Chapter 16
WKB Approximation

16.1 WKB Wave Functions

The WKB (Wentzel, Kramers, Brillouin) approximation is covered in most standard quantum mechanics texts. Basically, the WKB approximation is a type of *eikonal* approximation in which it is assumed the potential varies very slowly compared with the average de Broglie wavelength of a particle. In some sense, the quantum particle is acting somewhat like a classical particle. This is not quite the case, since the particle is still described by a wave function. It is like trying to have the best of both the classical and quantum worlds. Generally it is valid for high energies such that the de Broglie wavelength is large compared with distances over which the potential varies significantly.

Since this is a type of *semi-classical* approximation, it makes sense to look for a solution of Schrödinger's equation as a power series in $\hbar$. Terms to zeroth order in $\hbar$ correspond to a classical limit and the higher order terms provide quantum corrections. The WKB method generally works only in 1-D problems, but can be used in problems in 3-D with spherical symmetry, since the radial equation is an equation in one variable. I consider only one-dimensional motion in the x direction in this chapter, but return to the radial equation in discussing scattering theory.

The time independent Schrödinger equation is

$$\psi'' + k^2(x)\psi = 0 \tag{16.1}$$

where

$$k(x) = \sqrt{\frac{2m}{\hbar^2}[E - V(x)]} = p(x)/\hbar \tag{16.2}$$

and primes indicate derivatives with respect to x. For the moment I assume that $E > V(x)$ so that $k(x)$ is real and positive. If k were a constant, then the solution of Eq. (16.1) would be $\psi(x) = e^{\pm ikx}$. This suggests that I try a solution of the form

P.R. Berman, *Introductory Quantum Mechanics*, UNITEXT for Physics,
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$$\psi(x) = e^{iS(x)/\hbar} \tag{16.3}$$

and obtain equations for $S(x)$ that can be solved to give $S(x)$ as a power series in $\hbar$. If I do so, I need retain only those terms varying as $\hbar^0$ or $\hbar$, since higher order terms do not contribute to Eq. (16.3) in the limit that $\hbar \to 0$.

To obtain such a series solution for $S(x)$, I first calculate the derivatives of $\psi(x)$,

$$\psi' = \left[iS'(x)/\hbar\right] e^{iS(x)/\hbar}; \tag{16.4a}$$

$$\psi'' = -\left[S'(x)/\hbar\right]^2 e^{iS(x)/\hbar} + \left[iS''(x)/\hbar\right] e^{iS(x)/\hbar}, \tag{16.4b}$$

and substitute the expression for ψ'' into Eq. (16.1) to arrive at

$$\left[S'(x)\right]^2 = \hbar^2 k^2(x) + i\hbar S''(x). \tag{16.5}$$

Note that

$$p^2(x) = \hbar^2 k^2(x) \tag{16.6}$$

is independent of $\hbar$.

It looks like I haven't accomplished much since I started from a linear differential equation for $\psi(x)$ and ended up with a highly nonlinear differential equation for $S(x)$. The idea is to solve Eq. (16.5) iteratively, assuming that $S(x)$ is slowly varying so that the second derivative term in Eq. (16.5) can be treated as a small correction. This is equivalent to solving for $S(x)$ as a power series in $\hbar$. To lowest order

$$S'(x) = \pm\hbar k(x) = \pm p(x). \tag{16.7}$$

I use this to approximate

$$S''(x) = \pm p'(x), \tag{16.8}$$

and substitute this result back into Eq. (16.5) to obtain

$$\begin{aligned}
\left[S'(x)\right]^2 &= p^2(x) \pm i\hbar p'(x); \\
S'(x) &= \pm p(x)\sqrt{1 \pm i\hbar p'(x)/p^2(x)} \\
&\approx \pm p(x) + i\hbar \frac{p'(x)}{2p(x)} \\
&= \pm\hbar k(x) + i\hbar \frac{k'(x)}{2k(x)},
\end{aligned} \tag{16.9}$$

having used the fact that the sign of the $i\hbar p'(x)$ term is correlated with the sign of the $\pm p(x)$ factor.

The solution of this equation, neglecting integration constants, is

$$\begin{aligned} S(x) &= \pm\hbar \int k(x)dx + i\hbar \int \frac{k'(x)}{2k(x)}dx \\ &= \pm\hbar \int k(x)dx + \frac{i\hbar}{2} \int \frac{d}{dx} \ln [k(x)]\, dx \\ &= \pm\hbar \int k(x)dx + \frac{i\hbar}{2} \ln [k(x)]\,, \end{aligned} \tag{16.10}$$

leading to

$$\begin{aligned} \psi_{WKB}(x) &= e^{iS(x)/\hbar} = \exp\left\{\pm i \int k(x)dx - \frac{1}{2} \ln [k(x)]\right\} \\ &= \frac{C}{\sqrt{k(x)}} \exp\left\{\pm i \int k(x)dx\right\}, \end{aligned} \tag{16.11}$$

where the integration constants have been absorbed into the normalization constant C.

