In the earlier examples (infinite square-well and barrier), $V$ changed instantaneously at the boundaries.

If $V$ changes gradually, then $|E - V|$ becomes arbitrarily small. Therefore,

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

also becomes arbitrarily small. But this then invalidates the assumption that

$$\left| \frac{A''}{A} \right| \ll \left| \frac{p^2}{\hbar^2} \right|$$

that forms the basis of the WKB approximation; i.e., as

$$E - V \rightarrow 0 \quad \text{or} \quad |p(x)| \rightarrow 0,$$

the wavelength becomes infinite so the requirement that $V(x)$ varies little over a wavelength becomes impossible to meet.
The solution is to approximate $V(x)$ by a straight line in this region, solve the T.I.S.E. for the linear $V(x)$, and then match the solution to the WKB solutions in two overlap regions:

- the point at which $E = V$ is called the turning point: e.g., $p(x)$ turns from real to imaginary at this point.

- the region in which the potential is assumed to be linear is called the patching region. $\psi$ in this region will be called $\psi_p$.

Let’s define the turning point as $x = 0$.

Away from the turning point, if $|E - V|$ is large,

$$
\psi \simeq \frac{1}{\sqrt{p(x)}} \left[ B e^{\frac{i}{\hbar} \int_{x}^{0} p(x')dx'} + C e^{-\frac{i}{\hbar} \int_{x}^{0} p(x')dx'} \right], \quad x < 0
$$

$$
\psi \simeq \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar} \int_{0}^{x} |p(x')|dx'}, \quad x > 0.
$$
FIGURE 8.7: Enlarged view of the right-hand turning point.
In the patching region, we linearize $V(x)$:

$$V(x) \simeq E + V'(0)x.$$  

Substituting this into the T.I.S.E. gives

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

or defining

$$\alpha \equiv \left(\frac{2m}{\hbar^2} V'(0)\right)^{1/3}$$,

where $\alpha$ has dimension of inverse length,

$$\frac{d^2\psi_p}{dx^2} = \alpha^3 x \psi_p.$$  

Now define the dimensionless variable $z \equiv \alpha x$, $dx = \frac{1}{\alpha} dz$, to get

$$\frac{d^2\psi_p}{dz^2} = z \psi_p.$$  \textit{Airy equation}
This second-order differential equation is called the Airy equation, and the two linearly independent solutions are called the Airy functions: \( Ai(z) \) and \( Bi(z) \).

Some of their properties are listed below (from Griffith).

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

<table>
<thead>
<tr>
<th>Differential Equation:</th>
<th>( \frac{d^2y}{dz^2} = zy. )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solutions:</strong></td>
<td>Linear combinations of Airy Functions, ( Ai(z) ) and ( Bi(z) ).</td>
</tr>
<tr>
<td><strong>Integral Representation:</strong></td>
<td>( Ai(z) = \frac{1}{\pi} \int_0^\infty \cos \left( \frac{s^3}{3} + sz \right) ds, )</td>
</tr>
<tr>
<td></td>
<td>( Bi(z) = \frac{1}{\pi} \int_0^\infty \left[ e^{-\frac{s^3}{3} + sz} + \sin \left( \frac{s^3}{3} + sz \right) \right] ds. )</td>
</tr>
<tr>
<td><strong>Asymptotic Forms:</strong></td>
<td>( Ai(z) \sim \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-\frac{2}{3}z^{3/2}} ) ( z \gg 0; ) ( Ai(z) \sim \frac{1}{\sqrt{\pi(-z)^{1/4}}} \sin \left[ \frac{2}{3} (-z)^{3/2} + \frac{\pi}{4} \right] ) ( z \ll 0. )</td>
</tr>
<tr>
<td></td>
<td>( Bi(z) \sim \frac{1}{\sqrt{\pi(-z)^{1/4}}} e^{\frac{2}{3}z^{3/2}} ) ( z \gg 0; ) ( Bi(z) \sim \frac{1}{\sqrt{\pi(-z)^{1/4}}} \cos \left[ \frac{2}{3} (-z)^{3/2} + \frac{\pi}{4} \right] ) ( z \ll 0. )</td>
</tr>
</tbody>
</table>
We will be interested in the asymptotic forms at large positive \( z \) and large negative \( z \):

