WKB (Wentzel-Kramers-Brillouin) Approximation

1. We apply the WKB method to approximate solutions to equations of the form

\[ \varepsilon^2 y'' + q(x)y = 0, \quad \varepsilon \ll 1, \quad (1) \]

\[ y'' + q(\varepsilon x)^2 y = 0, \quad \varepsilon \ll 1, \quad (2) \]

and

\[ -y'' + q(x)y = \lambda^2 p(x)y, \quad \lambda \gg 1. \quad (3) \]

2. Example: The wave function \( \Psi(x, t) \) in one space dimension satisfies the Schrödinger equation

\[ i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi, \]

where \( V \) is the potential, \( m \) the mass and \( \hbar = h/2\pi \), \( h \) being Planck’s constant. We separate variables by setting

\[ \Psi(x, t) = \phi(t)y(x). \]

We set the \( x \) and \( t \) terms equal to the constant \( E \) and obtain the equation

\[ \frac{\hbar^2}{2m} y'' + (E - V(x))y = 0, \quad (4) \]

which is the time-independent Schrödinger equation. Set

\[ q(x) = E - V(x), \]

and

\[ \frac{\hbar^2}{2m} = \varepsilon^2 \]

to obtain an equation of the form (1).

3. The Nonoscillatory Case: If \( q(x) < 0 \) over the interval of interest, set \( q(x) = -k(x)^2 \), where \( k(x) > 0 \). The equation becomes

\[ \varepsilon^2 y'' - k(x)^2 y = 0. \quad (5) \]

Were \( k(x) \equiv k_0 \), a real constant, then (5) would have linearly independent, nonoscillatory solutions of the form \( \exp(\pm k_0 x/\varepsilon) \). This suggests the change of variable

\[ y = e^\frac{u(x)}{\varepsilon}. \quad (6) \]

The function \( u \) satisfies the equation

\[ \varepsilon u'' + u^2 - k(x)^2 = 0. \]
We set $u' = v$ to get
\begin{equation}
\varepsilon v' + v^2 - k(x)^2 = 0. \tag{7}
\end{equation}

4. Plug the regular perturbation expansion
\[ v = v_0 + \varepsilon v_1 + \cdots. \]

into (7):
\[ \varepsilon (v_0 + \varepsilon v_1 + \cdots)' + (v_0 + \varepsilon v_1 + \cdots)^2 - k(x)^2 = 0. \]

Matching powers of $\varepsilon$ gives the equations
\[ O(1): \quad v_0^2 - k(x)^2 = 0, \]
\[ O(\varepsilon): \quad 2v_0 v_1 = -v_0'. \]

From the $O(1)$ equation we obtain
\[ v_0(x) = \pm k(x). \]

Put this in the $O(\varepsilon)$ equation to get
\[ v_1(x) = -\frac{k'(x)}{2k(x)}. \]

Thus $v$ has the expansion
\begin{equation}
v(x) = \pm k(x) - \varepsilon \frac{k'(x)}{2k(x)} + O(\varepsilon^2). \tag{8}
\end{equation}

And since $v = u'$,
\[ u(x) = \pm \int_{\xi}^{x} k(z) \, dz - \frac{\varepsilon}{2} \ln \frac{k(x)}{k(\xi)} + O(\varepsilon^2), \tag{9}\]
where $\xi$ is arbitrary. Thus
\begin{align*}
y_\pm(x) &= e^{\frac{u(x)}{\varepsilon}} \\
&= \left[ \frac{k(\xi)}{k(x)} \right]^{\frac{1}{2}} e^{\pm \frac{1}{\varepsilon} \int_{\xi}^{x} k(z) \, dz} e^{O(\varepsilon)} \\
&= \left[ \frac{k(\xi)}{k(x)} \right]^{\frac{1}{2}} e^{\pm \frac{1}{\varepsilon} \int_{\xi}^{x} k(z) \, dz} (1 + O(\varepsilon)). \tag{10}
\end{align*}

In (10), we have approximations of two linearly independent solutions to (5), one with the plus sign and the other the minus. Thus, to leading order, any solution $y$ to (5) will have the WKB approximation
\begin{equation}
y(x) \approx y_\alpha(x) = \frac{c_1}{\sqrt{k(x)}} e^{\frac{1}{\varepsilon} \int_{\xi}^{x} k(z) \, dz} + \frac{c_2}{\sqrt{k(x)}} e^{-\frac{1}{\varepsilon} \int_{\xi}^{x} k(z) \, dz}, \tag{11}
\end{equation}
for constants $c_1$ and $c_2$.

