.6 shows the probability distribution associated to the approximate wave function, plotted together with the function $1/p(x)$. (Compare the discussion preceding Conclusion 15.5.)

We now derive the results in Claim 15.7. The Airy function $\mathrm{Ai}(u)$ is known to have the following asymptotic behavior:

$$\mathrm{Ai}(u) \approx \frac{1}{2\sqrt{\pi}u^{1/4}} \exp\left\{-\frac{2}{3}u^{3/2}\right\}, \quad u \to +\infty, \tag{15.32}$$

and

$$\mathrm{Ai}(u) \approx \frac{1}{\sqrt{\pi}(-u)^{1/4}} \cos\left(\frac{2}{3}(-u)^{3/2} - \frac{\pi}{4}\right), \quad u \to -\infty. \tag{15.33}$$

For u tending to $-\infty$, the asymptotics in (15.33) can be obtained by a straightforward application of the "method of stationary phase," as explained in Exercise 9. For u tending to $+\infty$, repeated integrations by parts (Exercise 8) show that $\mathrm{Ai}(u)$ decays faster than any power of u, which is all

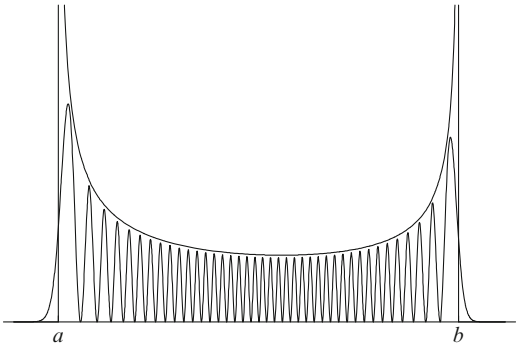

FIGURE 15.6. The probability distribution of the approximate wave function, plotted against the function $1/p(x)$.

that is strictly required for the main theorem of Sect. 15.6. To obtain the precise asymptotics in (15.32), one should deform the contour of integration to obtain a different integral representation of $\mathrm{Ai}(u)$, and then apply some variant of the method of stationary phase, such as Laplace's method or the method of steepest descent. See Sect. 4.7 of [30] for one approach to this analysis.

We will use the Airy function on an interval around the turning points with a length that goes to zero as $\hbar$ tends to zero (so that the linear approximation to the potential gets better and better) but with a length that is large compared to $\hbar^{2/3}$ (so that the value of u at the ends of the interval will be large, putting us into the asymptotic region of the Airy function). See Sect. 15.6 for more information.

We use the linear approximation $V(x) \approx (a-x)F_0$ to the potential near $x = a$, where $F_0 = -V'(a)$, which turns the Schrödinger equation (15.6) into the Airy equation, as previously noted. Now, the linear approximation to V yields

$$p \approx \sqrt{2mF_0}\sqrt{x-a} \tag{15.34}$$

and

$$\frac{1}{\hbar}\int_a^x p(y)\,dy \approx \frac{\sqrt{2mF_0}}{\hbar}\frac{(x-a)^{3/2}}{3/2} = \frac{2}{3}(-u)^{3/2}. \tag{15.35}$$

From here it is a simple matter to check, using (15.33), that

$$\frac{\sqrt{\pi}}{(2mF_0\hbar)^{1/6}}\mathrm{Ai}(u) \approx \frac{1}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_a^x p(y)\,dy - \frac{\pi}{4}\right)$$

for $x > a$, where the approximation holds in an intermediate region where x is close to a but not *too* close to a. Thus, if we scale our solution ψ_1 to the Schrödinger equation so that it is approximated by $\pi^{1/2}(2mF_0\hbar)^{-1/6}$ times $\mathrm{Ai}(u)$ near $x = a$, it should satisfy (15.27) in the classically allowed

region (but away from the turning points). It is then straightforward to verify, using (15.32), that this multiple of $\mathrm{Ai}(u)$ satisfies (15.25) for x near $-\infty$. The analysis of ψ_2 is entirely similar.

Finally, to compare the approximations (15.27) and (15.28), we note that

$$-\frac{1}{\hbar}\int_x^b p(y)\,dy + \frac{\pi}{4} = \left(\int_a^x p(y)\,dy - \frac{\pi}{4}\right) - \phi,$$

where

$$\phi = \frac{1}{\hbar}\int_a^b p(y)\,dy - \pi/2.$$

Now, if ϕ is an odd multiple of π, then $\cos(\theta-\phi) = -\cos\theta$ and if ϕ is an even multiple of π, then $\cos(\theta-\phi) = \cos\theta$. For all other values of ϕ (Exercise 4), $\cos(\theta-\phi)$ is not a constant multiple of $\cos\theta$. Thus, (15.31) is a necessary and sufficient condition for the two approximate solutions to agree up to a constant in the classically allowed region.