If the energy is less than $V(x)$, this equation is replaced by

$$\psi_{WKB}(x) = \frac{C}{\sqrt{\kappa(x)}} \exp\left\{\pm \int \kappa(x)dx\right\}, \tag{16.12}$$

where

$$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[V(x) - E]} > 0. \tag{16.13}$$

It is not too difficult to estimate the validity conditions for the WKB approximation. From Eq. (16.10) a necessary condition for the validity of the approach requires the second term be smaller than the first, or

$$\left|\frac{k'(x)}{2k^2(x)}\right| \ll 1; \tag{16.14a}$$

$$\hbar\left|\frac{p'(x)}{2p^2(x)}\right| \ll 1. \tag{16.14b}$$

Since

$$p'(x) = -\frac{\sqrt{2m}}{2}\frac{dV/dx}{\sqrt{E-V}}, \tag{16.15}$$

the validity condition can be written as

$$\hbar \frac{\sqrt{2m}}{4} \left| \frac{dV/dx}{\sqrt{E-V}} \right| \ll \left| p^2(x) \right| = \frac{h^2}{\lambda_{dB}^2(x)};$$

$$\lambda_{dB}(x) \left| \frac{dV}{dx} \right| \ll \sqrt{\frac{|E-V|}{2m}} \frac{8\pi h}{\lambda_{dB}(x)} = 8\pi \frac{\left| p^2(x) \right|}{2m}, \tag{16.16}$$

where $\lambda_{dB}(x) = h/\,|p(x)|$. The potential must change slowly compared to the kinetic energy over distances of order of a wavelength for the WKB approximation to be valid.

Equation (16.16) is a necessary condition for the validity of the WKB approximation, but it is not sufficient. If higher order terms in the expansion used to solve Eq. (16.5) are included, they lead to additional phases in the exponent appearing in Eq. (16.3). As I have stressed, when terms appear in an exponent, they must have an absolute value much less than unity for them to be neglected. If you carry out the expansion to next order, you will see that the condition

$$[\lambda_{dB}(x)]^2 \left| \frac{d^2V}{dx^2} \right| \ll \frac{\left| p^2(x) \right|}{2m} \tag{16.17}$$

must also be satisfied.

16.2 Connection Formulas

As long as conditions (16.16) and (16.17) are satisfied, the WKB method can be used to approximate the eigenfunctions for a particle moving in a potential $V(x)$. Let's check to see when we can expect this to be the case for the potentials shown in Fig. 16.1. (a) Assuming that conditions (16.16) and (16.17) hold, then the WKB approximation is valid for all x, and the WKB eigenfunctions for a given energy correspond to particles moving to the right or left. If you construct a wave packet having average energy E greater than the barrier height incident from the left, you will find that there is no reflected wave, the wave packet and simply moves to the right, adjusting its kinetic energy to changes in the barrier height. (b) In this case, the WKB approximation necessarily breaks down at the point discontinuities in the potential since $dV/dx = \infty$ at these points. In the exact quantum problem, there is always a reflected wave. We have seen already that the reflection coefficient is independent of $\hbar$ for step potentials in the high energy limit. In Fig. 16.1c–f, the WKB approximation necessarily fails at the *classical turning points* a and b since the momentum $p(x) = 0$ at such points.

Even when there are classical turning points for a given energy, it is still possible to use the WKB approximation. One proceeds by calculating the WKB wave functions in the regions away from the turning points and piecing together the solutions using the *exact* solutions in the vicinity of the turning points. At each

