8. WKB Approximation

The WKB approximation, named after Wentzel, Kramers, and Brillouin, is a method for obtaining an approximate solution to a time-independent one-dimensional differential equation, in this case the Schrödinger equation. Its principal applications for us will be in calculating bound-state energies and tunneling rates through potential barriers.

Note that both examples involve what is called the 'classical turning point', the point at which the potential energy V is approximately equal to the total energy E. This is the point at which the kinetic energy equals zero, and marks the boundaries between regions where a classical particle is allowed and regions where it is not.

If $E > V$, a classical particle has a non-zero kinetic energy and is allowed to move freely. *If* V were a constant, the solution to the one-dimensional Schrödinger equation would be $\psi(x) = Ae^{\pm ikx}$, where $k \equiv \sqrt{2m(E-V)}/\hbar$. This wf is oscillatory with constant wavelength $\lambda = 2\pi/k$ and constant amplitude A.

If V is not a constant, but instead varies very *slowly* on a distance scale of λ, then it is reasonable to suppose that ψ remains practically sinusoidal, except that the wavelength and amplitude change *slowly* with x (on a scale of λ).

Analogous comments can be made for the regions where $E < V$, wherein the solution to the Schrödinger equation for constant V is $\psi(x) = Ae^{\pm\kappa x}$, $\kappa \equiv \sqrt{2m(V-E)}/\hbar$. In these regions, a classical particle would not be allowed, but a quantum particle is said to 'tunnel'.

The WKB method involves implementing this basic point-of-view within the two kinds of regions. In-between these two types of regions lie the ‘classical turning points’ at which the two wf’s must be properly matched, leading to boundary conditions between the regions.

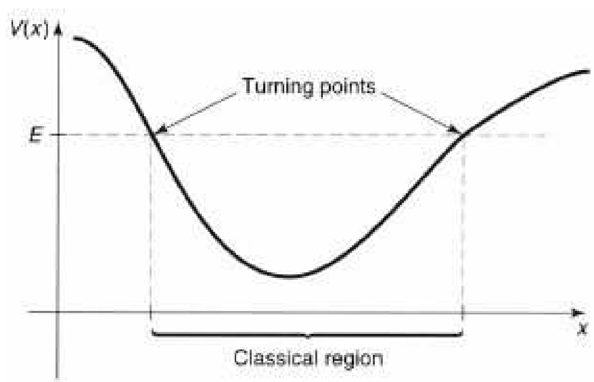


Figure 8.1 - Classically, the particle would be confined to the region where $E \geq V(x)$.

$E > V$: a 'classically allowed' region

The Schrödinger equation, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$, can be rewritten without approximation as $\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$, where $p(x) \equiv \sqrt{2m[E - V(x)]}$ is the classical formula for momentum. If $E > V$, then $p(x)$ is real and, with no loss of generality, one can write $\psi(x) = A(x)e^{i\phi(x)}$ where A and ϕ are both real functions of x.

Substituting this expression for ψ into the rewritten Schrödinger equation, we find $A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$. The real and imaginary parts of this equation must both hold. After some manipulation, these two eqs. become $A'' = A[(\phi')^2 - \frac{p^2}{\hbar^2}]$ and $(A^2\phi')' = 0$, which are together equivalent to the original Schrödinger equation.

The second equation is easily solved, leading to $A = \frac{C}{\sqrt{\phi'}}$ where C is a (real) constant.

The first equation cannot be solved in general, leading to the principal approximation of the WKB method:
assume that A varies sufficiently slowly that $A''/A \ll$ both $(\phi')^2$ and $p^2/\hbar^2$.

Then we can set the factor in brackets equal to zero, or $\frac{d\phi}{dx} = \pm\frac{p}{\hbar} \Rightarrow \phi(x) = \pm\frac{1}{\hbar}\int dx\, p(x)$.

Putting the solutions to both equations together, $\psi(x) \cong \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int dx\, p(x)}$, where C is now complex to absorb a constant of integration.

