Example 1 : Particle in a box

$$\delta y'' = -y \quad \text{as} \quad \delta \to 0$$

with $y(0) = 0, \quad y(1) = 1.$

comparing to our notation $\varepsilon^2 y'' = Q(x) y$

$$\delta = \varepsilon^2, \quad Q(x) = -1$$

$$\Rightarrow y(x) \sim \frac{c_1}{(-)^{1/4}} \exp\left[\frac{1}{\sqrt{\delta}} \int \sqrt{-1} \, dx'\right]$$

$$+ \frac{c_2}{(-)^{1/4}} \exp\left[-\frac{1}{\sqrt{\delta}} \int \sqrt{-1} \, dx'\right]$$

$$\sim c_1' \, e^{\frac{ix}{\sqrt{\delta}}} + c_2' \, e^{-\frac{ix}{\sqrt{\delta}}}$$

Imposing the b.c.'s,

$$y(x) \sim \sin(x/\sqrt{\delta}) / \sin(1/\sqrt{\delta})$$

which is the exact solution.

Example 2: Particle in a linear Potential

$$y'' = xy$$

We will soon see that WKB regime is $x \gg 1$. Physically,

$$\underbrace{\frac{\hbar^2}{2m}}_{\varepsilon^2} \frac{d^2\psi}{dx^2} = (V(x) - E)\psi \equiv -p^2(x)\psi$$

and WKB holds when $|p(x)|^2 \gg \left|\frac{dp}{dx}\right|$.
(equivalently, $|d\lambda / dx| \ll 1$ where $\lambda \sim 1/p$)
(we will derive a more rigorous condition later).

In this case, $|p(x)|^2 = x \quad \left|\frac{dp}{dx}\right| = 1$.

So for WKB to hold, $x \gg 1$.

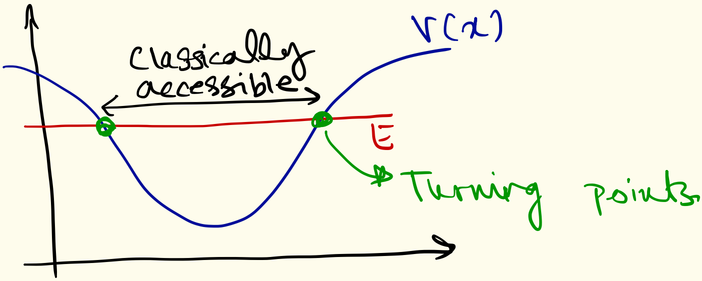
Here, $Q(x) = x, \quad \varepsilon = 1$.

$$\Rightarrow y(x) \sim \frac{c_1}{x^{1/4}} \exp\left[\int^x \sqrt{x'}\, dx'\right] + \frac{c_2}{x^{1/4}} \exp\left[-\int^x \sqrt{x'}\, dx'\right]$$

$$\sim \frac{c_1}{x^{1/4}} \exp\left[\frac{2}{3} x^{3/2}\right] + \frac{c_2}{x^{1/4}} \exp\left[-\frac{2}{3} x^{3/2}\right]$$

Matched WKB Asymptotics

WKB clearly breaks down when $Q(x) = 0$ i.e. $V(x) = E$, which correspond to classical turning points.



The requirement for the validity of WKB are actually more stringent. This is because WKB is an asymptotic expansion and is generally, <u>not</u> convergent.

Recall the difference between an asymptotic series and convergent series:

Asymptotic series:

$$f(x) \sim \sum_{n=0}^{\infty} a_n (x - x_0)^n \quad \text{as } x \to x_0$$

if

$$\left| f(x) - \sum_{n=0}^{N} a_n (x-x_0)^n \right| \ll (x-x_0)^N$$

for every fixed N, as $x \to x_0$.

Convergent series:

$$\left| f(x) - \sum_{n=0}^{N} a_n (x-x_0)^n \right| \to 0 \quad \text{as}$$

$N \to \infty$ for fixed x.

assuming $|x - x_0| < R$ where R is the radius of convergence.

for WKB to work, one requires,

$$S_1(x) \ll \frac{S_0(x)}{\varepsilon} \quad \text{as} \quad \varepsilon \to 0$$

$$S_2(x) \ll \frac{S_1(x)}{\varepsilon} \quad \text{as} \quad \varepsilon \to 0$$

$$\vdots$$

$$S_{n+1}(x) \ll \frac{S_n(x)}{\varepsilon} \quad \text{as} \quad \varepsilon \to 0.$$

uniformly in x.