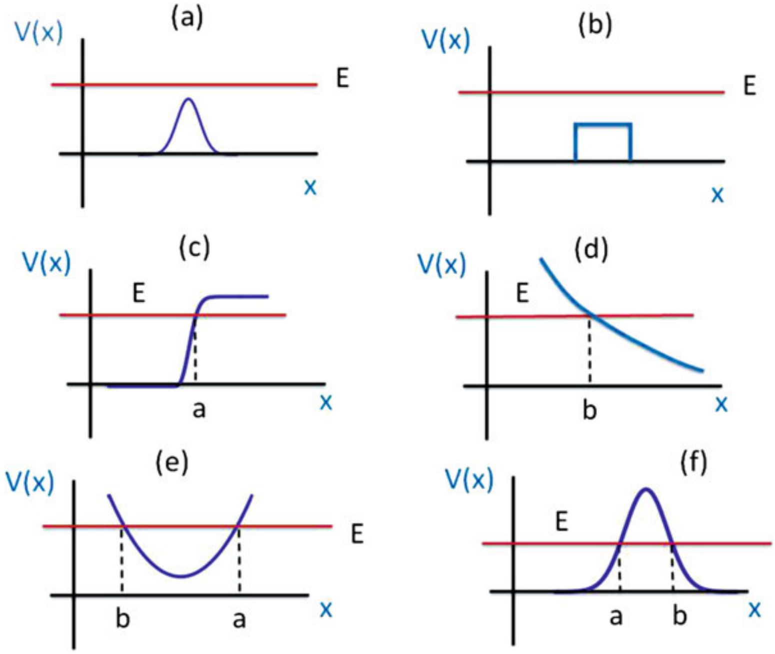

Fig. 16.1 The WKB approximation fails at point discontinuities in the potential and at the classical turning points. The classical turning point a has the classical region to the left and the classical turning point b has the classical region to the right. (**a**) smooth barrier (**b**) square barrier (**c**) classical region to left of turning point (**d**) classical region to right of turning point (**e**) bound states (**f**) barrier with tunneling

classical turning point, the spatially dependent de Broglie wavelength $\lambda_{dB}(x) = h/p(x) = 2\pi/k(x)$ is infinite. It is generally assumed that the potential varies linearly with x in the region of a turning point and that the slope is sufficiently small to insure that the exact solution for a linear potential (which are so-called Airy functions) extends into the region where the WKB wave functions are valid. In this manner, one arrives at a number of *connection formulas* which tell you how to piece together the solutions. I give a derivation of one of the connection formulas in the Appendix; derivations can also be found in most textbooks on quantum mechanics.

The connection formulas must be written for the two possible cases of a turning point with the classically allowed region to the right or to the left of the turning point:

Turning point at $x = b$ (classically allowed region to the right):

$$\frac{A}{\sqrt{\kappa(x)}} \exp\left\{-\int_x^b \kappa(x')dx'\right\} + \frac{B}{\sqrt{\kappa(x)}} \exp\left\{\int_x^b \kappa(x')dx'\right\}$$
$$\leftrightarrow \frac{2A}{\sqrt{k(x)}} \cos\left\{\int_b^x k(x')dx' - \frac{\pi}{4}\right\} - \frac{B}{\sqrt{k(x)}} \sin\left\{\int_b^x k(x')dx' - \frac{\pi}{4}\right\}. \quad (16.18)$$

Turning point at $x = a$ (classically allowed region to the left):

$$\frac{2A}{\sqrt{k(x)}} \cos\left\{\int_x^a k(x')dx' - \frac{\pi}{4}\right\} - \frac{B}{\sqrt{k(x)}} \sin\left\{\int_x^a k(x')dx' - \frac{\pi}{4}\right\}$$
$$\leftrightarrow \frac{A}{\sqrt{\kappa(x)}} \exp\left\{-\int_a^x \kappa(x')dx'\right\} + \frac{B}{\sqrt{\kappa(x)}} \exp\left\{\int_a^x \kappa(x')dx'\right\}. \quad (16.19)$$

16.2.1 Bound State Problems

If you look at Fig. 16.1e, you can deduce that there is a discrete infinity of bound states for this potential. You can estimate the bound state energies using the WKB approximation. The answer should be good for the high energy states. To do so, begin on the left ($x < b$) with an exponentially decreasing function and use

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left\{-\int_x^b \kappa(x)dx\right\} \rightarrow \frac{2}{\sqrt{k(x)}} \cos\left\{\int_b^x k(x)dx - \frac{\pi}{4}\right\} \quad (16.20)$$

to connect the solution to the region $b < x < a$. To connect the wave function in the region $b < x < a$ to one in the region $x > a$, I rewrite the right-hand side of Eq. (16.20) as

$$\begin{aligned}
&\frac{2}{\sqrt{k(x)}} \cos\left\{\int_b^x k(x)dx - \frac{\pi}{4}\right\} \\
&= \frac{2}{\sqrt{k(x)}} \cos\left\{-\int_x^a k(x)dx + \int_b^a k(x)dx - \frac{\pi}{4}\right\} \\
&= \frac{2}{\sqrt{k(x)}} \cos\left\{\int_x^a k(x)dx - \int_b^a k(x)dx - \frac{\pi}{4} + \frac{\pi}{2}\right\} \\
&= \frac{2}{\sqrt{k(x)}} \cos\left\{\int_x^a k(x)dx - \frac{\pi}{4}\right\} \cos\left\{\int_b^a k(x)dx - \frac{\pi}{2}\right\} \\
&\quad + \frac{2}{\sqrt{k(x)}} \sin\left\{\int_x^a k(x)dx - \frac{\pi}{4}\right\} \sin\left\{\int_b^a k(x)dx - \frac{\pi}{2}\right\}. \quad (16.21)
\end{aligned}$$