15.6 A Rigorous Error Estimate

The preceding sections give a treatment of the WKB approximation that is typical of many books in the literature. This treatment gives the idea that energies E satisfying the corrected Bohr–Sommerfeld Condition (Condition 15.1) should be approximate eigenvalues for the Hamiltonian operator $\hat{H}$, without specifying the sense in which this approximation holds. In this section, we prove a rigorous estimate, as follows.

Theorem 15.8 *For any potential V and range $[E_1, E_2]$ of energies satisfying Assumption 15.3, there is a constant C such that the following holds. For any energy $E \in [E_1, E_2]$ satisfying Condition 15.1, there exists a nonzero function ψ belonging to* $\mathrm{Dom}(\hat{H})$ *such that*

$$\|\hat{H}\psi - E\psi\| < C\hbar^{9/8}\,\|\psi\|\,. \tag{15.36}$$

As noted already in Sect. 15.3, an estimate of the form $\|\hat{H}\psi - E\psi\| < \varepsilon\|\psi\|$ implies that there is a point $\tilde{E}$ in the spectrum of $\hat{H}$ with $|E-\tilde{E}| < \varepsilon$. (See Exercise 4 in Chap. 10.) Since, under our assumptions on V, the spectrum of $\hat{H}$ is purely discrete, we conclude that for each number $E \in [E_1, E_2]$ satisfying Condition 15.1, there is an actual eigenvalue $\tilde{E}$ for $\hat{H}$ with

$$|E - \tilde{E}| < C\hbar^{9/8}. \tag{15.37}$$

If E satisfies Condition 15.1, then the estimate (15.37) actually holds with $\hbar^{9/8}$ replaced by $\hbar^2$ on the right-hand side. It is not, however, possible to obtain such an optimal estimate by the methods we are using

in this chapter. Specifically, the approximate eigenvector ψ constructed in the proof of Theorem 15.8 *does not* satisfy an estimate of the form $\|\hat{H}\psi - E\psi\| < C\hbar^2$. One can, however, construct an approximate eigenvector by different methods—for example, the method in [31]—that satisfies an order-$\hbar^2$ error estimate, for any E satisfying the corrected Condition 15.1. Nevertheless, the error bound in (15.37) is small compared to the typical spacing between the energy levels, which is of order $\hbar$.

Recall, as we noted at the beginning of Sect. 15.4, that a Schrödinger operator with potential V that is smooth and tends to $+\infty$ at $\pm\infty$ is essentially self-adjoint on $C_c^\infty(\mathbb{R})$. The operator $\hat{H}$ in Theorem 15.8 is, more precisely, the unique self-adjoint extension of the Schrödinger operator defined on $C_c^\infty(\mathbb{R})$.

15.6.1 Preliminaries

Our construction of the approximate eigenfunction ψ will be essentially by the WKB approximation as outlined in Claim 15.7. That is to say, we will define ψ using scaled Airy functions near the turning points and by the standard WKB functions in the classically allowed and classically forbidden regions. There is, however, a difficulty with this approach, which is that at the boundary between different regions, the scaled Airy function does not *exactly* match the WKB functions, but only approximately. What this means is that if we define ψ by the WKB formula in, say, an interval of the form $(-\infty, a-\varepsilon)$ and we define ψ by a scaled Airy function on $(a-\varepsilon, a+\varepsilon)$, then ψ may be discontinuous at $a-\varepsilon$. Even if we scale ψ by a constant on one of these intervals to eliminate the discontinuity in ψ itself, the derivative of ψ will still probably be discontinuous. But if the derivative of ψ is discontinuous, ψ is not actually in the domain of $\hat{H}$, and the left-hand side of (15.36) does not make sense. (Compare Sect. 5.2.)

The condition that ψ' be continuous is not just a technicality: If we did not worry about continuity of ψ', then we could *always* match the scaled Airy function to the WKB functions, just by multiplying the various functions by constants, regardless of whether or not the energy satisfies the corrected Bohr–Sommerfeld Condition. In that case, we would be claiming that *any* number $E \in [E_1, E_2]$ is within $C\hbar^{9/8}$ of an eigenvalue of $\hat{H}$, which is false already for the harmonic oscillator.

