The WKB method is important both as a practical means of approximating solutions to the Schrödinger equation, and also as a conceptual framework for understanding the classical limit of quantum mechanics. The WKB approximation is valid whenever the wavelength $\lambda$ is small in comparison to an appropriate scale length $L$ of the system,

$$\lambda \ll L. \quad (4.1)$$

This condition is not restricted to quantum mechanics, but rather can be applied to any wave system (water waves, electromagnetic waves, etc.), where it leads to approximation schemes which are mathematically very similar to the WKB method in quantum mechanics. For example, in optics the method is called the “eikonal method,” and in general the method is referred to as “short wave-length asymptotics.” By whatever name, the method is an old one, which antedates quantum mechanics (it was apparently first used by Liouville and Green in the first half of the nineteenth century). In the 1920’s the method was applied to quantum mechanics by Wentzel, Kramers and Brillouin, whose names give the initials WKB. In quantum mechanics, $\lambda$ is interpreted as the de Broglie wavelength, and $L$ is normally the scale length of the potential energy. Thus, the WKB method is valid if the wavefunction oscillates many times before the potential energy changes significantly.

To motivate the WKB method, let us consider a one-dimensional problem with potential energy $V(x)$. The Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \quad (4.2)$$

First we take the case $V = \text{const}$, and assume $E > V$. Then a solution of the Schrödinger equation is

$$\psi(x) = Ae^{ipx/\hbar}, \quad (4.3)$$

where $A$ is the constant amplitude and where

$$p = \hbar k = \sqrt{2m(E - V)}. \quad (4.4)$$

This is for a wave travelling to the right; the wave travelling to the left has momentum $-p$. The momentum $p$ is related to the de Broglie wavelength by

$$\lambda = \frac{2\pi}{k} = \frac{2\pi \hbar}{p}. \quad (4.5)$$
If $V(x)$ is not constant but slowly varying on the scale of a wavelength, then it is reasonable that over distances on the order of a few wavelengths, the solution will still look like the wave function in a constant potential, but presumably with a slowly varying momentum and wavelength. That is, $p$ and $\lambda$ become functions of $x$,

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

and

$$\lambda = \lambda(x) = \frac{2\pi\hbar}{p(x)}$$

According to these formulas, both $p$ and $\lambda$ vary on the scale length of the potential $V$, which by assumption is large in comparison to the wavelength. We also expect the amplitude $A$ to vary on the scale length of the potential, since if $V$ is constant, then so is $A$. These expectations are borne out in various exact solutions of one dimensional problems, such as the harmonic oscillator solutions illustrated in Figs. 4.1 and 4.2.

![Fig. 4.1. Normalized harmonic oscillator eigenfunction for $n = 20$. Distance $x$ is measured in units of $(\hbar/m\omega)^{1/2}$.](image1)

![Fig. 4.2. Same as Fig. 4.1, except $n = 40$.](image2)

The phase of the wave advances by $2\pi$ every wavelength, and so is not slowly varying on the scale of a wavelength. Furthermore, since the wavelength is not constant but varies by a small amount from one oscillation to the next, the accumulated phase over some interval in $x$ must be obtained by integration. We can obtain a differential equation for the phase
\( \phi \) of the wave by noting that \( \Delta \phi = 2\pi \) when \( \Delta x = \lambda = \lambda(x) \), or, approximating \( \Delta \phi / \Delta x \) by a derivative,

\[
\frac{d\phi}{dx} = \frac{2\pi}{\lambda(x)} = \frac{p(x)}{\hbar}.
\]  

(4.8)

Thus, we have

\[
\phi(x) = \frac{1}{\hbar} \int_{x_0}^{x} p(x') \, dx',
\]  

(4.9)

where \( x_0 \) is some lower limit where the phase is taken to vanish. The quantity \( \int p \, dx \) is known in classical mechanics as the action and is denoted by \( S \). Altogether, we expect the solution of the Schrödinger equation to have the approximate form,

\[
\psi(x) = A(x)e^{iS(x)/\hbar},
\]  

(4.10)

where

\[
p(x) = \frac{dS}{dx},
\]  

(4.11)

when the potential varies slowly on the scale of a wavelength. Equation (4.10) is the WKB ansatz for one-dimensional problems.