\[
\begin{align*}
z \gg 0: & \\
Ai(z) & \simeq \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-\frac{2}{3}z^{3/2}}, \\
Bi(z) & \simeq \frac{1}{\sqrt{\pi}z^{1/4}} e^{\frac{2}{3}z^{3/2}},
\end{align*}
\]

\[
\begin{align*}
z \ll 0: & \\
Ai(z) & \simeq \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin \left[ \frac{2}{3}(-z)^{3/2} + \frac{\pi}{4} \right], \\
Bi(z) & \simeq \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos \left[ \frac{2}{3}(-z)^{3/2} + \frac{\pi}{4} \right].
\end{align*}
\]

Both \( Ai(z) \) and \( Bi(z) \) are oscillatory for negative \( z \); the significant difference in behavior is for positive \( z \). As \( z \) increases, \( Ai(z) \to 0 \) while \( Bi(z) \to \infty \).

Thus, the (approximate) wave function in the neighborhood of \( x = 0 \) is

\[\psi_p = aAi(\alpha x) + bBi(\alpha x).\]
FIGURE 8.8: Graph of the Airy functions.
We will now try to match this function with the WKB solutions on either side of the patching region. Note that this is more than just matching the ”boundary conditions”. We will force the functions to be identical in the overlap regions.

The overlap regions must be close enough to the turning point so that $V(x)$ is approximately linear in $x$ and yet far enough away from the turning point so that the WKB approximation is reliable. In practical applications, there usually exists such a region.
In the $\psi_{WKB}$ formulae, we need $\int |p(x)| \, dx$. In the overlap regions,

$$V \simeq E + V'(0)x$$

so

$$p(x) \simeq \sqrt{2m(E - \frac{\hbar}{m} - V')x} = \hbar \alpha^{3/2} \sqrt{-x}.$$

In overlap region 2, $x > 0$,

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

Thus,

$$\psi_{WKB} = \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar} \int_0^x |p(x')| \, dx'} = \frac{D}{\sqrt{\hbar \alpha^{3/4} x^{1/4}}} e^{-\frac{2}{3} (\alpha x)^{3/2}}.$$
Meanwhile we assume that

\[ z = \alpha x = \left( \frac{2m}{\hbar^2} V'(0) \right)^{1/3} x \]

is large so that we can use the large-\(z\) asymptotic form for the Airy functions. Again, in practical applications we can define a region in which \( z = \alpha x \) is large, but a linear approximation for \( V(x) \) is still valid.

In the large-\(z\) limit,

\[ \psi_p(x) \simeq \frac{a}{2\sqrt{\pi} (\alpha x)^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi} (\alpha x)^{1/4}} e^{\frac{2}{3}(\alpha x)^{3/2}}. \]
\[ \psi_{\text{WKB}} = \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar} \int_0^x |p(x')| \, dx'} = \frac{D}{\sqrt{\hbar \alpha}^{3/4} x^{1/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}}. \]

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

Comparing the two solutions, \( \psi_{\text{WKB}} \) and \( \psi_p \), in overlap region 2, we see that the only way \( \psi_{\text{WKB}} = \psi_p \) is if \( b = 0 \) and

\[ a = \sqrt{\frac{4\pi}{\alpha \hbar}} D. \]

\[ \Rightarrow \quad \psi_p = a Ai(\alpha x). \]
Now we repeat the procedure for overlap region 1.

Again \( p(x) = \hbar \alpha^{3/2} \sqrt{-x} \), but this time \( x \) is negative, so

\[
\int_x^0 p(x') \, dx' \simeq \frac{2}{3} \hbar (\alpha x)^{3/2}
\]

and the WKB wave function is

\[
\psi_{\text{WKB}} = \frac{1}{\sqrt{\hbar \alpha^{3/4} (-x)^{1/4}}} \left[ Be^{i\frac{2}{3} (-\alpha x)^{3/2}} + Ce^{-i\frac{2}{3} (-\alpha x)^{3/2}} \right].
\]

For the patching function \( \psi_p \), we already found \( b = 0 \) and therefore restrict ourselves to \( \psi_p = a \text{Ai}(\alpha x) \). Using the large negative \( z \) form of the Airy functions, we get

