WKB Approximation

\[-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\]

\[\frac{\hbar}{i} \frac{d}{dx} S(x)\]

\[\psi(x) = A(x) e^{i\frac{\hbar}{\epsilon} S(x)}\]

Slow varying potential \(\Rightarrow\)

\[S(x) = \pm \int_{x'}^x p_{cl}(x') \, dx'\]

\[p_{cl}^2(x) = 2m (E - V(x))\]

\[A(x) = \frac{1}{|p_{cl}(x)|}\]

Form of solution
\[ \psi(x) = \begin{cases} \frac{c_I}{\sqrt{P_{cc}(x)}} \cos \left( \int \sqrt{P_{cc}(x')} \, dx' \right) & \text{region I} \\ + i \int \sqrt{P_{cc}(x')} \, dx' & \text{region II} \\ - \int \sqrt{P_{cc}(x')} \, dx' & \text{region III} \end{cases} \]

Normally one would assume \( \psi(x) \) and its first derivative are continuous at the classical turning points \( A \) and \( B \).

The problem is that the condition for the approximation to be valid breaks down at the classical turning points.
In order to satisfy the boundary conditions, approximate the potential near the classical turning points by a linear potential

\[ V(x) \approx V(x_A) + \frac{dV}{dx}(x_A)(x - x_A) \]

\[ V(x) \approx V(x_B) + \frac{dV}{dx}(x_B)(x - x_B) \]

\[ S \text{ olve } \]

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \left[ V(x_A) + \frac{dV}{dx}(x_A)(x - x_A) \right] \psi = E \psi \]

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \left[ V(x_B) + \frac{dV}{dx}(x_B)(x - x_B) \right] \psi = E \psi \]
Note for the turning point, 

\[ E = V(x_a) = V(x_b) \]

we also use the notation 

\[ \frac{dV}{dx} (x_a) = -F_a \]
\[ \frac{dV}{dx} (x_b) = -F_b \]

which represent constant forces.

The third step is to match the WKB solutions to the solutions of 

\[ \frac{d^2 \psi}{dx^2} = -\frac{2m}{\hbar^2} F_a (x - x_a) \psi \]
\[ \frac{d\psi}{dx} = -\frac{2m}{\hbar^2} F_b (x - x_b) \psi \]

To solve equations of this general form
Let
\[ \sigma = -\left(\frac{2mF}{\hbar^2}\right)^{1/3} (X - X_\pm) \]

\[ (\pm = A \lor B) \]

\[ \frac{d}{dx} = \frac{d\sigma}{dx} \frac{d}{d\sigma} = -\left(\frac{2mF}{\hbar^2}\right)^{1/3} \frac{d}{d\sigma} \]

\[ \frac{d^2}{dx^2} = \left(\frac{2mF}{\hbar^2}\right)^{2/3} \frac{d^2}{d\sigma^2} \]

With this change of variable, the Schrödinger equation becomes

\[ \left(\frac{2mF}{\hbar^2}\right)^{2/3} \frac{d^2}{d\sigma^2} = -\frac{2mF}{\hbar^2} \left(-\left(\frac{\hbar}{2mF}\right)^{1/3} \sigma \right) \]

\[ = \left(\frac{2mF}{\hbar^2}\right)^{2/3} \sigma \]

Canceling the \(\left(\frac{2mF}{\hbar^2}\right)^{2/3}\) gives the following equation

\[ \frac{d^2}{d\sigma^2} A(X) = 6 A(X) \]
This equation is called Airy's equation. The solutions are called Airy functions. This is a second order linear differential equation. It has 2 independent solutions

\[ \text{Ai}(\sigma) \text{ and } \text{Bi}(\sigma) \]

where

\[ \text{Ai}(\sigma) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i(s\sigma + \frac{s^3}{3})} ds \]

\[ = \frac{1}{\pi} \int_{0}^{\infty} \cos(s + \frac{s^3}{3}) ds \]