Before proceeding with this ansatz, let us examine the conditions for validity for the WKB approximation more thoroughly. If we substitute Eq. (4.7) into Eq. (4.1) and ignore the \( 2\pi \) because we are only interested in order of magnitude estimates, then we can write

\[
\hbar \ll pL.
\]  

(4.12)

Because of relations like this, people often say that the WKB approximation is valid when \( \hbar \) is “small,” or in the limit “\( \hbar \to 0 \).” Of course such statements have no precise meaning, because \( \hbar \) is a constant, not a variable, whose value in any case depends on the units chosen. To state the condition in a more careful manner, we can say that WKB theory is valid when \( \hbar \) is small in comparison typical actions of the problem, such as the quantity \( pL \) indicated above. Other quantities with the dimensions of action include an energy times a time or an angular momentum. For example, in a 1-dimensional oscillator, we can identify \( L \) with the amplitude of the oscillation and \( p \) with the maximum momentum (the amplitude of the momentum), whereupon the product \( pL \) becomes essentially the phase space area of the orbit, which is essentially the quantity known in classical mechanics as the action of the orbit. But as we will see later when we examine the Bohr-Sommerfeld quantization conditions, the action of the orbit is approximately equal to \( n\hbar \), where \( n \) is the quantum number of the oscillator. In this case, the condition (4.12) becomes \( \hbar \ll n\hbar \), or

\[
n \gg 1.
\]  

(4.13)
This is another way of thinking about the conditions of validity of WKB theory: the theory holds when the quantum numbers are large.

On the other hand, the condition of validity of classical mechanics is that all actions should be large in comparison to \( \hbar \), something which is normally true for macroscopic systems. This is the same as the conditions of validity of WKB theory, so the WKB method can be thought of as using classical mechanics to approximate quantum mechanics. Sometimes the WKB method is called *semiclassical*; in the Russian literature, it is regularly called the *quasiclassical approximation*.

Let us now generalize the WKB problem to three dimensions, by making obvious changes of notation. First, we will take the Schrödinger equation to be

\[
\frac{-\hbar^2}{2m} \nabla^2 \psi + V(x) \psi = E \psi, \tag{4.14}
\]

and we generalize Eq. (4.10) into

\[
\psi(x) = A(x) e^{iS(x)/\hbar}. \tag{4.15}
\]

We will take this as the WKB ansatz in three dimensions. As before, the amplitude \( A(x) \) is assumed to be slowly varying on the scale of a wavelength, and we will assume that \( S(x) \) is related to a de Broglie momentum by

\[
p = p(x) = \nabla S(x), \tag{4.16}
\]

which is the generalization of Eq. (4.11). The meaning of this equation is best understood from a picture. Since the phase of the wave (4.15) is proportional to \( S(x) \), a surface of constant phase, that is, a wave front, is given by \( S(x) = S_0 = \text{const} \). Such a wave front is indicated schematically in Fig. 4.3. Lying behind the given wave front are two others, lagging in phase by \( 2\pi \) and \( 4\pi \). Thus, the distance between the fronts in a direction perpendicular to the fronts is the de Broglie wavelength \( \lambda \). But \( \nabla S \) is a vector perpendicular to the fronts, whose magnitude is the rate of change of \( S \) in the perpendicular direction. This rate of change can also be written as \( 2\pi \hbar / \lambda \), which for a plane wave is the momentum \( p \). Therefore in the WKB problem, we identify \( \nabla S \) with a local momentum, as indicated by Eq. (4.16).

The relation (4.16) can also be understood analytically. Let \( x_0 \) be a some point of space, and let \( \xi \) be a displacement from \( x_0 \) which may be of the order of one or two wavelengths, but which is small in comparison to the scale length of the potential. Let us assume \( \psi(x) \) has the WKB form (4.15), and let us approximate \( \psi \) at \( x = x_0 + \xi \). Since the amplitude is slowly varying on the scale of the wavelength, we can set \( A(x) \approx A(x_0) \). But the phase must be expanded,

\[
S(x) \approx S(x_0) + \xi \cdot p_0, \tag{4.17}
\]
where \( p_0 = \nabla S(x_0) \). This gives
\[
\psi(x) = A(x_0) e^{iS(x_0)/\hbar} e^{i p_0 \cdot \xi/\hbar},
\]
which is a plane wave in \( \xi \) multiplied by a constant amplitude and phase. This shows that locally (on the scale of a few wavelengths) the wave function (4.15) looks like a plane wave with momentum \( p_0 \).

Thus, the 3-dimensional WKB wave (4.15) is associated with a momentum field \( p = p(x) = \nabla S \) on configuration space. This field, being the gradient of a scalar, satisfies \( \nabla \times p(x) = 0 \), and is related to the function \( S \) by
\[
S(x) = \int_{x'}^x p(x') \cdot dx'.
\]
Integrals of this form are well known in classical mechanics, where the function \( S(x) \) is called Hamilton's characteristic function.