To work around the difficulty described in the previous paragraphs, we must put in a transition region over which we smoothly pass from one function to the other, using the "join" construction described in Sect. 15.6.4. Thus, we define the function ψ in Theorem 15.8 as follows. We use the formulas in Claim 15.7 in the indicated intervals, except that multiply the functions (15.28), (15.29), and (15.30) by -1 when n is odd. We use the scaled Airy functions (15.26) and (15.29) on intervals of the form $(a-\varepsilon, a+\varepsilon)$ and $(b-\varepsilon, b+\varepsilon)$, respectively, for some ε depending on $\hbar$ in a manner to be determined later. We then put in four transition regions, each

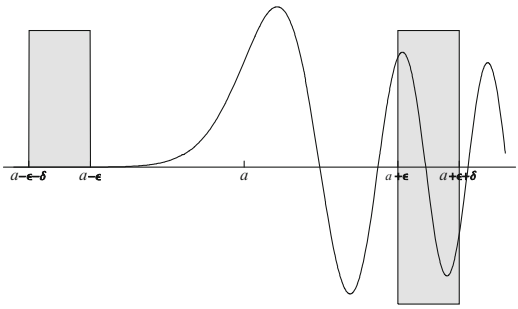

FIGURE 15.7. The approximate eigenfunction ψ, with the transition regions shaded.

having length δ, where δ also depends on $\hbar$ in a manner to be determined later. The first transition region, for example, is the interval $(a-\varepsilon-\delta, a-\varepsilon)$ between the first classically forbidden region and the first turning point. In each transition region, we change over smoothly from one function to another. See Fig. 15.7 for an illustration of the transition regions around the turning point $x = a$.

Suppose $\hat{H}_0$ denotes the Schrödinger operator with potential V, with domain equal to $C_c^\infty(\mathbb{R})$. Then, as we have noted, $\hat{H}_0$ is essentially self-adjoint, and we are letting $\hat{H}$, which coincides with the adjoint operator $\hat{H}_0^*$, denote the unique self-adjoint extension of $\hat{H}_0$. Now, the domain of $\hat{H}_0^*$ consists of all functions $\psi \in L^2(\mathbb{R})$ such that the Schrödinger operator, computed in the distributional sense, again belongs to $L^2(\mathbb{R})$. In particular, if ψ is smooth, then ψ belongs to the domain of $\hat{H} = \hat{H}_0^*$ if and only if ψ is in $L^2(\mathbb{R})$ and $-(\hbar^2/2m)\psi'' + V\psi$ is also in $L^2(\mathbb{R})$.

Because of the joins, our approximate eigenfunction is ψ actually infinitely differentiable on all of $\mathbb{R}$. And since $V(x)$ tends to $+\infty$ at $\pm\infty$, the exponential WKB functions (15.25) and (15.30) have rapid decay at infinity, which shows that ψ is in $L^2(\mathbb{R})$. Furthermore, for x near $\pm\infty$, the calculation (15.17) applies, with $A(x) = Cq(x)^{-1/2}$. We obtain, after a short calculation,

$$\begin{aligned} &-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) \\ &= -\frac{\hbar^2}{2m}\left(\frac{5}{16}\left(\frac{V'(x)}{V(x)-E}\right)^2 - \frac{1}{4}\frac{V''(x)}{V(x)-E}\right)\psi(x). \end{aligned} \tag{15.38}$$

Since V'/V and V''/V are assumed to be bounded near infinity and $\psi(x)$ tends to $+\infty$ at $\pm\infty$, we see that the Schrödinger operator applied to ψ is bounded by a constant times ψ near infinity and is thus square integrable. This shows that ψ is in the domain $\hat{H}$.

In Sect. 15.6.2, we will take the width 2ε of the region around the turning points to be of order $\hbar^{1/2}$. In that case, the L^2 norm of our approximate

wave function is of order 1 (bounded and bounded away from zero) as $\hbar$ tends to zero, despite the blow-up of order $\hbar^{-1/6}$ very near the turning points. Although this result is not hard to verify (Exercise 10), if anything, the norm would be blowing up as $\hbar$ tends to zero, which would only help us in showing that $\|\hat{H}\psi - E\psi\|$ is small compared to $\|\psi\|$.

To prove Theorem 15.8, we must estimate the contributions to the quantity $\|\hat{H}\psi - E\psi\|$ from four different types of regions: the classically allowed region, the classically forbidden regions, the regions near the turning points, and the transition regions. These estimates will occupy the remainder of this section, with the analysis in the transition regions being the most involved. In particular, it is essential that the derivative of scaled Airy function *almost* match the derivative of the WKB function in the transition region, as in the second part of Lemma 15.9.

15.6.2 The Regions Near the Turning Points

We use a scaled Airy function in an interval around each turning point. [We use (15.26) near $x = a$ and either (15.29) or the negative thereof near $x = b$, depending on whether n is even or odd.] We now verify that taking these intervals to have length of order $\hbar^{1/2}$ will give satisfactory estimates. If ψ denotes one of the scaled Airy functions, then ψ satisfies a Schrödinger equation in which the potential V is replaced by a linear approximation $\tilde{V}$ near one of the turning points, which means that