I can now use the connection formula (16.19) to extend the solution to the $x > a$ region; however, in doing so, the sin term leads to an exponentially increasing wave function, which is not physical. The only way to avoid this is to have

$$\sin\left\{\int_b^a k(x)dx - \frac{\pi}{2}\right\} = 0, \quad (16.22)$$

which implies that

$$\int_b^a k(x)dx = \left(n + \frac{1}{2}\right)\pi \tag{16.23}$$

(n is a positive integer or zero) or

$$\int_b^a p(x)dx = \left(n + \frac{1}{2}\right)\pi\hbar; \quad n = 0, 1, 2 \ldots. \tag{16.24}$$

This is the *semiclassical quantization condition*. Note that the WKB approximation breaks down near the turning points, which is the reason that it may not be possible to normalize the entire wave function.

If the potential is infinite for $x < 0$, then you start from the right of the turning point at $x = a$ and work backwards towards the turning point at $x = b = 0$ to obtain

$$\frac{2}{\sqrt{k(x)}}\cos\left\{\int_x^a k(x)dx - \frac{\pi}{4}\right\} \leftarrow \frac{1}{\sqrt{\kappa(x)}}\exp\left\{-\int_a^x \kappa(x)dx\right\}. \tag{16.25}$$

Since the wave function must vanish at $x = 0$, you are led to the requirement that

$$\int_0^a k(x)dx - \frac{\pi}{4} = \left(n + \frac{1}{2}\right)\pi \tag{16.26}$$

or

$$\int_0^a k(x)dx = \left(n + \frac{3}{4}\right)\pi; \quad n = 0, 1, 2 \ldots. \tag{16.27}$$

If the potential is infinite at *both* $x = a$ and $x = b$, this equation is replaced by

$$\int_b^a k(x)dx = (n + 1)\pi; \quad n = 0, 1, 2 \ldots. \tag{16.28}$$

16.3 Examples

Equation (16.24) may not give the correct energies, but it always gives a good idea of how the energy levels scale with n at high energy. For example, consider the potential

$$V(x) = V_0 |x/x_0|^q = \alpha |x|^q, \tag{16.29}$$

with $q > 0$, $V_0 > 0$, $x_0 > 0$, and

$$\alpha = V_0/x_0^q. \tag{16.30}$$

The classical energy for a particle having mass m moving in this potential is

$$E = \frac{p^2}{2m} + \alpha |x|^q \tag{16.31}$$

and the classical turning points $[p(x) = 0]$ occur at

$$a = -b = (E/\alpha)^{1/q}, \tag{16.32}$$

leading to the quantization condition

$$\begin{aligned}
&\int_{-(E/\alpha)^{1/q}}^{(E/\alpha)^{1/q}} \sqrt{2m\,(E - \alpha\,|x|^q)}dx \\
&= 2\int_0^{(E/\alpha)^{1/q}} \sqrt{2m\,(E - \alpha\,|x|^q)}dx = \left(n + \frac{1}{2}\right)\pi\hbar.
\end{aligned} \tag{16.33}$$

The integral is tabulated and one finds

$$\sqrt{2m\pi}\frac{E^{\left(\frac{1}{q}+\frac{1}{2}\right)}}{\alpha^{1/q}}\frac{\Gamma(1+1/q)}{\Gamma(3/2+1/q)} = \left(n + \frac{1}{2}\right)\pi\hbar, \tag{16.34}$$

where Γ is the gamma function. Solving for the energy, I find

$$\frac{E_{q,n}}{V_0} = C_{q,n}\left(\frac{1}{\beta^2}\right)^{\frac{q}{q+2}}, \tag{16.35}$$

where

$$C_{q,n} = \left[\frac{\Gamma(3/2+1/q)\sqrt{\pi}}{\Gamma(1+1/q)}\left(n + \frac{1}{2}\right)\right]^{2q/(q+2)} \tag{16.36a}$$

and

$$\beta^2 = \frac{2mV_0x_0^2}{\hbar^2}. \tag{16.36b}$$

For the harmonic oscillator potential with $q = 2$ and $\alpha = m\omega^2/2$, it follows that $V_0 = m\omega^2x_0^2/2$,

$$\beta^2 = \frac{4V_0^2}{\hbar^2\omega^2}, \tag{16.37}$$

$$C_{2,n} = \frac{\Gamma(2)\sqrt{\pi}}{\Gamma(3/2)}\left(n+\frac{1}{2}\right) = 2\left(n+\frac{1}{2}\right), \tag{16.38}$$

and

$$E_{2,n} = \left(n+\frac{1}{2}\right)\hbar\omega. \tag{16.39}$$

The fact that I got the exact answer is an "accident." In the classically allowed region, the WKB wave function looks nothing like the true wave function for the $n = 0$ state. With increasing n, by choosing the WKB wave functions to agree with the exact wave functions at the origin (with this choice the WKB wave functions are not normalized), you will find that the WKB and exact wave functions are in good agreement as long as you stay away from the turning points.