The WKB ansatz (4.15) was based on some approximations, and is not by itself a systematic expansion of the wavefunction. But we can easily generalize it. First we bring the amplitude up into the exponent by writing
\[
\psi(x) = \exp \left\{ \frac{i}{\hbar} [S(x) - i\hbar \ln A(x)] \right\},
\]
which suggests that the WKB ansatz amounts to an expansion of the logarithm of the wavefunction $\psi$ in powers of $\hbar$, beginning with the power $\hbar^{-1}$, in which the leading term is the action $S$ and the next term is $-i \ln A$. Therefore we extend this expansion to all orders, writing

$$\psi(x) = \exp \left[ \frac{i}{\hbar} W(x) \right], \quad (4.21)$$

where

$$W(x) = W_0(x) + \hbar W_1(x) + \hbar^2 W_2(x) + \ldots, \quad (4.22)$$

and where

$$W_0(x) = S(x), \quad W_1(x) = -i \ln A(x). \quad (4.23)$$

It is now seen that the WKB ansatz, in its generalized form (4.21), only involves the assumptions that the logarithm of the wave function can be expanded in powers of $\hbar$, and that the leading term is $O(\hbar^{-1})$. These seem like mild assumptions, but, in fact, the WKB expansion does not always work, and even when it does work, it is only an asymptotic expansion, not a convergent one.

In any case, we may now substitute Eq. (4.21) into the Schrödinger equation (4.14), and express the latter in terms of $W$ instead of $\psi$. After a little algebra, we find

$$\frac{1}{2m} \langle \nabla W \rangle^2 - \frac{i\hbar}{2m} \nabla^2 W + V = E. \quad (4.24)$$

No approximations have been made yet, and this is exactly equivalent to the Schrödinger equation (4.14), although the shift from $\psi$ to its logarithm has made the Schrödinger equation nonlinear. Next we expand $W$ as in Eq. (4.22), substitute into Eq. (4.24), and collect terms order by order. At order $\hbar^0$, we find

$$\frac{1}{2m} (\nabla W_0)^2 + V(x) = E, \quad (4.25)$$

or

$$\frac{1}{2m} (\nabla S)^2 + V(x) = E. \quad (4.26)$$

This is the well known Hamilton-Jacobi equation of classical mechanics. At order $\hbar^1$, we find

$$\frac{1}{m} \nabla W_0 \cdot \nabla W_1 - \frac{i}{2m} \nabla^2 W_0 = 0, \quad (4.27)$$

or by Eq. (4.23),

$$\nabla S \cdot \nabla \ln A + \frac{1}{2} \nabla^2 S = 0. \quad (4.28)$$
It is convenient to transform this equation further by writing \( \rho(x) = |A(x)|^2 \), which by Eq. (4.15) is equivalent to \( \rho = |\psi|^2 \), so that \( \rho \) is the quantum probability density on configuration space. Then Eq. (4.28) can be written as a divergence:

\[
\nabla \cdot (\rho \nabla S) = 0.
\]

This equation is called the amplitude transport equation. With motivation we can go to higher orders in \( \hbar \), but all the interesting classical mechanics and most of the practical interest lies in the first two orders.

Now for some comments on these two principal results, the Hamilton-Jacobi equation (4.26) and the amplitude transport equation (4.29). First, the Hamilton-Jacobi equation was known almost a hundred years before quantum mechanics. It was originally discovered in restricted form by Hamilton, in his researches into the variational principles of mechanics. It is interesting that Hamilton was explicitly pursuing optical analogies, in which variational principles can be used to find light rays, and it is often commented that had he pushed this analogy a little further, he would have discovered wave mechanics. In fact, Schrödinger himself seems to have been guided by WKB solutions of various wave equations when he invented his own wave equation. After Hamilton, Jacobi generalized the equation which now bears both their names, and developed the theory which shows how the solutions of the equations of motion in classical mechanics are implicitly contained in the solution \( S \) of the Hamilton-Jacobi equation. This is not the place to describe how this comes about—such matters are taught in Physics 205A. Suffice it to say that in Hamilton-Jacobi theory, the function \( S \) is interpreted as the generating function of the canonical transformation which trivializes the classical equations of motion.