Note that $\psi^2 \cong \frac{|C|^2}{p(x)}$, which implies that the probability of finding a particle is smaller in those regions where it is ‘moving rapidly’, classically speaking.

This result can now be applied to the following problem: suppose that we start with the infinite square well, in which V is such that the walls rise vertically at, say, $x = 0$ and a. Let's vary that potential, however, by allowing $V(x)$ to vary moderately in the bottom of the infinite square well, a 'lumpy' potential.

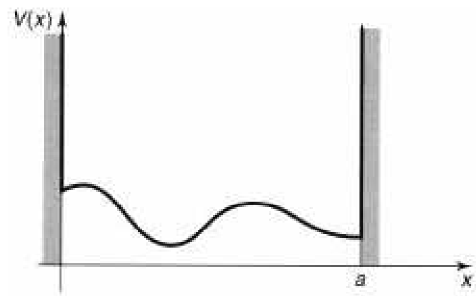


Figure 8.2 - An infinite 'square' well with a 'bumpy' bottom.

As before, the vertical walls require that the wf vanish at $x = 0$ and a. But, the variation of $V(x)$ in-between must be accounted for. Using the above approach, we find that the conditions on the constant of motion, k, appropriate to the square well, are replaced by $\int_0^a dx\, p(x) = n\pi\hbar$.

Note that this result reduces to the earlier result for the infinite square well when $V(x)$ is constant.

$E < V$: a tunneling region

Keeping the same definition of $p(x)$, it is now not real but imaginary. A similar set of manipulations leads to the solution: $\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int dx\, |p(x)|}$.

This equation allows us to treat the case of tunneling through a barrier by an otherwise free electron, for situations where the barrier potential $V(x) > E$ is abrupt and finite but not constant. It is shown in the text that the transmission coefficient is given by: $T \cong e^{-2\gamma}$, where $\gamma \equiv \frac{1}{\hbar} \int_0^a dx\, |p(x)|$.

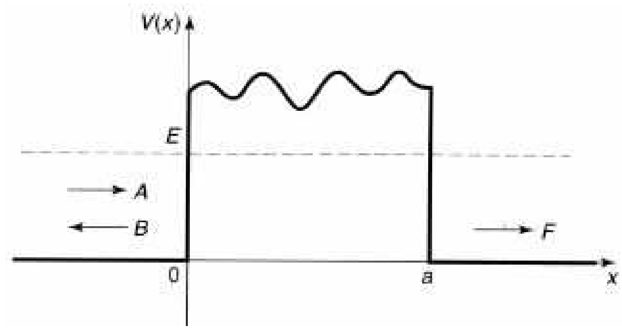


Figure 8.3 - Scattering from a rectangular barrier with a 'bumpy' top.

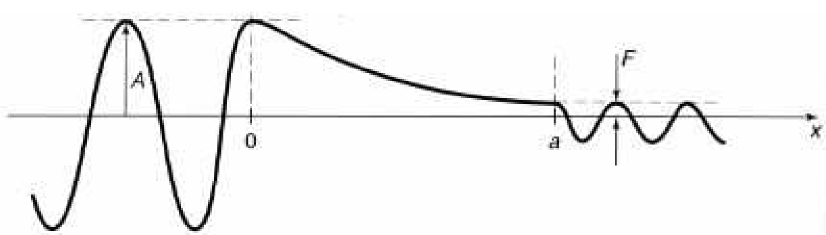


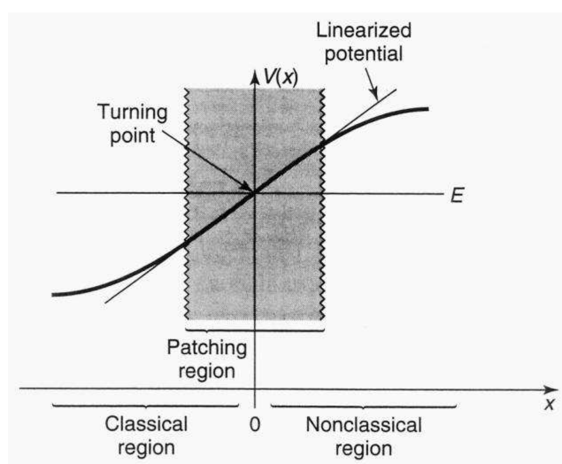
Figure 8.4 - Qualitative structure of the wavefunction for scattering from a high, broad barrier.