For arbitrary q, the energies vary as

$$E_{q,n} \sim (n+1/2)^{2q/(q+2)}. \tag{16.40}$$

For $q = 4$, $C_{4,n} = 2.185\,(n+1/2)^{4/3} = 0.867, 3.75, 7.41, 11.6$ for $n = 0, 1, 2, 3$, while the numerical solution of the Schrödinger equation[1] yields $C_{4,n} = 1.06, 3.80, 7.46, 11.6$. Not so great for $n = 0$, but not too bad for $n \geq 1$. As $q \to \infty$, the potential approximates an infinite square well potential having width $2x_0$ and the WKB energies vary as $(n+1/2)^2$. The WKB energies given by Eq. (16.35) of the high-lying n states nearly coincide with the exact results, but the $n = 0$ state energy is off by a factor of 4, since a better quantization condition to use is the one given in Eq. (16.28), rather than that given in Eq. (16.23), because the potential walls approximate those of an infinite potential well. In certain cases, the WKB approximation may provide a lower bound for the ground state energy.[2]

The condition given in Eq. (16.16) for the WKB approximation to be valid reduces to

$$\frac{q}{4\beta}\left|\frac{x}{x_0}\right|^{q-1}\left|C_{q,n}\left(\frac{1}{\beta^2}\right)^{\frac{q}{q+2}} - \left|\frac{x}{x_0}\right|^q\right|^{-3/2} \ll 1. \tag{16.41}$$

[1] I took these values from the lecture notes of Professor Klaus Schulten on the web site http://www.ks.uiuc.edu/Services/Class/PHYS480/.

[2] L.F. Barrágan-Gil and A. Camacho, Modern Physics Letters **22**, 2675–2687 (2007) prove that a lower bound to the ground state energy can be obtained using WKB considerations for potentials that vary as x^q for $x > 0$ and are infinite for $x < 0$, provided $1 < q < 5/2$. However the lower bound they obtain is lower than that which would be calculated using the WKB quantization condition.

It turns out that inequality (16.41) holds over a large range of parameter space. It is violated near $x/x_0 = 0$ if $q \ll 1$ (the derivative of the potential diverges at the origin if $q < 1$) and near the turning points. The worst violations (that is, over the largest range of x/x_0) occur for $n = 0$ and for q of order unity. It is not readily apparent to me how the validity condition for the WKB *wave function* given in Eq. (16.41) translates into one for the accuracy of the *energy levels* calculated using the WKB approximation. That is, although the violation of inequality (16.41) for $n = 0$ decreases with increasing q for fixed β, the relative error in the $n = 0$ energy calculated in the WKB approximation increases with increasing q. As was mentioned previously, this can be associated with using the wrong quantization condition as the potential begins to approximate the infinite square well potential.[3] For fixed q and β, the WKB approximation becomes better with increasing n.

The connection formulas can also be used to calculate the reflection and transmission coefficients for the barrier shown in Fig. 16.1f. You start with the WKB wave function for $x > b$ in the form

$$\frac{2F}{\sqrt{k(x)}} \cos\left\{\int_b^x k(x)dx - \frac{\pi}{4}\right\} - \frac{G}{\sqrt{k(x)}} \sin\left\{\int_b^x k(x)dx - \frac{\pi}{4}\right\} \tag{16.42}$$

and choose G such that this is in the form of a wave moving to the right only, that is, something varying as $T \exp\left\{i\left[\int_b^x k(x)dx - \frac{\pi}{4}\right]\right\}$. You then propagate this solution all the way back to $x < a$ using the connection formulas and write the wave function for $x < a$ in the form of a wave moving to the right plus one moving to the left as

$$A \exp\left\{i\left[\int_x^a k(x)dx - \frac{\pi}{4}\right]\right\} + R \exp\left\{-i\left[\int_x^a k(x)dx - \frac{\pi}{4}\right]\right\}. \tag{16.43}$$

The (intensity) transmission coefficient is then $|T/A|^2$ and the reflection coefficient is $|R/A|^2$. The result for the transmission coefficient is the same as that given by Eq. (6.120) for a square barrier, if the quantity κd is replaced by $\int_a^b \kappa(x)dx$, where d is the width for the square barrier and a and b are the classical turning points. You are asked to prove this in the problems.