In recent years there has arisen new interest in the Hamilton-Jacobi equation and its connection to the Schrödinger equation via WKB theory, due to current researches into chaos theory. It happens that the Hamilton-Jacobi equation possesses global solutions only in the case that the classical motion is regular (not chaotic), and therefore only in this case can classical mechanics be used to construct asymptotic forms for the quantum wave function. In other words, the Schrödinger equation has no solutions in the WKB form (a local plane wave) in the case that the classical motion is chaotic. This in turn implies that the morphology and many other features of the quantum wave function depend on the nature (regular or chaotic) of the classical motion.

In principle, in finding the WKB wave function we should first solve the Hamilton-Jacobi equation for the action \( S \), and then substitute this into the amplitude transport equation and solve for the amplitude \( A \). The amplitude transport equation is actually
equivalent to the continuity equation for the probability flux,
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad (4.30) \]
where the first term vanishes because we are dealing with a time-independent problem, and where the probability flux in the second term is given by
\[ \mathbf{J}(x) = \rho(x) \mathbf{v}(x) = \rho(x) \frac{p(x)}{m} = \rho \frac{\nabla S}{m}. \quad (4.31) \]
Here we think of the momentum field \( p(x) = \nabla S \) as representing the momentum at position \( x \) of swarm of classical particles of energy \( E \) which fill up configuration space and which follow the classical equations of motion. In this interpretation, \( \mathbf{J} \) is proportional to the particle flux.

A brief comment is in order on the time-dependent WKB problem. Consider the time-dependent Schrödinger equation,
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x, t) \psi = i\hbar \frac{\partial \psi}{\partial t}, \quad (4.32) \]
and let the WKB ansatz be
\[ \psi(x, t) = A(x, t) e^{iS(x, t)/\hbar}. \quad (4.33) \]
Then at order \( \hbar^0 \) we find
\[ \frac{1}{2m} (\nabla S)^2 + V(x, t) + \frac{\partial S}{\partial t} = 0, \quad (4.34) \]
which is also well known in classical mechanics as the time-dependent version of the Hamilton-Jacobi equation. The solution \( S(x, t) \) to this equation is known as Hamilton’s principal function, and is given in terms of a line integral (usually taken along classical orbits),
\[ S(x, t) = \int_{x_0}^{x} \mathbf{p} \cdot d\mathbf{x} - H \, dt = \int L \, dt, \quad (4.35) \]
where \( L \) is the classical Lagrangian. It would take us too far afield to explain the precise meaning of this line integral in classical mechanics; however, we will see Hamilton’s principal function appear again when we study the Feynman path integral. At order \( \hbar^1 \), the time-dependent problem gives rise to a time-dependent version of the amplitude transport equation,
\[ \frac{\partial \rho}{\partial t} + \frac{1}{m} \nabla \cdot (\rho \nabla S) = 0, \quad (4.36) \]
which is obviously just the continuity equation (4.30) in time-dependent form.

WKB theory is most practical and easiest to apply in 1-dimensional problems, partly because of the difficulties of chaos in higher dimensions. Therefore we will henceforth
restrict consideration to time-independent, 1-dimensional, kinetic-plus-potential problems, for which the Schrödinger equation is Eq. (4.2). We transcribe the Hamilton-Jacobi equation (4.26) over to the one-dimensional case, whereupon we find

\[
\frac{1}{2m} \left( \frac{dS}{dx} \right)^2 + V(x) = E, \tag{4.37}
\]

and likewise the amplitude transport equation (4.29) becomes

\[
\frac{d}{dx} \left( \rho \frac{dS}{dx} \right) = 0, \tag{4.38}
\]

where \( \rho(x) = [A(x)]^2 \). The 1-dimensional WKB ansatz itself is given by Eq. (4.10).

The Hamilton-Jacobi equation is easily solved. We simply solve Eq. (4.37) for \( \frac{dS}{dx} \),

\[
\frac{dS}{dx} = p(x) = \pm \sqrt{2m[E - V(x)]}, \tag{4.39}
\]

and integrate to obtain

\[
S(x) = \pm \int^x p(x') \, dx'. \tag{4.40}
\]

The lower limit of integration serves merely to define the overall phase of the WKB wave function (4.10), and has no physical significance. As for the amplitude transport equation (4.38), it can be integrated immediately to give

\[
A(x) = \text{const} \sqrt{p(x)}. \tag{4.41}
\]

The constant present in this solution is equivalent to the normalization and/or phase convention for \( \psi \). We will worry about normalization later, and for now set this constant equal to anything convenient.