The turning points

At the classical turning points, the vanishing of the classical particle momentum prevents us from making the principal assumption of the WKB method; *i.e.*, that A''/A is small on the scales of $(\phi')^2$ and $p^2/\hbar^2$. This breakdown is obvious from the forms of the solutions: ψ becomes infinite as $p(x) \to 0$. This difficulty can be handled in the following way.

Clearly, we have no trouble with the case in which the potential rises abruptly (*i.e.*, a step function), wherein the region is vanishingly small in which $p \to 0$. It is reasonable to hope that we can handle the general case if we approximate the variation of the potential with a linear dependence on x.

Figure 8.7 - The right-hand turning point.



Let the 'right-hand' turning point occur at $x = 0$. In the vicinity of $x = 0$, let $V(x) \cong E + V'(0)x$. Substituting this into the Schrödinger equation, we get $\frac{d^2\psi}{dx^2} = \alpha^3 x\psi$, where $\alpha \equiv [\frac{2m}{\hbar^2}V'(0)]^{\frac{1}{3}}$. If we let $z \equiv \alpha x$, then $\frac{d^2\psi}{dz^2} = z\psi$. This is Airy's equation, which is 'well known', having solutions called the Airy functions.

The Airy functions, which are described in the text, are denoted by $Ai(z)$ and $Bi(z)$. These functions are both sinusoidal functions of $(-z)^{\frac{3}{2}}$ for $z \ll 0$. For $z \gg 0$, $Ai(z) \propto e^{-\frac{2}{3}z^{\frac{3}{2}}}$ and $Bi(z) \propto e^{+\frac{2}{3}z^{\frac{3}{2}}}$. Thus they are well suited to match a sinusoidal function (in z) on the left with an exponential function on the right (or *vice versa*, if necessary, with a suitable change of variables).