However, since the asymptotic expansion appears in the exponent, there is a more stringent requirement: If one truncates the series at order N, then $\varepsilon^N S_{N+1}(x) \ll 1$ as $\varepsilon \to 0$. This ensures that

$$\exp(\varepsilon^N S_{N+1}(x)) = 1 + O(\varepsilon^N S_{N+1}(x))$$

$$\Rightarrow \quad \frac{y(x) - \exp\left[\frac{1}{\varepsilon}\sum_{n=0}^{N} \varepsilon^{N} S_N(x)\right]}{y(x)}$$

$$\sim \quad \varepsilon^{N} S_{N+1}(x) \ll 1 .$$

as $\varepsilon \to 0$.

Lets once more look at the first three terms in the expansion:

$$y(x) \sim e^{\frac{S_0(x)}{\varepsilon} + S_1(x) + \varepsilon S_2(x)}$$

If we keep just the first term in the exponent, then the condition $S_1(x) \ll 1$ is generally not satisfied. This is geometrical optics. Keeping the first two terms is better since is $S_2(x)$ is bounded in the region of interest then $\varepsilon S_2(x) \ll 1$ is indeed satisfied.

This is 'physical optics' approximation.

Consider the example of Airy's function again,

$$S_0 = \pm \frac{2}{3} x^{3/2}$$

$$S_1 = -\frac{1}{4} \log(x)$$

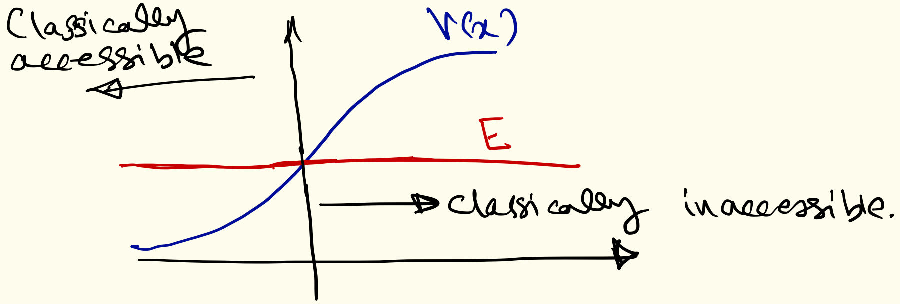
$$S_2 = \pm \frac{5}{48} x^{-3/2} \quad \text{(check!)}$$

Since $\varepsilon = 1$, $\left|\frac{S_0}{\varepsilon}\right| \gg |S_1| \gg |\varepsilon S_2|$

as $x \to \infty$ is indeed satisfied.

Patched WKB Solutions

We first consider only one turning point, located at $x = 0$ with $x<0$ as the classically accessible region.

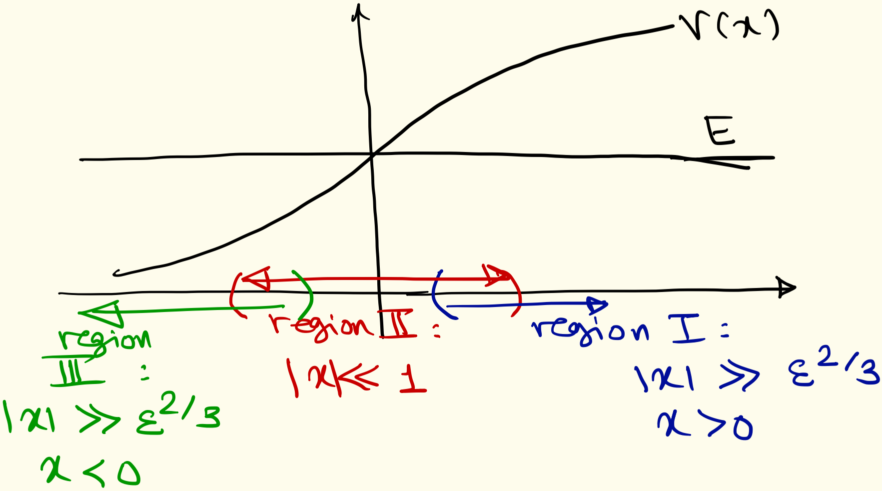


The Schrodinger's eqn is:

$$\varepsilon^2 y'' = Q(x)\, y \qquad Q(x) = V(x) - E$$

$Q(x) \sim ax$ near $x=0$ with $a>0$.

Let's divide the x-axis into three regimes:



The main point of WKB theory is that regions I and III, where physical optics approximation does work have non-zero overlap with region II, which encloses the turning point. Let's see how.

Let's determine the boundary of region I : since $Q(x) \sim ax$, $S_0(x) \sim \pm \frac{2}{3} x^{3/2}$

$S_1(x) \sim -\frac{1}{4}\log(x)$, $S_2(x) \sim \pm x^{-3/2}$

We require $\dfrac{S_0(x)}{\varepsilon} \gg S_1(x)$

$$\frac{S_1(x)}{\varepsilon} \gg S_2(x)$$

or, $\dfrac{x^{3/2}}{\varepsilon} \gg |\log(x)|$

and $\dfrac{|\log(x)|}{\varepsilon} \gg x^{-3/2}$

Both conditions imply that

$\boxed{x \gg \varepsilon^{2/3}}$ This is the lower limit for WKB to work, assuming $Q(x) \sim x$.