The solution (4.41) of the amplitude transport equation has a simple classical interpretation. It is possible to define a probability density \( \rho_{cl}(x) \) in classical mechanics in terms of a time average of a particle going around an orbit. This probability density is only normalizable in the case of a bound (periodic) orbit, so let us consider that case. Let \( T \) be the period of the orbit, and let \( dt/T \) be the fraction of a period which the particle spends on some small interval \( dx \). Then we can define \( \rho_{cl} \) by

\[
\rho_{cl}(x) dx = \frac{dt}{T}, \tag{4.42}
\]

or,

\[
\rho_{cl}(x) = \frac{1}{T} \frac{1}{|v(x)|}. \tag{4.43}
\]
where \( v(x) \) is the velocity at point \( x \). Usually the particle will pass over the interval \( dx \) twice per period with velocities \( \pm v(x) \), and the time \( dt \) should include both passes. But in the WKB approximation, the quantum probability density is \( \rho(x) = A^2 = \text{const}/p(x) \), which is the same as \( \rho_c(x) \), since \( p = mv \). Thus, we expect the amplitude of the WKB wave to be smallest where the classical particle is moving most rapidly and larger where the classical particle slows down. These features are obvious in the harmonic oscillator wave functions in Figs. 4.1 and 4.2.

![Diagram](image)

**Fig. 4.4.** A 1-dimensional potential \( V(x) \) rising to the right. Point \( x_0 \) is a classical turning point.

To proceed further it helps to have a specific shape of potential in mind. Consider the potential sketched in Fig. 4.4, in which \( V(x) \) rises to the right and some total energy \( E \) is indicated. The point \( x_0 \) where \( E = V(x_0) \) is the classical turning point, with the classically allowed region (region I) to the left, and the classically forbidden region (region II) to the right.

First we treat region I, the classically allowed region, where \( x < x_0 \) and \( E > V(x) \). In this region we define the function \( p(x) \) by

\[
p(x) = \sqrt{2m[E - V(x)]},
\]

which is exactly as in Eq. (4.39), except that we are now committing ourselves to the positive square root. In other words, we henceforth agree that the function \( p(x) \) is the positive square root in the classically allowed region. We integrate this to obtain \( S(x) \),

\[
S(x) = \int_{x_0}^{x} p(x') \, dx',
\]

which again is exactly as in Eq. (4.40) except that now we are agreeing that henceforth \( S(x) \) is defined with the plus sign in the integral. Thus, the two solutions to the Hamilton-Jacobi
equation (4.37) are \( S(x) \) and \(-S(x)\). We are also taking the lower limit of the integral in Eq. (4.45) to be \( x_0 \), the classical turning point. This is merely a matter of convenience, but it means that \( S(x) \) is real and negative in region I, and increasing to the right \( \text{[since } \frac{dS}{dx} = p(x) > 0 \text{]} \). As for the amplitude transport equation, we write its solution as

\[
A(x) = \frac{1}{\sqrt{p(x)}}.
\]

(4.46)

Altogether, the general WKB solution of the Schrödinger equation in region I is

\[
\psi_1(x) = c_1 \frac{e^{iS(x)/\hbar}}{\sqrt{p(x)}} + c_2 \frac{e^{-iS(x)/\hbar}}{\sqrt{p(x)}},
\]

(4.47)

where \( c_1 \) and \( c_2 \) are arbitrary complex constants. We notice that the first term is a wave travelling to the right, and the second, a wave travelling to the left; the general solution is a linear combination of such waves.

Next we treat region II, the classically forbidden region, where \( x > x_0 \) and \( E < V(x) \). In this region we define the function \( p(x) \) by

\[
p(x) = i\sqrt{2m[V(x) - E]} = i|p(x)|.
\]

(4.48)

We introduce a function \( K(x) \), defined by

\[
K(x) = \int_{x_0}^{x} |p(x')| \, dx' = \int_{x_0}^{x} \sqrt{2m[V(x') - E]} \, dx',
\]

(4.49)

and we take \( S(x) = iK(x) \). Again, the lower limit \( x_0 \) is the classical turning point. In this region \( p(x) \) is pure imaginary, and \( K(x) \) is real, positive, and increasing to the right. We also write the amplitude in the form,

\[
A(x) = \frac{1}{\sqrt{|p(x)|}}.
\]

(4.50)

Thus, the general WKB solution in region II is

\[
\psi_{II}(x) = c_3 \frac{e^{K(x)/\hbar}}{\sqrt{|p(x)|}} + c_4 \frac{e^{-K(x)/\hbar}}{\sqrt{|p(x)|}},
\]

(4.51)

where \( c_3 \) and \( c_4 \) are a new pair of complex constants. We notice that the first term is a wave which is growing exponentially as we move to the right, while the second is damping exponentially to the right. (It is necessary to say, “to the right,” because a wave which is growing to the right is damping to the left, and vice versa.)