5. **Example**: Find the WKB approximation to the solution of the equation

\[
\begin{cases}
\varepsilon^2 y'' - (1 + x)^2 y = 0, & \text{for } x > 0, \varepsilon \ll 1, \\
y(0) = 1, \\
y(\infty) = 0.
\end{cases}
\]

Take $\xi = 0$. The WKB approximation has the form

\[
y_a(x) = \frac{c_1}{\sqrt{1 + x}} e^{\frac{1}{\varepsilon} \int_0^x (1 + z) \, dz} + \frac{c_2}{\sqrt{1 + x}} e^{-\frac{1}{\varepsilon} \int_0^x (1 + z) \, dz}.
\]  
(12)

The second boundary condition forces us to take $c_1 = 0$. The first boundary condition then implies that $c_2 = 1$. Hence, to leading order,

\[
y(x) \approx y_a = \frac{1}{\sqrt{1 + x}} e^{-\frac{1}{\varepsilon} \int_0^x (1 + z) \, dz} = \frac{1}{\sqrt{1 + x}} e^{-\frac{1}{\varepsilon} \left( x + \frac{x^2}{2} \right)}.
\]  
(13)

6. **The Oscillatory Case**: When $q(x) > 0$ over the interval of interest, we set $q(x) = k(x)^2$, where $k(x) > 0$. The equation becomes

\[
\varepsilon^2 y'' + k(x)^2 y = 0.
\]  
(14)

W were $k(x) \equiv k_0$, a real constant, then (14) would have oscillatory solutions of the form $\exp(\pm i k_0 x / \varepsilon)$. This suggests the change of variable

\[
y = e^{i u(x) / \varepsilon},
\]  
(15)

for some real-valued function $u(x)$. The same analysis as the foregoing yields WKB approximations to linearly independent solutions to equation (14):

\[
y_{\pm}(x) = \frac{1}{\sqrt{k(x)}} e^{\pm i \int_\xi^x k(z) \, dz}.
\]  
(16)

To finish the derivation, use the Coates-Euler formula $e^{i\theta} = \cos \theta + i \sin \theta$, to rewrite $y_{\pm}$ terms of sines and cosines. Then use these to form the the WKB approximation to the general solution to (14):

\[
y(x) \approx y_a(x) = \frac{c_1}{\sqrt{k(x)}} \sin \left( \frac{1}{\varepsilon} \int_\xi^x k(z) \, dz \right) + \frac{c_2}{\sqrt{k(x)}} \cos \left( \frac{1}{\varepsilon} \int_\xi^x k(z) \, dz \right),
\]  
(17)
for constants $c_1$ and $c_2$. We can multiply and divide the above expression by

$$A = (c_1^2 + c_2^2)^{\frac{1}{2}},$$

and then rewrite it as

$$\frac{A}{\sqrt{k(x)}} \cos \left( \frac{1}{\varepsilon} \int_{\xi}^{x} k(z) \, dz - \phi \right), \tag{18}$$

where

$$\phi = \arctan \frac{c_1}{c_2}$$

is the phase.

7. **Example**: Consider the time-independent Schrödinger equation (4). If $E > V(x)$, we have the oscillatory case. Since $\hbar$ is small, we can apply the WKB method to obtain the approximate solution

$$y_a(x) = \frac{A}{(E - V(x))^{\frac{1}{4}}} \cos \left( \frac{\sqrt{2m}}{\hbar} \int_{\xi}^{x} \sqrt{E - V(z)} \, dz - \phi \right).$$