$$\hat{H}\psi - E\psi = (V(x) - \tilde{V}(x))\psi. \tag{15.39}$$

The difference between $V(x)$ and its linear approximation $\tilde{V}(x)$ grows at most quadratically with the distance from the turning point. Meanwhile, the asymptotics of the Airy function tell us that it can be bounded as $|\mathrm{Ai}(u)| \leq Cu^{-1/4}$. (This is terrible estimate for small u, but still true.) Now u, as defined in (15.22), is of order $\hbar^{-2/3}$ times the distance to the turning point. Since, also, there is factor of $\hbar^{-1/6}$ in (15.26) and the distance from the turning point is at most of order $\hbar^{1/2}$, we find that

$$|\hat{H}\psi - E\psi| \leq C(\hbar^{1/2})^2\hbar^{-1/6}(\hbar^{-2/3}\hbar^{1/2})^{-1/4} = C\hbar^{7/8}$$

over the interval around each turning point. Finally, if a function f satisfies $|f| \leq D$ on an interval of length L, then the L^2 norm of f over that interval will be at most $D\sqrt{L}$. Thus, over the interval around the turning points,

$$||\hat{H}\psi - E\psi|| \ = O(\hbar^{7/8}\hbar^{1/4}) = O(\hbar^{9/8}).$$

15.6.3 The Classically Allowed and Classically Forbidden Regions

The expression (15.38) for $\hat{H}\psi - E\psi$, derived from (15.17), applies both in the classically allowed region and in the classically forbidden regions. Let us

consider first the classically allowed region. Although (15.38) is nominally of order $\hbar^2$, we use this expression on an interval whose ends get closer and closer to the turning point as $\hbar$ tends to zero. Since, also, the expression in (15.38) is blowing up at the turning points, the contribution to $\|\hat{H}\psi - E\psi\|$ from this interval is of order larger than $\hbar^2$.

We have taken the interval around the turning point to have length 2ε that is of order $\hbar^{1/2}$, and we will also take (Sect. 15.6.4) the transition regions to have length δ that is of order $\hbar^{1/2}$. Thus, we use the oscillatory WKB function on an interval of the form $(a+\gamma, b-\gamma)$, where $\gamma = \varepsilon + \delta$ is of order $\hbar^{1/2}$. Now, the formula for ψ in the classically allowed regions has a factor of $1/\sqrt{p(x)}$ times a bounded quantity (the cosine factor). Since $V'(a)$ is assumed to be nonzero, $V(x) - E$ behaves like a constant times $(x-a)$ and so $1/\sqrt{p(x)}$ behaves like a constant time $(x-a)^{-1/4}$ for x approaching a, with similar behavior near the other turning point.

Meanwhile, the more problematic term in (15.38) is the term having $(V(x)-E)^2$ in the denominator. Keeping in mind the $1/\sqrt{p}$ blowup of ψ itself, this term behaves like $(x-a)^{-9/4}$ as x approaches a. Thus, we may estimate the norm of $\hat{H}\psi - E\psi$ over the left half of the classically allowed region as

$$\begin{aligned} ||\hat{H}\psi - E\psi|| &\leq C\hbar^2 \left(\int_{(a+b)/2}^{a+\gamma} (x-a)^{-9/2}\, dx \right)^{1/2} \\ &= C'\hbar^2 (\gamma^{-7/2} - ((a+b)/2)^{7/2})^{1/2}. \end{aligned}$$

Since γ is of order $\hbar^{1/2}$, the contribution to $\|\hat{H}\psi - E\psi\|$ from the interval $(a+\gamma, (a+b)/2)$ will consist of a term of order $\hbar^2\hbar^{-7/8} = \hbar^{9/8}$, plus lower-order terms. The estimate over the other half of the classically allowed region is similar.

Meanwhile, in the first classically forbidden region, we also apply (15.38). By Assumption 15.3, V'/V and V''/V are bounded near infinity. Thus, $V'/(V-E)$ and $V''/(V-E)$ will also be bounded near infinity, and thus also bounded on $(-\infty, a-1)$, since $V-E$ is strictly positive on this interval and tends to $+\infty$ as x tends to $-\infty$. We see, then, that the norm of $\hat{H}\psi - E\psi$ over $(-\infty, a-1)$ is bounded by a constant times $\hbar^2 \|\psi\|$.

The norm of $\hat{H}\psi - E\psi$ over an interval of the form $(a-1, a-\gamma)$ can be analyzed similarly to the classically allowed region. The estimates from this region are better, however, because of the exponentially decaying factor in the definition of the WKB function. Thus, the contribution to $\|\hat{H}\psi - E\psi\|$ from the classically forbidden region $(-\infty, a-\gamma)$ is certainly no larger than order $\hbar^{9/8}$, and similarly for the other classically forbidden region.

