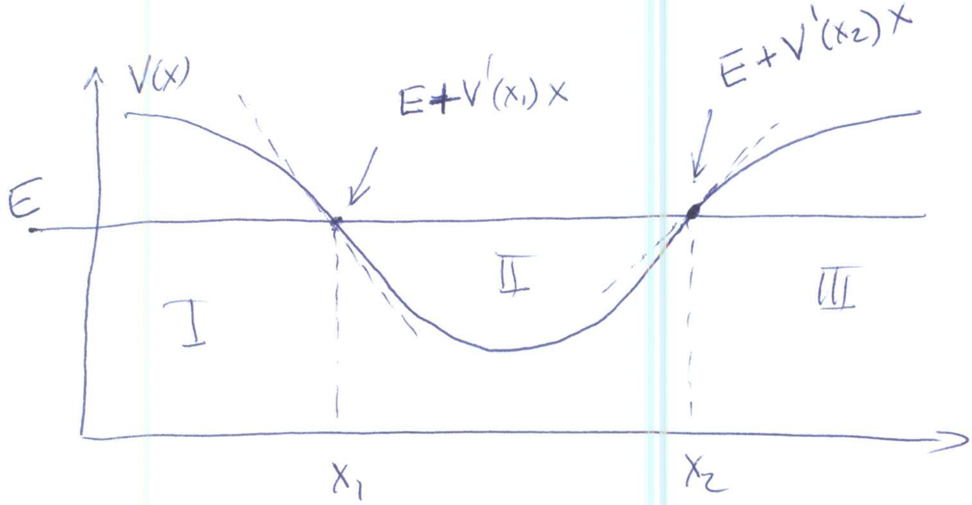
The connection formulae in WKB



Let us consider this general potential V(x)

In region I, for to the left of x_1 the WKB solution is

$$\varphi_I = \frac{1}{\sqrt{\varkappa}} \exp\left[\cdot\int_{x_1}^{x} \varkappa\, dx\right] \qquad \varkappa^2 = \frac{2m}{\hbar^2}\left[V-E\right] > 0$$

In region III

$$\varphi_{III} = \frac{A}{\sqrt{\varkappa}} \exp\left[-\int_{x_2}^{x} \varkappa\, dx\right]$$

In the classically allowed region:

$$\varphi_{II}^{-}(x) = \frac{C}{\sqrt{k}} \sin\left[\int_{x_1}^{x} k\, dx + \delta\right] \qquad x_1 < x \qquad k^2 = \frac{2m}{\hbar^2}(E-V) > 0$$

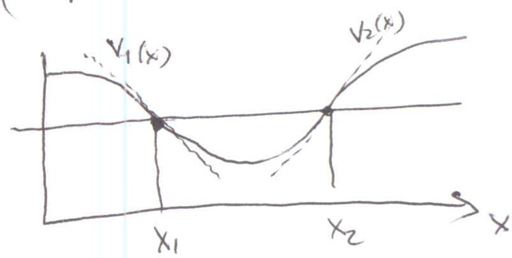
$$\varphi_{II}^{+}(x) = \frac{B}{\sqrt{k}} \sin\left[\int_{x}^{x_2} k\, dx + \delta\right) \qquad x < x_2$$

If $\varphi_I, \varphi_{II}^-, \varphi_{II}^+, \varphi_{III}$ were valid representations at any point, the constants of those functions could be obtained by simply matching those component solutions. However, the WKB solutions are invalid at the classical turning points.