At some point, the linear approximation breaks down.

Taylor expanding $Q(x) \sim ax + bx^2$

$\Rightarrow$ The leading WKB term is

$$\exp \frac{1}{\varepsilon} \int^x \sqrt{Q(t)}\, dt$$

$$\sim \exp \frac{1}{\varepsilon} \int^x \sqrt{at + bt^2}\, dt$$

$$\sim \exp \frac{1}{\varepsilon} \frac{a^{1/2} x^{3/2}}{\varepsilon} + \frac{x^{5/2}}{\varepsilon} \frac{b}{\sqrt{a}}$$

If we only want to keep the first term, then $\boxed{\varepsilon \gg x^{5/2}}$

Thus, the part of region I, where the linear approximation works is

$$\boxed{\varepsilon^{2/3} \ll x \ll \varepsilon^{2/5}}$$

Now we want to match this onto region II, where we solve the differential eqn: $\varepsilon^2 y''' = axy$ directly. Defining $t = \varepsilon^{-2/3} a^{1/3} x$, this becomes $d^2y/dt^2 = ty$ whose soln. is the Airy's functions.

$$y \sim a\, Ai(t) + b\, Bi(t)$$

where for $t \gg 1$,

$$Ai(t) \sim t^{-1/4} e^{-\frac{2}{3} t^{3/2}}$$

$$Bi(t) \sim t^{-1/4} e^{+2/3\, t^{3/2}}$$

For these asymptotics to be valid we require $t \gg 1$ or $x \gg \varepsilon^{2/3}$.

Of course we still need $x \ll 1$ so that the eqn $\varepsilon^2 y'' = axy$ is valid to begin with. Thus, there is a overlap between region I ($\varepsilon^{2/3} \ll x \ll \varepsilon^{2/5}$) and region II ($\varepsilon^{2/3} \ll x \ll 1$), namely,

$$\varepsilon^{2/3} \ll x \ll \varepsilon^{2/5}.$$

In this region,

$$y_{II}(x) \sim a\, x^{-1/4} \varepsilon^{1/6} e^{-\frac{2a^{1/2}x^{3/2}}{3\varepsilon}} + b\, x^{-1/4} \varepsilon^{1/6} e^{+\frac{2a^{1/2}x^{3/2}}{\varepsilon 3}}$$

$$y_I(x) \sim c\, a^{-1/4} x^{-1/4} e^{-\frac{2a^{1/2}x^{3/2}}{3\varepsilon}}$$

Thus, chosing $c \sim \varepsilon^{1/6} a$, the two solutions can be 'matched'.

Let's do similar matching between region II and III:

In region II, we already determined that the coefficient of $Bi(x)$ vanishes. Thus, we need the asymptotic expression for $Ai(x)$ for large, negative x. It is given by,

$$Ai(t) \sim (-t)^{-1/4} \sin\left[\frac{2}{3}(-t)^{3/2} + \frac{\pi}{4}\right]$$

$$\sim (-x)^{-1/4} \varepsilon^{1/6} \sin\left[\frac{2}{3\varepsilon}(-x)^{3/2} + \frac{\pi}{4}\right]$$

This needs to be matched onto the WKB soln. in the linear regime of region III: $(\varepsilon^{2/5} \gg |x| \gg \varepsilon^{2/3})$

$$y_{III}(x) \sim c_1 \frac{1}{[-|x|]^{1/4}} \exp \frac{1}{\varepsilon} \int^x \sqrt{-|x'|}\, dx'$$

$$+ c_2 \frac{1}{[-|x|]^{1/4}} \exp\left[-\frac{1}{\varepsilon} \int^x \sqrt{-|x'|}\, dx'\right]$$

$$\sim \frac{c_1}{|x|} \cdot \exp\left[\frac{i}{\varepsilon} |x|^{3/2} \frac{2}{3} + \frac{i\pi}{4}\right]$$

$$+ \frac{c_2}{|x|} \exp\left[-\frac{i}{\varepsilon} |x|^{3/2} \frac{2}{3} + \frac{i\pi}{4}\right]$$

Choosing $c_1 \sim \varepsilon^{1/6}$

$$c_2 \sim \varepsilon^{1/6} \times -1 \times e^{-\frac{i\pi}{2}}$$

does the trick of matching with $y_{II}(x)$ (i.e. the asymptotics of $Ai(x)$).