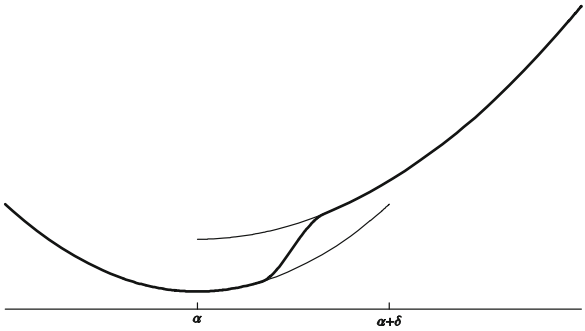

FIGURE 15.8. The join of two functions over the interval $[\alpha, \alpha+\delta]$ (*thick curve*).

15.6.4 The Transition Regions

Given two smooth functions ψ_1 and ψ_2 and some interval of the form $[\alpha, \alpha+\delta]$, we now define a "join" $\psi_1 \sqcup \psi_2$ of ψ_1 and ψ_2, where $\psi_1 \sqcup \psi_2(x)$ is equal to $\psi_1(x)$ for $x < \alpha$ and equal to $\psi_2(x)$ for $x > \alpha + \delta$, and where $\psi_1 \sqcup \psi_2$ is smooth everywhere. Let χ be a smooth function on $[0,1]$ that is identically equal to 0 in a neighborhood of 0 and identically equal to 1 in a neighborhood of 1. Then define $\psi_1 \sqcup \psi_2$ by

$$(\psi_1 \sqcup \psi_2)(x) = \psi_1(x) + (\psi_2(x) - \psi_1(x))\chi((x-\alpha)/\delta).$$

(See Fig. 15.8.) By direct calculation, we have

$$\begin{aligned}(\hat{H} - EI)(\psi_1 \sqcup \psi_2) = (\hat{H}\psi_1 - E\psi_1) \sqcup (\hat{H}\psi_2 - E\psi_2) \\ - \frac{1}{\delta}\frac{\hbar^2}{m}(\psi_2'(x) - \psi_1'(x))\chi'((x-a)/\delta) \\ - \frac{1}{\delta^2}\frac{\hbar^2}{2m}(\psi_2(x) - \psi_1(x))\chi''((x-a)/\delta). \qquad (15.40)\end{aligned}$$

In our constructing our approximate eigenfunction, we use five different formulas in five different regions: the two classically forbidden regions, the classically allowed region, and the regions near the two turning points. Since none of these functions exactly matches the function in the next interval, we put in a total of four joins in order to produce a function that is in the domain of $\hat{H}$. We choose the width δ of the interval on which the join takes place to be of the same size as the intervals around the turning points, namely, order $\hbar^{1/2}$.

The most critical case is the transition from the region near the turning points to the classically allowed region. Consider, for example, the scaled Airy function ψ_1 in (15.26) and the oscillatory WKB function ψ_2 in (15.27). There are two contributions to the mismatch between these two functions. First, there is a discrepancy between the Airy function and its leading-order asymptotics. Second, there is an error in the approximations (15.34)

and (15.35), which come from the discrepancy between the potential $V(x)$ and its linear approximation $\tilde{V}(x)$ near $x = a$. We need to consider both contributions to the mismatch in our estimation of $\psi_1 - \psi_2$ and of $\psi_1' - \psi_2'$.

Lemma 15.9 *Let ψ_1 denote the scaled Airy function in (15.26), let $\tilde{\psi}_1$ denote the same function with the Airy function replaced by the right-hand side of (15.33), and let ψ_2 denote the oscillatory WKB function in (15.27). If $x - a$ is positive and of order $\hbar^{1/2}$, we have*

$$|\psi_1(x) - \tilde{\psi}_1(x)| = O(\hbar^{1/8})$$
$$|\tilde{\psi}_1(x) - \psi_2(x)| = O(\hbar^{1/8})$$

and

$$|\psi_1'(x) - \tilde{\psi}_1'(x)| = O(\hbar^{-5/8})$$
$$|\tilde{\psi}_1'(x) - \psi_2(x)| = O(\hbar^{-5/8}).$$

Before giving the proof of this lemma, let us verify that these estimates are sufficient to control the contribution to $\|\hat{H}\psi - E\psi\|$ from the transition region $(a + \varepsilon, a + \varepsilon + \delta)$ between the first turning point and the classically allowed region, where both ε and δ are taken to be of order $\hbar^{1/2}$. We must consider each of the three lines in (15.40). The L^2 norm of the first line is of order at most $\hbar^{9/8}$, by precisely the same argument as in Sect. 15.6.3.