The technique of matching φ_I ~~to~~ φ_{II}^- and φ_{II}^+ ~~to~~ φ_{III} is as follows. The SE is solved exactly at the turning points for potentials that approximate $V(x)$ in these domains. The asymptotic forms of those exact solutions are then used. Following this idea, we write

$$V(x) \simeq V_1(x) = E - F_1(x - x_1)$$

(F_1 is a constant)



Similarly

$$V(x) \simeq V_2(x) = E + F_2(x - x_2)$$

The SE then appears as

$$\frac{d^2\varphi}{dx^2} + \frac{2mF_1}{\hbar^2}(x - x_1)\varphi = 0 \qquad x \text{ near } x_1$$

$$\frac{d^2\varphi}{dx^2} - \frac{2mF_2}{\hbar^2}(x - x_2)\varphi = 0 \qquad x \text{ near } x_2$$

Now if we substitute

$$y = -\left(\frac{2mF_1}{\hbar^2}\right)^{1/3}(x - x_1)$$

and

$$y = \left(\frac{2mF_2}{\hbar}\right)^{1/3}(x - x_2)$$

Both of the equations above then reduce to the same equation

$$\frac{d^2\varphi}{dy^2} - y\varphi = 0$$

The solutions to this equation are called Airy functions. They are usually denoted as $Ai(x)$ and $Bi(x)$

In our problem $\varphi(x)$ must approach zero when $x \ll x_1$ and $x \gg x_2$.

Both of these regions correspond to large positive values of $|y|$. $Ai(y)$ has the following asymptotic form

$$Ai(y) \approx \frac{1}{2\sqrt{\pi}\, y^{1/4}} \exp\left[-\frac{2}{3} y^{3/2}\right] \qquad y>0$$

$$Ai(y) \sim \frac{1}{\sqrt{\pi}\,(-y)^{1/4}} \sin\left[\frac{2}{3}(-y)^{3/2} + \frac{\pi}{4}\right] \qquad y<0$$

In the vicinity of x_1 we obtain

$$p^2 = 2m(E-V_1) \simeq 2mF_1(x-x_1) = -(2mF_1\hbar)^{2/3} y$$

$$2mF_1\,dx = -(2mF_1\hbar)^{2/3} dy$$

To the left of x_1 $p^2 = -\hbar^2 \varkappa^2$, so

$$\hbar^2 \varkappa^2 = (2mF_1\hbar)^{2/3} y$$

and we may write

$$\int_{x_1}^{x} \varkappa\, dx = -\int_0^y \sqrt{y}\, dy = -\frac{2}{3} y^{3/2}$$

To the right of x_1, in the oscillatory well domain
$p^2 = \hbar^2 k^2$ and $\hbar^2 k^2 = -(2mF_1\hbar)^{2/3} y$
So y is negative in this domain. The integral of k gives

$$\int_{x_1}^{x} k\, dx = -\int_0^y \sqrt{-y}\, dy = \frac{2}{3}(-y)^{3/2} \qquad y<0$$

In these same respective domains φ_1 and φ_{II}^- appear as

$$\varphi_I = \frac{1}{y^{1/4}} \exp\left(-\frac{2}{3} y^{3/2}\right)$$

$$\varphi_{II}^- = \frac{c}{(-y)^{1/4}} \sin\left(\frac{2}{3}(-y)^{3/2} + \delta\right)$$

These agree with the asymptotic form above if $c=2$ and $\delta = \frac{\pi}{4}$

In this manner we find that the WKB appr. in $\underline{I}$

$$\varphi_I(x) = \frac{1}{\sqrt{k}} \exp\left(\int_{x_1}^{x} \varkappa\, dx\right) \qquad x < x_1$$

mathes with WKB approximation

$$\varphi_{II}^{-}(x) = \frac{2}{\sqrt{k}} \sin\left(\int_{x_1}^{x} k\, dx + \frac{\pi}{4}\right) \qquad \text{in} \qquad x_1 < x$$

In like manner we find that in region $\underline{III}$

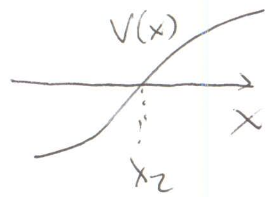
$$\varphi_{III} = \frac{A}{\sqrt{\varkappa}} \exp\left(-\int_{x_2}^{x} \varkappa\, dk\right.$$

the WKB approximation matches with the WKB approximation

$$\varphi_{II}^{+} = \frac{2A}{\sqrt{k}} \sin\left(\int_{x}^{x_2} k\, dx + \frac{\pi}{4}\right)$$

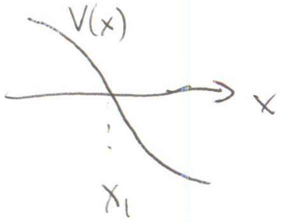
in region $\underline{II}$. The remaining constant A is determined in matching φ_{II} to φ_{II}^{+}.