16.4 Summary

The WKB approximation is generally referred to as a semi-classical approximation since it is valid in the limit of large energies, where the de Broglie wave length is large over distances in which the potential varies significantly. It always fails at classical turning points, but connection formulas can be used to connect the WKB

[3] See H. Friedtich and J. Trost, *Nonintegral Maslov indices*, Physical Review A **54**, 1136–1145 (1996). I thank R. Shakeshaft for pointing out this reference to me.

wave functions in regions on both sides of the turning point. The WKB method provides a relatively simple way for estimating the energies of all but the lowest energy bound states in one-dimensional problems. The equation that allows you to do this, Eq. (16.24), is essentially the Bohr quantization condition.

16.5 Appendix: Connection Formulas

To illustrate how the connection formulas can be derived, I consider the case where the turning point is at $x = a$ such that the classical region is to the left of the turning point. The basic idea is to expand the potential in the region of the turning point and keep only the term that is linear in $x - a$. That is, in the region of the turning point I approximate

$$V(x) \approx V(a) + \left.\frac{dV}{dx}\right|_{x=a} (x-a), \tag{16.44}$$

such that

$$E - V(x) \approx -\left.\frac{dV}{dx}\right|_{x=a} (x-a), \tag{16.45}$$

since $E = V(a)$. From Fig. 16.1 you can see that the slope is positive at the turning point at $x = a$. The next step is to obtain an exact solution of Schrödinger's equation for this potential and hope that the solution remains valid at distances sufficiently far from $x = a$ to join with the WKB solutions. This will normally be the case if the general validity conditions for the WKB approximation given in Eqs. (16.16) and (16.17) are satisfied, provided the first derivative of the potential at the turning point does not vanish.

In the region of the turning point, Schrödinger's equation is

$$\frac{d^2\psi}{dx^2} - K^2(x)\psi = 0, \tag{16.46}$$

where

$$K^2(x) = \frac{2m}{\hbar^2}\left.\frac{dV}{dx}\right|_{x=a} (x-a) = \begin{cases} -k^2(x) & x < a \\ \kappa^2(x) & x > a \end{cases} \tag{16.47}$$

is positive for $x > a$ and negative for $x < a$. In terms of a dimensionless variable z defined by

$$z = \left[\frac{2m}{\hbar^2}\left.\frac{dV}{dx}\right|_{x=a}\right]^{1/3} (x-a), \tag{16.48}$$

Eq. (16.46) is transformed into

$$\frac{d^2\psi}{dz^2} - z\psi = 0. \tag{16.49}$$

This is a well-known (to those who know it well) differential equation of mathematical physics known as Airy's equation, having independent solutions denoted by $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ (Mathematica symbols AiryAi[z] and AiryBi[z]). The general solution of Eq. (16.49) is

$$\psi(z) = C_1\mathrm{Ai}(z) + C_2\mathrm{Bi}(z). \tag{16.50}$$

The idea is to use the asymptotic forms of the Airy functions to join the solution for $\psi(z)$ to the WKB solutions in the regions $x < a$ and $x > a$. The WKB validity condition given in Eq. (16.16) corresponds to the requirement that $|z| \gg 1$. To see this, I use Eq. (16.45) and assume that $dV/dx > 0$ is constant in the region near the turning point to write

$$\frac{dV}{dx} = \left|\frac{E - V(x)}{|x-a|}\right| = \frac{|p(x)|^2}{2m\,|x-a|}. \tag{16.51}$$

Condition (16.16) then reduces to

$$\frac{dV}{dx} = \frac{|p(x)|^2}{2m\,|x-a|} \ll \frac{8\pi\,|p(x)|^2}{2m\lambda_{dB}(x)} \tag{16.52}$$

or

$$|x-a| \gg \hbar/4\,|p(x)|\,, \tag{16.53}$$

which corresponds to

$$|z|^3 = \frac{2m}{\hbar^2}\frac{dV}{dx}\,|x-a|^3 = \frac{2m}{\hbar^2}\frac{|p(x)|^2\,|x-a|^3}{2m\,|x-a|} = \frac{|p(x)|^2\,|x-a|^2}{\hbar^2} \gg \frac{1}{16}. \tag{16.54}$$

I need the asymptotic forms of $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ for $|z| \gg 1$.