Thus the WKB 'connection formulae' are:

$$y_I(x) \sim \frac{1}{[Q(x)]^{+1/4}} \exp\left[-\frac{1}{\varepsilon}\int_0^x \sqrt{Q(t)}\,dt\right]$$

$$x > 0, \quad x \gg \varepsilon^{2/3}.$$

$$y_{II}(x) \sim \varepsilon^{-1/6} \, Ai\left(\varepsilon^{-2/3} a^{1/3} x\right)$$

$$|x| \ll 1.$$

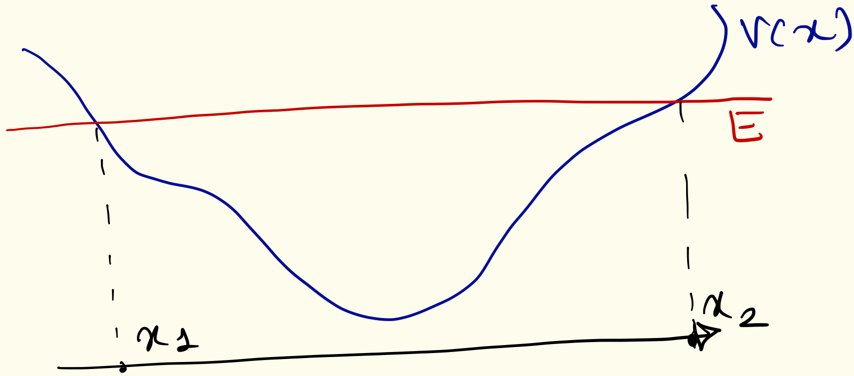
$$y_{III}(x) \sim \frac{1}{[-Q(x)]^{1/4}} \sin\left[\int_x^0 \frac{1}{\varepsilon} \sqrt{-Q(t)}\,dt + \frac{\pi}{4}\right]$$

$$x < 0, \quad |x| \gg \varepsilon^{2/3}.$$

Note the order we solved the problem: region I $\to$ region II $\to$ region III. This is the only order the logic works here.

Two Turning Points:

Bohr - Sommerfeld Quantization



Approaching from $x > x_2$.

For $x - x_2 \gg \varepsilon^{2/3}$,

$$\psi \sim [Q(x)]^{-1/4} \exp\left[-\frac{1}{\varepsilon}\int_{x_2}^{x} \sqrt{Q(t)}\, dt\right]$$

for $x_1 < x < x_2$

$$\psi \sim C_1 [Q(x)]^{-1/4} \sin\left[\frac{1}{\varepsilon}\int_{x}^{x_2} \sqrt{Q(t)}\, dt + \pi/4\right]$$

Approaching from $x < x_1$.

for $\quad |x - x_1| \gg \varepsilon^{2/3} \quad x < x_1$

$$\psi \sim [a(x)]^{-1/4} \exp -\frac{1}{\varepsilon}\int_x^{x_1} \sqrt{a(t)}\, dt$$

and
$$\psi \sim C_2[-a(x)]^{-1/4} \sin\left[\frac{1}{\varepsilon}\int_{x_1}^{x} \sqrt{-a(t)}\, dt + \pi/4\right]$$

Now we have two different looking expressions for the region $x_1 < x < x_2$.

They must match.

$$C_2 \sin \frac{1}{\varepsilon}\left[\int_{x_1}^{x} \sqrt{-a(t)}\, dt + \pi/4\right]$$

$$= C_1 \sin\left[\frac{1}{\varepsilon}\int_x^{x_2} \sqrt{-a(t)}\, dt + \pi/4\right]$$

$$= -C_1 \sin\left[-\frac{1}{\varepsilon}\int_x^{x_2} \sqrt{-a(t)} - \frac{\pi}{4}\right]$$

$$= -c_1 \sin\left[\frac{1}{\varepsilon}\int_{x_1}^{x}\sqrt{a(t)}\,dt + \pi/4 - \left[\frac{1}{\varepsilon}\int_{x_1}^{x_2}\sqrt{a(t)}\,dt + \frac{\pi}{2}\right]\right]$$

Choosing $c_1 = (-)^n c_2$

and $$\int_{x_1}^{x_2}\sqrt{a(t)}\,dt = \left(n+\frac{1}{2}\right)\pi,$$

the equation is solved.

Thus we obtain the quantization condition.

$$\frac{\int_A^B \sqrt{a(t)}\,dt}{\varepsilon} = \left(n+\frac{1}{2}\right)\pi$$

Recall that $a = V(x) - E$

$$\varepsilon^2 = \frac{\hbar^2}{2m} \Rightarrow \int_A^B \sqrt{\frac{[E - V(x)]}{\hbar^2/2m}}\,dx = \left(n+\frac{1}{2}\right)\pi$$