There are in total four connection formulas, which serve to relate WKB component wave functions across turning points. In the preceding analysis we uncovered two of them. Carrying through a parallel analysis and employing the asymptotic forms of $Bi(y)$ gives the remaining two relatios. The complete list is the following



$$\frac{2}{\sqrt{k}} \cos\left(\int_{x}^{x_2} k\, dx - \frac{\pi}{4}\right) \leftrightarrows \frac{1}{\sqrt{\varkappa}} \exp\left(-\int_{x_2}^{x} \varkappa\, dx\right)$$

$$\frac{1}{\sqrt{k}} \sin\left(\int_{x}^{x_2} k\, dx - \frac{\pi}{4}\right) \rightleftarrows -\frac{1}{\sqrt{\varkappa}} \exp\left(\int_{x_2}^{x} \varkappa\, dx\right)$$

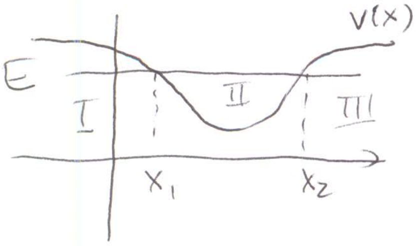


$$\frac{1}{\sqrt{\varkappa}} \exp\left(\int_{x_1}^{x} \varkappa\, dx\right) \rightleftarrows \frac{2}{\sqrt{k}} \cos\left(\int_{x_1}^{x} k\, dx - \frac{\pi}{4}\right)$$

$$-\frac{1}{\sqrt{k}} \exp\left(-\int_{x_1}^{x} \varkappa\, dx\right) \rightleftarrows \frac{1}{\sqrt{k}} \sin\left(\int_{x_1}^{x} k\, dx - \frac{\pi}{4}\right)$$

Bohr - Sommerfeld quantization rules

The energy levels of the finite well depicted below



may be obtained (approximately) by joining φ_{II}^- and φ_{II}^+ smoothly within the well. This gives

$$\sin\left(\int_{x_1}^{x} k\,dx + \frac{\pi}{4}\right) = A \sin\left(\int_{x}^{x_2} k\,dx + \frac{\pi}{4}\right)$$

if we denote

$$\eta = \int_{x_1}^{x_2} k\,dx \qquad a \equiv \int_{x}^{x_2} k\,dx + \frac{\pi}{4}$$

the continuity condition becomes

$$\sin\left(\eta + \frac{\pi}{2} - a\right) = A \sin a$$

or

$$\sin\left(\eta + \frac{\pi}{2}\right)\cos a - \cos\left(\eta + \frac{\pi}{2}\right)\sin a = A \sin a$$

The solution to this equation which gives A, constant and independent of a, is obtained by setting

$$\eta + \frac{\pi}{2} = (n+1)\pi \qquad n = 0, 1, 2, \ldots$$

(writing $n+1$ instead of n ensures that η is nonnegative)

Corresponding values of A are $(-1)^n$

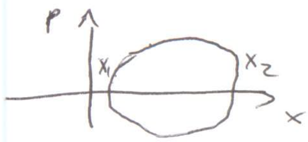
Thus, the continuity of φ_{II} implies the condition

$$\eta = \int_{x_1}^{x_2} k\,dx = \left(n + \frac{1}{2}\right)\pi$$

or given the relation $p = \hbar k$, it appears as

$$\int_{x_1}^{x_2} p\,dx = \left(n + \frac{1}{2}\right)\frac{h}{2}$$

In the corresponding classical motion the particle oscillates between x_1 and x_2. In Cartesian x, p space this "orbit" is a closed loop with area $\oint p\,dx$



$$\oint p\,dx = \left(n + \frac{1}{2}\right)h$$