For the second and third lines, we recall that if a function f is bounded by C, then the L^2 norm of f over an interval of length L is at most $C\sqrt{L}$. Since we are taking the length δ of our transition interval to be of order $\hbar^{1/2}$, the L^2 norm of the second line of (15.40) is of order

$$\frac{1}{\hbar^{1/2}} \hbar^2 \hbar^{-5/8} \hbar^{1/4} = \hbar^{9/8}.$$

Meanwhile, the contribution from the third line of (15.40) is of order

$$\frac{1}{\hbar} \hbar^2 \hbar^{1/8} \hbar^{1/4} = \hbar^{11/8}.$$

Thus, the contribution to $\|\hat{H}\psi - E\psi\|$ from the transition region $(a+\varepsilon, a+\varepsilon+\delta)$ is of order at most $\hbar^{9/8}$.

The analysis of the transition between the classically allowed region and the region around $x = b$ is entirely similar. The analysis of the transitions between the regions near the turning points and the classically forbidden regions is also similar, but much less delicate, because all of the functions involved are very small in the transition region. When $(a - x)$ is positive and of order $\hbar^{1/2}$, for example, u, as defined in (15.22) will be of order $\hbar^{-1/6}$ and so $u^{3/2}$ is of order $\hbar^{-1/4}$. Thus, the exponential factor in leading-order asymptotics of the Airy function for $u > 0$ will behave like $\exp(-C\hbar^{-1/4})$, which is very small for small $\hbar$, certainly smaller than any power of $\hbar$. Since

all the factors in front of the exponential will behave like $\hbar$ to a power, the overall contribution to $\|\hat{H}\psi - E\psi\|$ from the transition between the region near the turning points and the classically forbidden region is smaller than any power of $\hbar$. Thus, none of the transition regions contributes an error worse that $O(\hbar^{9/8})$.

Proof of Lemma 15.9. We consider only the estimates for the derivatives of the functions involved. The analysis of the functions themselves is similar (but easier) and is left as an exercise to the reader (Exercise 11).

We begin by considering $\psi_1' - \tilde{\psi}_1'$. With a little algebra, we compute that

$$\frac{d\psi_1}{dx} - \frac{d\tilde{\psi}_1'}{dx} = -\sqrt{\pi}(2mF_0)^{1/6}\hbar^{-5/6}(\mathrm{Ai}'(u) - \widetilde{\mathrm{Ai}}'(u)) \tag{15.41}$$

where u is as in (15.22) and where $\widetilde{\mathrm{Ai}}$ is the function on the right-hand side of (15.33).

Now, $\mathrm{Ai}(u)$ has an asymptotic expansion for $u \to -\infty$ given by

$$\mathrm{Ai}(u) = \widetilde{\mathrm{Ai}}(u)(1 + Cu^{-3/2} + \cdots),$$

and $\mathrm{Ai}'(u)$ has the asymptotic expansion obtained by formally differentiating this with respect to u. [See Eq. (7.64) in [30].] From this, we obtain

$$\mathrm{Ai}'(u) - \widetilde{\mathrm{Ai}}'(u) = \widetilde{\mathrm{Ai}}'(u)O((-u)^{-3/2}) + \widetilde{\mathrm{Ai}}(u)O((-u)^{-5/2}). \tag{15.42}$$

From the explicit formula for $\widetilde{\mathrm{Ai}}$, we see that $\widetilde{\mathrm{Ai}}(u)$ is of order $(-u)^{-1/4}$. Meanwhile, the formula $\widetilde{\mathrm{Ai}}'(u)$ will contain two terms, the larger of which will be of order $u^{1/4}$. Thus, the slower-decaying term on the right-hand side of (15.42) is the first one, which is of order $(-u)^{-5/4}$. Now, in the transition regions, u behaves like $\hbar^{-2/3}\hbar^{1/2} = \hbar^{-1/6}$. Thus, (15.42) goes like $\hbar^{5/24}$ and so (15.41) goes like $\hbar^{-5/6+5/24} = \hbar^{-5/8}$, as claimed.

We now consider $\tilde{\psi}_1' - \psi_2'$. By direct calculation, the derivatives of $\tilde{\psi}_1$ and ψ_2 each consist of two terms, a "dominant" obtained by differentiating the cosine factor and a "subdominant" term obtained by differentiating the coefficient of the cosine factor. In the case of $\tilde{\psi}_1'$, the dominant term in the derivative may be simplified to

$$-\frac{1}{\hbar}((2mF_0)(x-a))^{1/4}\sin\left(\frac{2}{3}(-u)^{3/2} - \frac{\pi}{4}\right). \tag{15.43}$$

According to Exercise 12, we have, when $x - a$ is of order $\hbar^{1/2}$, the estimates

$$((2mF_0)(a-x))^{1/4} = \sqrt{p} + \sqrt{p}O(\hbar^{1/2}) \tag{15.44}$$

and

$$\frac{2}{3}(-u)^{3/2} = \frac{1}{\hbar}\int_a^x p(y)\, dy + O(\hbar^{1/4}). \tag{15.45}$$

Since the derivative of $\sin\theta$ is bounded, a change of order $\hbar^{1/4}$ in the argument of a sine function produces a change of order $\hbar^{1/4}$ in the value of the sine. Thus, if we substitute (15.44) and (15.45) into (15.43), we find that the difference between the dominant term in $\tilde{\psi}_1'$ and the dominant term in ψ_1' is

$$\frac{1}{\hbar}\sqrt{p}O(\hbar^{1/4}) + \text{lower-order terms.}$$

Since $\sqrt{p}$ is of order $(x-a)^{1/4}$ or $\hbar^{1/8}$, we get an error of order $\hbar^{-5/8}$, as claimed.