The needed asymptotic forms are

$$\mathrm{Ai}(z) \sim \frac{1}{2\sqrt{\pi}} z^{-1/4} e^{-y} \qquad z \gg 1; \tag{16.55a}$$

$$\mathrm{Ai}(z) \sim \frac{1}{\sqrt{\pi}} (-z)^{-1/4} \cos\left(y - \frac{\pi}{4}\right) \qquad z \ll -1; \tag{16.55b}$$

$$\mathrm{Bi}(z) \sim \frac{1}{\sqrt{\pi}} z^{-1/4} e^{y} \qquad z \gg 1; \tag{16.55c}$$

$$\mathrm{Bi}(z) \sim -\frac{1}{\sqrt{\pi}} (-z)^{-1/4} \sin\left(y - \frac{\pi}{4}\right) \qquad z \ll -1, \tag{16.55d}$$

where

$$y = \frac{2}{3} |z|^{3/2} . \tag{16.56}$$

I am now in a position to connect the WKB solution for $x < a$ to that for $x > a$. To simplify matters I write the WKB solution in the form

$$\psi_{WKB}(x) = \begin{cases} \frac{A_1}{\sqrt{k(x)}} \cos\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) & \\ + \frac{A_2}{\sqrt{k(x)}} \sin\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) & x < a \\ \frac{B_1}{\sqrt{\kappa(x)}} e^{-\int_a^x \kappa(x')dx'} + \frac{B_2}{\sqrt{\kappa(x)}} e^{\int_a^x \kappa(x')dx'} & x > a \end{cases}, \tag{16.57}$$

while the exact asymptotic solution (for $z \gg 1$) near the turning point, obtained using Eqs. (16.50) and (16.55), is

$$\psi_{\mathrm{Airy}}(z) = \begin{cases} C_1 \frac{1}{\sqrt{\pi}} (-z)^{-1/4} \cos\left(y - \frac{\pi}{4}\right) & \\ -C_2 \frac{1}{\sqrt{\pi}} (-z)^{-1/4} \sin\left(y - \frac{\pi}{4}\right) & x < a \\ C_1 \frac{1}{2\sqrt{\pi}} z^{-1/4} e^{-y} + C_2 \frac{1}{\sqrt{\pi}} z^{-1/4} e^{y} & x > a \end{cases}. \tag{16.58}$$

In the range where the potential is linear, if $x < a$,

$$\int_x^a k(x')dx' = \sqrt{\frac{2m}{\hbar^2} \frac{dV}{dx}} \int_x^a \sqrt{a - x'}dx' = \frac{2}{3} \sqrt{\frac{2m}{\hbar^2} \frac{dV}{dx}} (a - x)^{3/2} = y, \tag{16.59}$$

and, if $x > a$,

$$\int_a^x \kappa(x')dx' = \sqrt{\frac{2m}{\hbar^2} \frac{dV}{dx}} \int_a^x \sqrt{x' - a}dx' = \frac{2}{3} \sqrt{\frac{2m}{\hbar^2} \frac{dV}{dx}} (x - a)^{3/2} = y. \tag{16.60}$$

Comparing Eqs. (16.57) and (16.58), and using Eqs. (16.47) and (16.48) to show that $-z = c\sqrt{k(x)}$ for $x < a$ and $z = c\sqrt{\kappa(x)}$ for $x > a$ (c = constant), I find that

$$B_1 = A_1/2; \quad B_2 = -A_2, \tag{16.61}$$

giving rise to the connection formula given in Eq. (16.19). The calculation proceeds in the same manner for the turning point at $x = b$, but the slope of the potential is negative at this turning point.

16.6 Problems

1. In the WKB approximation, what is the reflection coefficient when a wave packet is sent into a one-dimensional barrier with the energy above the barrier height? How and why does this differ from the problem of a rectangular barrier?

2. Use the WKB method to estimate the energy levels of a particle having mass m in the potential

$$V(z) = \begin{cases} mgz & z > 0 \\ \infty & z < 0 \end{cases} .$$

In this case, because of the infinite wall at the origin, the semi-classical quantization condition is given by Eq. (16.27). Compare your answer with the solutions $E_n = 2.338, 4.088, 5.521, 6.787$ for $n = 0, 1, 2, 3$ obtained from an exact solution of the Schrödinger equation, where E_n is expressed in units of $(\hbar^2 mg^2/2)^{1/3}$. Show that the exact solution for the ground state energy lies between the WKB value and the variational upper bound of $E_0 = 2.34477$ calculated in Problem 15.2–3