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

\[
= \frac{a}{\sqrt{\hbar \alpha^{3/4} (-x)^{1/4}}} \frac{1}{2i} \left( e^{i\pi/4} e^{i\frac{2}{3} (\alpha x)^{3/2}} - e^{-i\pi/4} e^{-i\frac{2}{3} (\alpha x)^{3/2}} \right).
\]
Comparing $\psi_{WKB} = \psi_p$ in overlap region 1, we see that they are the same if

$$\frac{a}{2i\sqrt{\pi}} e^{i\pi/4} = \frac{B}{\sqrt{\hbar} \alpha}$$

and

$$\frac{-a}{2i\sqrt{\pi}} e^{-i\pi/4} = \frac{C}{\sqrt{\hbar} \alpha}.$$

Putting this together with the constraint from overlap region 2, $a = \sqrt{\frac{4\pi}{\alpha \hbar}} D$, we can eliminate $a$ from the above two expressions and express $B + C$ in terms of $D$:

$$B = -i e^{i\pi/4} D \quad \text{and} \quad C = i e^{-i\pi/4} D.$$

Substituting these two expressions for $B$ and $C$ in the equation for $\psi_{WKB}$ (on previous page) gives the sine component only:

$$\psi_{WKB}(x) = \frac{2D}{\sqrt{p(x)}} \sin \left( \frac{1}{\hbar} \int_{x}^{0} p(x') \, dx' + \frac{\pi}{4} \right), \quad x < 0.$$
Summary:

By matching the solutions in the two overlap regions shown cross-hatched in the figure on the previous page, we have found the unknown coefficients $a, b, B, C$, in terms of $D$:

$$\psi(x) = \frac{2D}{\sqrt{p(x)}} \sin \left( \frac{1}{\hbar} \int_x^{x_2} p(x') \, dx' + \frac{\pi}{4} \right) \quad \text{if} \ x < x_2,$$

$$\psi(x) = \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar} \int_{x_2}^{x} |p(x')| \, dx'} \quad \text{if} \ x > x_2,$$

now expressed for a turning point at an arbitrary position $x_2$. 
FIGURE 7.36 WKB approximation for the fourth state of the harmonic oscillator, together with a graph of the Airy function. Also shown are the potential $V(\xi)$ and the fourth eigenenergy. Note the divergence of the WKB approximation at the turning point $\xi_4$. This calculation was performed previously by J. D. Powell and B. Craseman (*Quantum Mechanics*, Addison-Wesley, Reading, Mass., 1965). For extensive discussion of numerical techniques in the WKB analysis, see C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, New York, 1978.

(from “Intro to QM”, Liboff, 4th ed.)

\[
\xi^2 = \frac{m \omega_0}{\hbar} x^2
\]

Turning points for harmonic oscillator: $\xi_n^2 = (2n + 1)$
Example I: potential well with one vertical wall.

The solution has the above form but we must impose the boundary condition \( \psi(0) = 0 \):

\[
\psi(0) = \frac{2D}{\sqrt{p(0)}} \sin \left( \frac{1}{\hbar} \int_0^{x_2} p(x') dx' + \frac{\pi}{4} \right) = 0
\]
⇒ the argument of the sine function must be equal to \( n\pi, \ n = 1, 2, 3, \ldots \)

(Note that \( n \) cannot be 0 or less because the integral \( \int_0^{x_2} p(x')dx' \) is positive in this classical region.)

Thus,

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

or

\[
\int_0^{x_2} p(x')dx' = \left(n - \frac{\pi}{4}\right)\pi\hbar.
\]

This is the quantization condition on \( E \) since \( p(x) \equiv \sqrt{2m(E - V)} \). So, as usual, imposing boundary conditions leads to quantization of energy.
Application (for which we know the exact solution):

**Half-harmonic oscillator**

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

In this case,

\[
p(x) = \sqrt{2m(E - \frac{1}{2}m\omega^2 x^2)} \\
= \sqrt{2mE - m^2\omega^2 x^2} \\
= m\omega\sqrt{x_2^2 - x^2}
\]

where \(x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}\).

Note: at the turning point \(E = V\), by definition. Therefore \(p(x) = 0\) at the turning point. Also \(E = \frac{1}{2}m\omega^2 x_2^2\) or \(x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}\).