Finally, the subdominant terms in the derivatives of $\tilde{\psi}_1$ and ψ_2 are easily seen to be separately of order $\hbar^{-5/8}$. Thus, even without taking into account the cancellation between these terms, they do not change the order of the estimate. ■

15.6.5 Proof of the Main Theorem

We have estimated the contributions to $\|\hat{H}\psi - E\psi\|$ from each type of region: classically allowed and classically forbidden regions, the regions around the turning points, and the transition regions. In each case, we have found a contribution that is of order at most $\hbar^{9/8}\|\psi\|$. Thus, it remains only to verify that the constants in all estimates are bounded uniformly over the given range $E_1 \leq E \leq E_2$ of energies.

This verification is straightforward. Near the turning point $x = a$, for example, we need to estimate the difference between the potential $V(x)$ and its linear approximation $\tilde{V}(x)$ near $x = a$. As a consequence of the Taylor remainder formula, $|V(x) - \tilde{V}(x)|$ will be bounded by $C|x-a|^2/2$, where C is the maximum of $|V''(x)|$ over the interval from a to x. As E varies over $[E_1, E_2]$, the set of points where we have to evaluate $|V''(x)|$ will be bounded, meaning that C can be taken to be independent of E, for E in such a range.

Similarly, in the classically allowed region, the blow-up of $1/(V(x)-E)^2$ near $x = a(E)$ can be controlled by the minimum of $|V'(y)|$ for y between a and x. By assumption, $|V'(x)| > 0$ at all the turning points $a(E)$ and $b(E)$ with $E_1 \leq E \leq E_2$, and thus, by continuity, in some neighborhood of that set of turning points. Thus, blow-up of $1/(V(x)-E)^2$ will be controlled by the minimum of $|V'(x)|$ on an interval of the form $[a(E_2)+\alpha, a(E_1)+\alpha]$ for some small $\alpha > 0$. The remaining details of this verification are left to the reader.

15.7 Other Approaches

The main complicating factor in the WKB approximation is the singular behavior near the turning points. The turning points, meanwhile, are only problematic because we are working in the position representation. The

turning points, after all, are the points on the classical trajectory where the *position* of the particle achieves a maximum or a minimum. If we were to work in the momentum representation, the points where the *momentum* achieves a maximum or a minimum would instead be the problematic points. A. Voros [42] has proposed working in the Segal–Bargmann representation (Sect. 14.4). In Voros's analysis, there are no turning points and, thus, the analysis is much simpler. The problem with Voros's approach is that he only gives an approximation to the wave function on the classical energy curve. Even in simple cases, Voros's expression does not admit a holomorphic extension to the whole plane, but has branching behavior inside the classical energy curve. Thus, Voros's formula does not define an element of the quantum Hilbert space (which is a space of *entire* holomorphic functions), let alone an element of the domain of the Hamiltonian.

Nevertheless, it is possible to build approximate eigenfunctions as superpositions of coherent states, using formulas similar to those in Voros. This approach avoids dealing with turning points but still yields a rigorous eigenvalue estimate, with the same corrected Bohr–Sommerfeld condition as in Condition 15.1. See [31, 23, 7], or (in greater generality) [26].

15.8 Exercises

1. Show that if c_1 is any complex number, then we have an identity of the form
$$c_1 e^{i\theta} + \overline{c_1} e^{-i\theta} = R\cos(\theta - \delta)$$
for some real numbers R and δ.

2. Let $H(x,p) = p^2/2m + m\omega^2 x^2/2$ be the Hamiltonian for a harmonic oscillator having mass m and classical frequency ω. Show that a positive number E satisfies the corrected Bohr–Sommerfeld condition (Condition 15.1) if and only if E is of the form $(n+1/2)\hbar\omega$, where n is a non-negative integer.

   Note: In light of the results of Chap. 11, this calculation means that, in this very special case, the corrected Bohr–Sommerfeld condition gives the *exact* eigenvalues of the quantum Hamiltonian $\hat{H}$.

3. Suppose A and p are two nonzero, smooth functions satisfying (15.15). Show that $A(x) = C(p(x))^{-1/2}$ for some constant C.

   Hint: Think in terms of the logarithms of the functions involved.