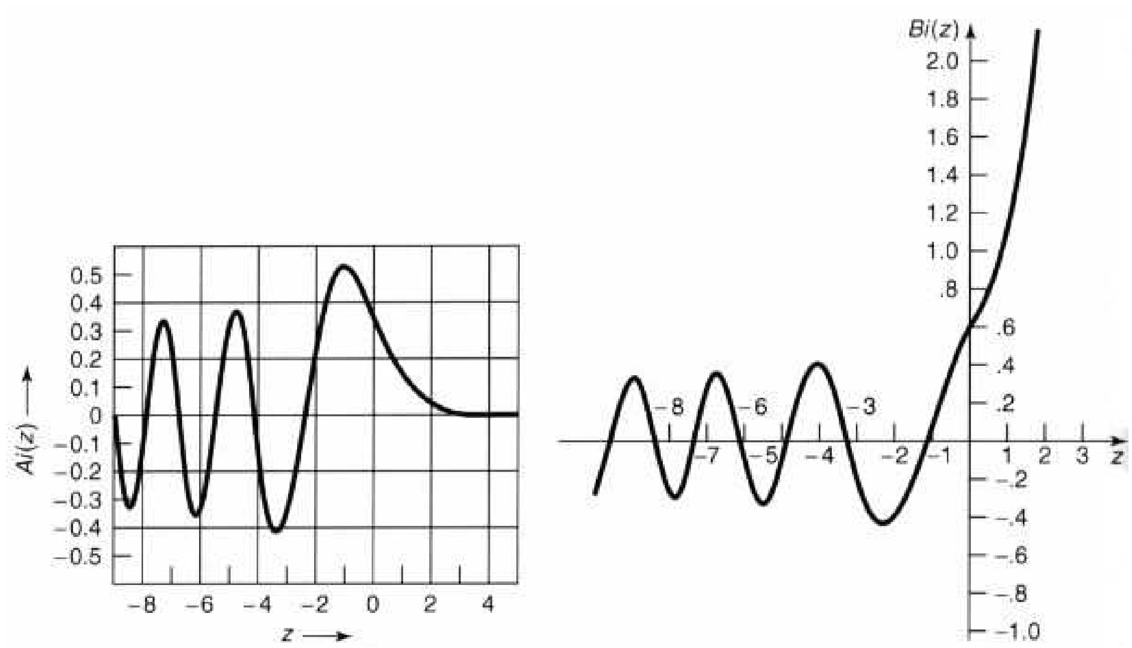


Figure 8.8 - Airy functions, of both types.

In order to use the Airy functions in the WKB solution to a problem, it is necessary to divide the region of the turning point into three regions: the patching region in which the Airy function is 'a good solution'; a region on each side of that in which the asymptotic forms of the Airy function overlap with the WKB solutions ('far' from the turning point).

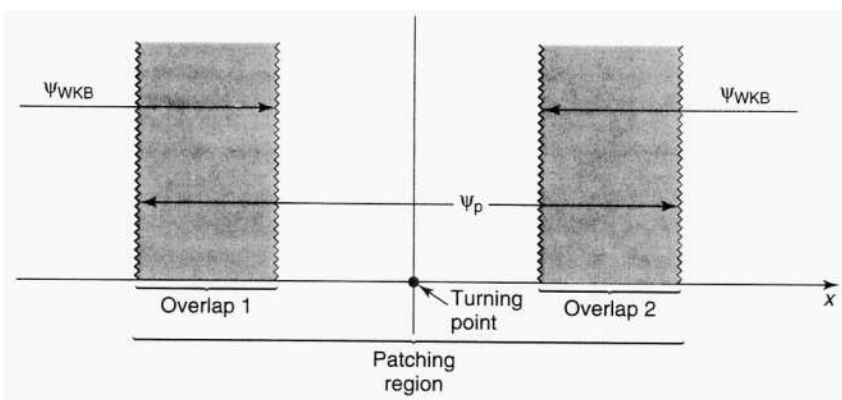


Figure 8.9 - Patching region and the two overlap zones.

Specifically, near the turning point we can write $p(x) \cong \sqrt{2m[E - E - V'(0)x]} = \hbar\alpha^{\frac{3}{2}}\sqrt{-x}$.

Thus, in overlap region 2, $\int_0^x dx' \, |p(x')| \cong \frac{2}{3}\hbar(\alpha x)^{\frac{3}{2}}$ and the WKB wf can be written $\psi(x) \cong \frac{D}{\sqrt{\hbar}\alpha^{\frac{3}{4}}x^{\frac{1}{4}}} e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}}$.

Using the asymptotic forms for $z \gg 0$, we can write the Airy functions in this same region as $\psi_p(x) \cong \frac{a}{2\sqrt{\pi}(ax)^{\frac{1}{4}}} e^{-\frac{2}{3}(ax)^{\frac{3}{2}}} + \frac{b}{\sqrt{\pi}(ax)^{\frac{1}{4}}} e^{+\frac{2}{3}(ax)^{\frac{3}{2}}}$.

Equating these two expressions leads to $a = \sqrt{\frac{4\pi}{\alpha\hbar}} D$ and $b = 0$.

Overlap region 1 is treated in a similar fashion, except that $b = 0$ and we use the asymptotic form of the Airy function Ai for $z \ll 0$.

These expressions lead to expressing the WKB solutions to the 'far' left using the same overall constant multiplier as on the 'far' right. Moving the turning point to x_2,

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

Having joined the two WKB solutions together correctly, one need refer no longer to the Airy connection formulas.