We now have two solutions, Eqs. (4.47) and (4.51), in regions I and II respectively, each with two constants. The two pairs of constants cannot be independent, since the general
solution to the Schrödinger equation (4.2) can only have two arbitrary constants overall. Therefore there must be a way of determining $c_3$ and $c_4$, given $c_1$ and $c_2$, and vice versa. The rules for doing this are called connection rules, and they amount to connecting the two WKB solutions through the turning point region which separates the classical allowed and classically forbidden regions.

Unfortunately, neither WKB solution (4.47) nor (4.51) is valid in the immediate neighborhood of the turning point. This is evident from the given forms of the solutions, because the momentum $p(x)$ goes to zero at the turning point, and the solutions diverge. The divergence in the amplitude of the nominal WKB solutions is nonphysical, in the sense that the exact solution to the Schrödinger equation has no divergence at turning points, as is apparent in the examples shown in Figs. 4.1 and 4.2. On the other hand, the divergence does have a classical rationale, because the classical probability density $\rho_{cl}$ does diverge at the turning points. The divergence in $\rho_{cl}$ integrable, in the sense that $\int \rho_{cl} dx$ is finite and $\rho_{cl}$ can be normalized, but there is a divergence in the density nonetheless. In the exact solution to the Schrödinger equation, quantum effects such as the uncertainty principle cause the classical singularity to be smoothed out, so that while it is true that the wave function becomes large at the turning points (see again Figs. 4.1 and 4.2), it does not diverge there. As a result of this smoothing out of the classical singularity, some of the wave function extends into the classically forbidden region.

The reason for the breakdown of the WKB solution at the turning point is easily seen from the condition (4.1), for when the momentum $p$ goes to zero, the de Broglie wavelength $\lambda$ becomes arbitrarily large, and the condition (4.1) is violated. Therefore to find the connection between the coefficients $(c_1, c_2)$ and $(c_3, c_4)$ we cannot simply extend the two WKB solutions up to one another at the turning point.

Instead, we require a separate solution, or at least an approximate one, which is valid in the immediate neighborhood of the turning point. A more careful analysis than we will present here shows that the WKB solutions (4.47) and (4.51) are valid except in a small region around the turning point, unless the slope $V'(x_0)$ of the potential at the turning point itself should be too small. We will not quantify what “small” precisely means in this context, but rather will proceed with the equations and see where they lead us.

In particular, let us approximate the potential in the neighborhood of the turning point by a straight line,

$$V(x) \approx V(x_0) + (x - x_0)V'(x_0), \quad (4.52)$$
valid when \( x - x_0 \) is small. Then using \( E = V(x_0) \), the Schrödinger equation (4.2) becomes

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V'(x_0)(x - x_0)\psi = 0.
\] (4.53)

To clean this up, we introduce a shifted and scaled variable \( z \) by the substitution,

\[
x = x_0 + az,
\] (4.54)

where \( a \) is a positive constant chosen to absorb all the physical constants in Eq. (4.53). We see that the variable \( z \) is zero at the turning point, negative in the classically allowed region, and positive in the classically forbidden region. The nicest choice for \( a \) is

\[
a = \left( \frac{\hbar^2}{2mV'(x_0)} \right)^{1/3},
\] (4.55)

which causes the Schrödinger equation to become

\[
\frac{d^2 \psi}{dz^2} - z\psi = 0.
\] (4.56)

Equation (4.56) is Airy’s differential equation, whose two linearly independent solutions are the functions \( \text{Ai}(z) \) and \( \text{Bi}(z) \). These functions are discussed in standard references on special functions of mathematical physics. See, for example, Abramowitz and Stegun, Handbook of Mathematical Functions. Since this book is published by Dover and is relatively cheap, I recommend that you buy a copy. Another valuable reference on special functions which is currently in print is Table of Integrals, Series, and Products by Gradshteyn and Ryzhik; older references such as Whittaker and Watson, Jahnke and Emde, Magnus and Oberhettinger, etc., are available in libraries.