3. Evaluate Eq. (16.35) for the potential $V(x) = V_0 \left|x/x_0\right|^q$ when $n = 0$ to get the WKB approximation to the ground state energy. Compare your result with the exact solutions $(E/V_0)\,\beta^{q/(q+2)} = 1.0188, 1, 1.02295, 1.06036, 1.1023$ for $q = 1, 2, 3, 4, 5$, with $\beta^2 = 2mV_0x_0^2/\hbar^2$. Also compare your result with the variational solution of Problem 15.2–3 by plotting the ratio of the variational to WKB solutions as a function of q. Show that the WKB solution is greater than the variational solution for $q < 2$ and less than the variational solution for $q > 2$. Also show that the WKB solution deviates more and more from the variational result with increasing q when $q > 2$. You may use the fact that the variational solution is

$$E/V_0 = \beta^{-\frac{q}{q+2}} \left[\frac{1}{\xi^2} + \frac{1}{2^{\frac{q}{2}}} \frac{\Gamma\left(\frac{1+q}{2}\right)}{\sqrt{\pi}} \xi^q \right]$$

with

$$\xi = \left[\frac{2^{\frac{q}{2}+1}}{q} \frac{\sqrt{\pi}}{\Gamma\left(\frac{1+q}{2}\right)} \right]^{\frac{1}{q+2}} .$$

4. Show that the WKB estimate of the energy levels of a particle having mass m in the potential

$$V(x) = \begin{cases} V_0 \left|x/x_0\right|^{\mu} & x > 0 \\ \infty & x < 0 \end{cases}$$

can be obtained from Eq. (16.36a) by replacing $(n + 1/2)$ with $(2n + 3/2)$. With this substitution, verify that the results are consistent with Problem 16.2 for $n = 0, 1, 2, 3$. For this potential, show that the variational approximation to the ground state energy is identical to that of Problem 15.4 if you use the same trial function. Plot the ratio of the variational to WKB solutions for the ground state energy as a function of q and determine the range of q for which it is possible (but not guaranteed) that the WKB ground state energy is a lower bound to the true energy.

5. For $q \to \infty$, show that the potential $V(x) = V_0 \left|x/x_0\right|^q$ approaches that of an infinite square well. Show that, as $q \to \infty$, Eq. (16.35) gives the correct energy for the infinite square well potential for $n \gg 1$ and 1/4 of the exact result for $n = 0$.

6. The Hamiltonian for the harmonic oscillator in dimensionless coordinates is $H' = \left(\eta^2 + \xi^2\right)/2$. The semiclassical quantization condition for the dimensionless energy levels ϵ_n of this Hamiltonian is

$$\int_{-\sqrt{2\epsilon}}^{\sqrt{2\epsilon}} \sqrt{2\left(\epsilon_n - \frac{\xi^2}{2}\right)} d\xi = \left(n + \frac{1}{2}\right)\pi; \quad n = 0, 1, \ldots,$$

where the dimensionless value of $k_n(x)$ is $\tilde{k}(\xi) = 2\epsilon_n - \xi^2$. Show that the WKB quantization condition gives the exact energies, $\epsilon_n = n + 1/2$. Plot the WKB wave function

$$\left(\tilde{\psi}_n\right)_{WKB} = \frac{C_n}{\sqrt{\tilde{k}_n(\xi)}} \cos\left[\int_{\xi}^{\sqrt{2n+1}} d\xi' \sqrt{\left(2n + 1 - \xi'^2\right)} - \frac{\pi}{4}\right]$$

in the classically allowed regime and compare it with the exact wave function

$$\tilde{\psi}_n(\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\xi^2/2} H_n(\xi)$$

for $n = 0$ and $n = 24$. Choose the constant C_n of the WKB wave function so it agrees with the exact wave function at $\xi = 0$ and plot the $n = 0$ case from $0 \le \xi \le 0.7$ and the $n = 24$ case from $0 \le \xi \le 6.7$ (that is to within about 0.3 from the classical turning point). The WKB energies are exact, but are the WKB wave functions also exact?

7. Use the connection formulas to extend the WKB solution of the previous problem to the region to the right of the classical turning point. Plot the approximate wave function for $n = 24$ using the WKB solutions in the regions $0 \le \xi \le 6.4$ and $\xi > 7.6$ and the Airy function solution given by Eq. (16.50) in the region $6.4 \le \xi \le 7.6$; on the same graph, plot the exact eigenfunction of the oscillator. [Hint: Show that the variable z defined by Eq. (16.48) is

$$z \to z_n = (2\xi)^{1/3}\left(\xi - \sqrt{(2n+1)}\right),$$

express $\tilde{k}_n(\xi)$ in terms of z_n, and compare Eqs. (16.57) and (16.58) to obtain the constants C_1 and C_2 appearing in Eq. (16.50).]

8–9. Use the WKB method to estimate the transmission coefficient for a smooth potential barrier when the energy is less than the barrier height. Show that the result is the same as that for a square barrier if the quantity $e^{-\kappa d}$ is replaced by $e^{-\int_a^b \kappa(x)dx}$, where d is the width for the square barrier and a and b are the classical turning points for the smooth barrier.