These are well defined functions like \( \sin x \) and \( \cos x \) or Bessel functions.
In fact,
\[ \text{Ai}(x) = \sqrt{\frac{x}{3\pi}} K_{i/3} \left( \frac{2}{3} x^{3/2} \right) \]
where \( K_{i/3} \) is a Bessel function with \( \nu = 1/3 \)

* some properties

1. \[ \int_{-\infty}^{\infty} \text{Ai}(\sigma) \, d\sigma = 1 \]

2. \[ \int_{-\infty}^{\infty} \text{Ai}(\sigma-x) \, \text{Ai}(\sigma-y) \, d\sigma = \delta(x-y) \]

3. The important properties for the WKB approximation are

\[ \lim_{\sigma \to -\infty} \text{Ai}(\sigma) = \frac{1}{\sqrt{4\pi}} e^{-\frac{1}{4} \sigma^2} \]

\[ \lim_{\sigma \to -\infty} \text{Ai}(\sigma) = \frac{1}{2\sqrt{\pi}} e^{-\frac{1}{4} \sigma^2} \cos \left( \frac{3}{2} \sigma^2 - \frac{\pi}{2} \right) \]
we want to compare the asymptotic solutions to the WKB solutions in the three regions.

To do this we need to express \( \sigma \) in terms of the classical moments:

\[
P_{\text{cl}}^{2}(x) = 2m \left( E - V(x_{\pm}) + F_{\pm}(x-x_{\pm}) \right)
\]

\[
P_{\text{cl}}^{-1}(x) = 2m F_{\pm}(x-x_{\pm})
\]

where \( F_{\pm} = -\frac{dV}{dx}(x_{\pm}) \) \( x_{\pm} = x_{A} \text{ or } x_{B} \)

\[
\sigma = -\left( \frac{2m F_{\pm}}{\hbar c} \right)^{1/3}(x-x_{\pm})
\]

\[
P_{\text{cl}}^{2}(x) = -2m F_{\pm} \left( \frac{\hbar c}{2m F_{\pm}} \right)^{1/3} \sigma
= -\left( \frac{2m F_{\pm}}{\hbar c} \right)^{2/3} \sigma
\]

\[
\sigma = -\frac{P_{\text{cl}}^{2}}{\left( \frac{2m F_{\pm}}{\hbar c} \right)^{2/3}}
\]
\[
\frac{2}{3} G^{3/2} = \frac{2}{3} \left(-\frac{P_{cl}}{(2mE \hbar)^{2/3}}\right)^{3/2}
\]

\[
= -\frac{2}{3} \frac{P_{cl}^3}{2mE \hbar}
\]

\[
\frac{2}{3} G^{3/2} = -\frac{P_{cl}^3}{3mE \hbar}
\]

\[
\frac{E}{\hbar} \int_{x_i}^{x_f} p_{cl}(x) \, dx = \frac{1}{\hbar} \int_{x_i}^{x_f} \sqrt{2mE (x-x_n)^3} \, dx
\]

\[
= \frac{2}{3} \frac{2 \sqrt{2mE}}{\hbar} (x-x_n)^{3/2} + \text{const}
\]

\[
= \frac{3}{2} \frac{\sqrt{2mE}}{\hbar} \left(\frac{P_{cl}}{2mE \hbar}\right)^{3/2}
\]

\[
= \frac{2}{3} \frac{P_{cl}}{2mE \hbar} = \frac{P_{cl}^3}{3mE \hbar}
\]

This means that the asymptotic forms of the Airy function can be expressed in terms of the classical momentum.

\[
\sigma^{1/4} = \left[\left(\frac{3}{2} \frac{P_{cl}^3}{3mE \hbar}\right)^{2/3}\right]^{1/4} = \text{const} \times P_{cl}^{1/4}
\]
the asymptotic form in terms of the classical momenta became

\[
\lim_{\sigma \to \infty} A_{\sigma}(\zeta) \rightarrow \frac{\text{const}}{2\sqrt{\pi}} \frac{1}{\sqrt{P_{cc}(\zeta)}} e^{-\int P_{cc}(x) \, dx / \sqrt{\zeta}}
\]

\[
\lim_{\sigma \to -\infty} A_{\sigma}(\zeta) \rightarrow \frac{\text{const}}{2\sqrt{\pi}} \frac{1}{\sqrt{P_{cc}(\zeta)}} \cos \left( \int P_{cc}(x) \, dx + \frac{\pi}{4} \right)
\]

The important properties are:

1) The constants are the same (they depend on the turning point).
2) They have the same form as the WKB solutions.