It helps to have some physical model in mind when studying the mathematical properties of the \( \text{Ai} \) and \( \text{Bi} \) functions. For this purpose, we notice that a potential \( V(x) \) which is linear in \( x \) occurs in the problem of a charged particle in a uniform electric field, where \( V(x) = qE_0x \), or of a massive particle in a uniform gravitational field, where \( V(x) = mgx \). Therefore, with appropriate scalings of variables as in Eq. (4.54), the \( \text{Ai} \) and \( \text{Bi} \) functions are the (exact) solutions of the Schrödinger equations for these two problems, as well as the approximate solutions for generic potentials near turning points.

The \( \text{Ai} \) and \( \text{Bi} \) functions are plotted in Figs. 4.5 and 4.6, respectively. The \( \text{Ai} \) function is the solution of Airy’s differential equation (4.56) which is decays exponentially as \( z \to \infty \), and therefore represents the physically allowable solution for a particle in the uniform gravitational field (with zero total energy, since the classical turning point is at \( z = 0 \)). As seen in Fig. 4.5, this function is oscillatory for \( z < 0 \), with the wavelength and amplitude of
the oscillations becoming smaller as \( z \) increases in the negative direction, corresponding to the increasing velocity or momentum of the particle falling in the gravitational field. The exponential damping of the function \( \text{Ai}(z) \) for \( z > 0 \) corresponds to tunnelling into the classically forbidden region. Finally, the function \( \text{Ai}(z) \) shows the characteristic behavior of the wave function at a turning point; the wave function has a large maximum near the turning point, which is a smoothed version of the classical singularity in the probability density. As for the \( \text{Bi}(z) \) function, it blows up exponentially in the region \( z > 0 \), and so is nonphysical for particles in gravitational fields; but we must retain this function for the general WKB problem. For \( z < 0 \), the function \( \text{Bi}(z) \) oscillates like the \( \text{Ai}(z) \) function, but \( 90^\circ \) out of phase.

Altogether, the general solution of the Schrödinger equation (4.2) in the neighborhood of a turning point has the form,

\[
\psi_{\text{tp}}(x) = c_a \text{Ai}(z) + c_b \text{Bi}(z),
\]

where \( c_a \) and \( c_b \) are a new pair of constants, and \( x \) and \( z \) are related by Eq. (4.54). We must now connect this solution with the solution \( \psi_1(x) \) to the left, and \( \psi_\Pi(x) \) to the right.

First, working to the left, we invoke the asymptotic forms for the \( \text{Ai} \) and \( \text{Bi} \) functions for large negative \( z \),

\[
\text{Ai}(z) = \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos \alpha(z), \quad z \ll 0,
\]

(4.58a)
\[
\text{Bi}(z) = \frac{1}{\sqrt{\pi}} (-z)^{1/4} \sin \alpha(z), \quad z \ll 0, \quad (4.58b)
\]

where
\[
\alpha(z) = -\frac{2}{3} (-z)^{3/2} + \frac{\pi}{4}. \quad (4.59)
\]

Notice that \(-z\) is positive in this region. Thus, we can write the wave function at the left of the turning point region in the form,
\[
\psi_{\text{tp}}(x) = \frac{1}{2\sqrt{\pi}} (-z)^{1/4} \left[ (c_a - ic_b)e^{i\alpha(z)} + (c_a + ic_b)e^{-i\alpha(z)} \right]. \quad (4.60)
\]

Compare this to the WKB solution in the classically allowed region,
\[
\psi_1(x) = \frac{1}{\sqrt{p(x)}} [c_r e^{i\varphi(x)} + c_\ell e^{-i\varphi(x)}], \quad (4.61)
\]

where
\[
\varphi(x) = \frac{S(x)}{\hbar} + \frac{\pi}{4}. \quad (4.62)
\]

In transcribing Eq. (4.47) over to Eq. (4.61) we have introduced extra phase shifts of \(\pi/4\) as a convenience, to make it easier to compare with the asymptotic forms of the \(\text{Ai}\) and \(\text{Bi}\) functions, and we have redefined the coefficients to compensate, so that \(c_1 = c_r e^{i\pi/4}\) and \(c_2 = c_\ell e^{-i\pi/4}\). The subscripts \(r\) and \(\ell\) on the new coefficients identifies the waves travelling to the right and left, respectively.