4. Show that $\cos(\theta - \delta)$, viewed as a function of θ, agrees, up to multiplication by a constant, with $\cos(\theta - \delta')$ if and only if $\delta - \delta'$ is an integer multiple of π.

5. If ψ is an eigenvector for $\hat{H}$ that is approximated by (15.25) near $-\infty$, one might hope to find an approximate expression for ψ in the classically allowed region by analytically continuing around the turning point in the complex plane. Even assuming V is analytic, however, it is fairly evident that analytic continuation in the upper half-plane does not give the same answer as in the lower half-planes. Nevertheless, one could use the average of the upper and lower half-plane results as a (totally nonrigorous) guess for the behavior of ψ in the classically allowed region.

   Show that the above approach gives the correct phase δ in the connection formula (15.21) but is off by a factor of 2 in the amplitude R.

6. Using integration by parts, show that the limit

$$\lim_{A\to+\infty} \int_0^A \cos\left(\frac{t^3}{3} + ut\right)\, dt$$

   exists.

   Hint: Multiply and divide by $t^2 + u$ (avoiding points where $t^2 + u = 0$ in the case $u < 0$).

7. In this exercise, we sketch an argument that the Airy function in (15.24) satisfies the differential equation $\psi''(u) - u\psi(u) = 0$. For the purposes of this exercise, let us say that $\int_0^\infty f(t)\, dt = C$ if $\int_0^A f(t)\, dt = C + g(A)$, where the function g is bounded and oscillates around an average value of zero.

   Assuming that it is legal to differentiate under the integral sign, verify that $\mathrm{Ai}(u)$ satisfies the stated equation.

   Hint: After differentiating under the integral, look for a term that can be integrated explicitly.

   Note: A more rigorous approach to this verification would be to integrate by parts as in Exercise 6 and *then* differentiate under the integral. This approach is, however, a bit messier.

8. By integrating by parts repeatedly in (15.24), show that $\mathrm{Ai}(u)$ decays faster than any power of u as u tends to $+\infty$.

   Hint: A key point is to show that the boundary terms in the integration by parts vanish at every stage. After performing the integrations by parts, estimate the resulting integral by using the inequality

$$\frac{1}{(t^2+u)^n} < \frac{1}{(t^2+1)^k}\frac{1}{u^{n-k}}, \quad u > 1,$$

   for some appropriate choice of k.

9. (a) For $u < 0$, make the change-of-variable $\tau = t/\sqrt{-u}$ in the integral formula for the Airy function, to obtain the expression

$$\mathrm{Ai}(u) = \frac{\sqrt{-u}}{\pi} \int_0^\infty \cos\left(\alpha\left(\frac{\tau^3}{3} - \tau\right)\right)\, d\tau, \tag{15.46}$$

where $\alpha = (-u)^{3/2}$.

(b) Suppose f is a smooth function on $[a, b]$ having a unique critical point x_0. Assuming that x_0 is in the interior of $[a, b]$ and that $f''(x_0) \neq 0$, the method of stationary phase asserts that

$$\int_a^b g(x) e^{i\alpha f(x)}\, dx = g(x_0) e^{i\alpha f(x_0)} e^{\pm i\pi/4} \sqrt{\frac{2\pi}{\alpha\, |f''(x_0)|}} + O\left(\frac{1}{\alpha}\right)$$

for α tending to $+\infty$, where the plus sign in the exponent is taken when $f''(x_0) > 0$ and the minus sign is taken when $f''(x_0) < 0$. (See, e.g., Eq. (5.12) in [30].)

Using this result, obtain the asymptotic formula (15.33).

Hint: Divide the integral in (15.46) into an integral over $[0, 2]$ and an integral over $[2, \infty)$. Use stationary phase for the first interval and integration by parts (as in Exercise 6) for the second interval.

10. Let ψ be the approximate eigenfunction for $\hat{H}$ defined in the beginning of Sect. 15.6. Show that the norm of ψ is bounded and bounded away from zero as $\hbar$ tends to zero.

Hint: First show that the L^2 norm of ψ over the intervals around the turning points goes like $\hbar^{-1/6}\hbar^{1/4}$. Then check that the functions $p(x)^{-1/2}$ and $q(x)^{-1/2}$ are square integrable near the turning points.

11. By imitating the arguments in the proof of Lemma 15.9, prove the estimates for $\psi_1 - \tilde{\psi}_1$ and $\tilde{\psi}_1 - \psi_2$ in the lemma.

12. By writing $V(x)$ as $F_0(a-x)$ plus an error term of order $(x-a)^2$, verify that the estimates (15.44) and (15.45) in the proof of Lemma 15.9 hold in the transition region. (Assume that $x - a$ is of order $\hbar^{1/2}$ in the transition region.)

Hint: The leading-order Taylor expansion of $(1+z)^a$ is $1+az+O(z^2)$, for any real number a.