The relevant factors in matching are the path of 2 and the phase.
\[ X < X_A \]

\[ \psi(x) = \frac{CA}{\sqrt{P_{cl}(x)}} \cdot \left[ -\int_{x_A}^{x} P_{cl}(y) dy \right]^1 \]

\[ X_A < x < X_B \]

\[ \psi(x) = \frac{CA}{2 \sqrt{P_{cl}(x)}} \cos \left( \frac{1}{2} \int_{X_A}^{x} P_{cl}(x') dx' - \frac{\pi}{4} \right) \]

\[ X > X_B \]

\[ \psi(x) = \frac{CB}{\sqrt{P_{cl}(x)}} \cos \left( \frac{1}{2} \int_{X_B}^{x} P_{cl}(x') dx' - \frac{\pi}{4} \right) \]

In order to get the quantization we need to use the two equations for \( X_A < x < X_B \). Clearly, we must have

\[ CB = \pm CA \quad \text{and} \quad \alpha \]

\[ \cos \left( \frac{1}{2} \int_{X_A}^{x} P_{cl}(x') dx' - \frac{\pi}{4} \right) = \pm \cos \left( \frac{1}{2} \int_{X_B}^{x} P_{cl}(x') dx' - \frac{\pi}{4} \right) \]
in order to compute then we note
\[ \cos \left( \frac{1}{\hbar} \int_{x}^{x_B} P_{cl}(x') dx' - \frac{\pi}{4} \right) = \]
\[ \cos \left( -\int_{x_A}^{x} P_{cl}(x') dx' + \int_{x}^{x_B} P_{cl}(x') dx' - \frac{\pi}{4} \right) = \]
\[ \cos \left( -\int_{x_A}^{x} P_{cl}(x') dx' + \int_{x}^{x_B} P_{cl}(x') dx' + \frac{\pi}{4} \right) = \]
\[ \pm \cos \left( \int_{x_A}^{x_B} P_{cl}(x') dx' - \frac{\pi}{4} \right) \]

The x dependence is in the red under linear factors
\[ \pm = \cos \left( -\frac{1}{\hbar} \int_{x_A}^{x_B} P_{cl}(x') dx' + \frac{\pi}{4} - \frac{\pi}{4} \right) \]
\[ \int_{x_A}^{x_B} P_{cl}(x') dx' = \pi n + \frac{1}{2} \pi \]
\[ \pm = \cos \left( n \pi + \frac{1}{2} \pi \right) \]

This is the WKB quantization condition.
Application - Harmonic oscillation

\[ P_{cl} = 2m \left( E - \frac{1}{2} kx^2 \right) \]

\[ P_{cl} = 0 \Rightarrow x_{\pm} = \pm \sqrt{\frac{2E}{k}} \]

\[(n - \frac{1}{2}) \pi \tau = \int_{-\sqrt{2E/k}}^{\sqrt{2E/k}} \sqrt{2m \left( E - \frac{1}{2} kx^2 \right)} \, dx \]

\[ = \sqrt{2mE} \int_{-\sqrt{2E/k}}^{\sqrt{2E/k}} \sqrt{1 - \frac{k}{2E} x^2} \, dx \]

Let \[ u = \sqrt{\frac{k}{2E}} x \quad du = \sqrt{\frac{2E}{k}} \, dx \]

\[ = \sqrt{2mE} \times \sqrt{\frac{2E}{k}} \int_{-1}^{1} \sqrt{1 - u^2} \, du \]

\[ \text{area of semicircle} \quad \Omega = \frac{1}{2} \pi \]

\[ \tau = \sqrt{\frac{m\Omega}{E}} \]

\[ \tau = \sqrt{\frac{k}{2m}} (n + \frac{1}{2}) \]

which is the exact oscillation eigenvalues.