Equations (4.60) and (4.61) must represent the same function. Furthermore, since the waves travelling to the left and right are linearly independent, the left and right travelling waves in the two equations must independently be equal. To show that this is true and to find the connections between the coefficients \((c_r, c_\ell)\) and \((c_a, c_b)\), we first approximate the momentum function \(p(x)\) near the turning point according to Eq. (4.52),
\[
p(x) = \sqrt{2m[E - V(x)]} = \sqrt{-2mV'(x_0)(x - x_0)} = \frac{\hbar}{a} (-z)^{1/2}, \quad (4.63)
\]

where we use Eqs. (4.54) and (4.55). This shows that the amplitude factors in Eqs. (4.60) and (4.61) are proportional, as they should be. Next, we integrate \(p(x)\) to find the action,
\[
\frac{S(x)}{\hbar} = \frac{1}{\hbar} \int_{x_0}^{x} p(x') \, dx' = \int_{0}^{z} (-z')^{1/2} \, dz' = -\frac{2}{3} (-z)^{3/2}, \quad (4.64)
\]

which shows that \(\alpha(z) = \varphi(x)\). Thus, the phases in Eqs. (4.60) and (4.61) are identical. Therefore we can read off the necessary relations between the coefficients, which are
\[
\frac{1}{2\sqrt{\pi}} (c_a - ic_b) = \sqrt{\frac{\alpha}{\hbar}} c_r, \quad (4.65a)
\]
\[
\frac{1}{2\sqrt{\pi}} (c_a + ic_b) = \sqrt{\frac{\alpha}{\hbar}} c_\ell. \quad (4.65b)
\]
This completes the connection between the classically allowed region and the turning point region.

To connect to the right, that is, between the turning point region and the classically forbidden region, we invoke the asymptotic forms of the $A_i$ and $B_i$ functions for large positive $z,$

$$A_i(z) = \frac{1}{2\sqrt{\pi}}z^{1/4}e^{-\beta(z)}, \quad z \gg 0,$$

$$B_i(z) = \frac{1}{\sqrt{\pi}}z^{1/4}e^{+\beta(z)}, \quad z \gg 0,$$

where

$$\beta(z) = \frac{2}{3}z^{3/2}.$$ (4.67)

Thus, the wave function to the right of the turning point region has the form,

$$\psi_{tp}(x) = \frac{1}{2\sqrt{\pi}z^{1/4}}\left[c_1e^{-\beta(z)} + 2c_2e^{+\beta(z)}\right],$$ (4.68)

whereas the WKB solution in the classically forbidden region has the form,

$$\psi_\kappa = \frac{1}{\sqrt{|p(x)|}}\left[c_3e^{\kappa(x)} + c_4e^{-\kappa(x)}\right],$$ (4.69)

where we now write $c_3$ and $c_4$ instead of $c_3$ and $c_4$ for the coefficients of the growing and damping terms (to the right), respectively, and where we set

$$\kappa(x) = \frac{1}{\hbar}K(x).$$ (4.70)

As before, Eqs. (4.68) and (4.69) must represent the same function. That the amplitudes are proportional is shown as before, for close to (but to the right of) the turning point we have

$$|p(x)| = \sqrt{2mV'(x_0)(x - x_0)} = \frac{\hbar}{\alpha}z^{1/2}.$$ (4.71)

As for the action integral, we have

$$\kappa(x) = \frac{1}{\hbar} \int_{x_0}^{x} |p(x')| \, dx' = \int_{0}^{z} z'/2 \, dz' = \frac{2}{3}z^{3/2} = \beta(z).$$ (4.72)

Therefore again we can read off the relations between the coefficients, which are

$$\frac{c_a}{2\sqrt{\pi}} = c_d\sqrt{\frac{\alpha}{\hbar}},$$

$$\frac{c_b}{\sqrt{\pi}} = c_g\sqrt{\frac{\alpha}{\hbar}}.$$ (4.73)
Finally, we can eliminate \((c_a, c_b)\) between Eqs. (4.65) and (4.73), and find the desired connection rules between the coefficients \((c_p, c_q)\) in the classically allowed region I, and the coefficients \((c_g, c_d)\) in the classically forbidden region II. These connection rules are summarized separately in Notes 5.

\[ V(x) \]

\[ E \]

**Fig. 4.7.** A 1-dimensional potential \(V(x)\) falling to the right. Point \(x_0\) is a classical turning point.

The case where the classically allowed region is to the right of a turning point, which is illustrated in Fig. 4.7, must also be analyzed. Here we again denote the turning point by \(x_0\), and region III \((x < x_0)\) is the classically forbidden region, while region IV \((x > x_0)\) is the classically allowed region. The derivation of the connection rules is exactly as above, and will not be repeated here. The connection rules themselves are summarized in Notes 5.