Since \(p(x_2) = 0\), \(x_2\) is the turning point.
The quantization condition is
\[ \int_0^{x_2} p(x) \, dx = \left(n - \frac{1}{4}\right) \pi \hbar, \quad n = 1, 2, 3, \ldots \]

So we need to evaluate the following integral
\[ \int_0^{x_2} p(x) \, dx = m\omega \int_0^{x_2} \sqrt{x_2^2 - x^2} \, dx. \]

Use integral table to find
\[ \int_0^a \sqrt{a^2 - x^2} \, dx = \frac{\pi}{4} a^2. \]
Thus,
\[ \int_0^{x_2} p(x) dx = m\omega \frac{\pi}{4} x_2^2 = \frac{\pi E}{2\omega} \]
and the quantization condition yields
\[ \frac{\pi E}{2\omega} = \left( n - \frac{1}{4} \right) \pi \hbar \]
or
\[ E_n = \left( 2n - \frac{1}{2} \right) \hbar \omega, \quad n = 1, 2, 3, \ldots \]
\[ = \left( \frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots \right) \hbar \omega. \]

These are the energies corresponding to the odd eigenfunctions of the full harmonic oscillator, which are the exact solutions of the half-harmonic oscillator. You did this problem (using the symmetry of the solutions and the boundary conditions) on a problem set in Physics 480.
Example II: potential well with no vertical walls.

In the region \( x_1 < x < x_2 \), matching at \( x_2 \) gave

\[
\psi(x) = \frac{2D}{\sqrt{p(x)}} \sin \left[ \frac{1}{\hbar} \int_{x}^{x_2} p(x') dx' + \frac{\pi}{4} \right], \quad x < x_2;
\]

matching at \( x_1 \) gives (see problem 8.9 in Griffith)

\[
\psi(x) = \frac{2D'}{\sqrt{p(x)}} \sin \left[ \frac{1}{\hbar} \int_{x_1}^{x} p(x') dx' + \frac{\pi}{4} \right], \quad x > x_1.
\]
In this case, applying the ”boundary conditions” means forcing the two wave functions in the well \((x_1 < x < x_2)\) to be the same:

\[
\frac{2D}{\sqrt{p(x)}} \sin \left[ \frac{1}{\hbar} \int_{x_2}^{x} p(x') dx' + \frac{\pi}{4} \right] = \frac{2D'}{\sqrt{p(x)}} \sin \left[ \frac{1}{\hbar} \int_{x_1}^{x} p(x') dx' + \frac{\pi}{4} \right]
\]

Clearly \(D\) and \(D'\) must have the same magnitude \((D = \pm D')\) and the difference in phase between the two sines must be a multiple of \(\pi\); for convenience we will write the r.h.s. (the reason will become clear on the next page) as

\[
-\frac{2D'}{\sqrt{p(x)}} \sin \left[ -\frac{1}{\hbar} \int_{x_1}^{x} p(x') dx' - \frac{\pi}{4} \right].
\]
Then the condition on the phase difference is

\[ \frac{1}{\hbar} \int_{x}^{x_2} p(x') dx' + \frac{\pi}{4} + \frac{1}{\hbar} \int_{x_1}^{x} p(x') dx' + \frac{\pi}{4} = n\pi \]

or, combining the integrals (this is why we multiplied the argument of the sine on the r.h.s. by $-1$):

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

This is the quantization condition that determines the energies for the typical case of a potential well with two sloping sides.
Compare it to the case of two vertical walls,
\[ \int_0^a p(x) dx = n\pi\hbar \]
and one vertical wall,
\[ \int_0^{x_2} p(x) dx = \left( n - \frac{1}{4} \right) \pi\hbar. \]
The three formulae differ only in the number that is subtracted from \( n \): 0, \( \frac{1}{4} \), or \( \frac{1}{2} \).

But the WKB approximation works best for large \( p \), or large \( |E - V| \), or large \( E \). Large \( E \) corresponds to large values of \( n \). For large \( n \), there is not a big difference between the above three formulae.
Conclusion: Through formulae like e.g.

\[ \int_{x_1}^{x_2} p(x) \, dx = \left( n - \frac{1}{2} \right) \pi \hbar \]

for a potential with two sloped walls, we can calculate the (approximate) allowed energies by simply evaluating one integral, without ever solving the Schrödinger equation.