The WKB Connection Formulae

The WKB formula

$$\psi(x) = A|k(x)|^{-1/2} \exp\left[i\int^x k(x')dx'\right] + B|k(x)|^{-1/2} \exp\left[-i\int^x k(x')dx'\right], \tag{1}$$

where $k(x) = \sqrt{2m[E - V(x)]}/\hbar$ for $E > V(x)$ and $k(x) = -i\kappa(x) = -i\sqrt{2m[V(x) - E]}/\hbar$ for $E < V(x)$, is valid only within regions where $|k'(x)| \ll |k(x)|^2$. In many problems, such regions of validity are separated by "breakdown regions," in which the WKB wave function diverges unphysically due to the vanishing (or near-vanishing) of $V(x) - E$.

In general, an accurate solution of the Schrödinger equation is required within each breakdown region to establish the connection between the constants A and B describing the WKB wave functions in the allowed regions on either side.

However, a relatively simple analytical approach works when a WKB region with $E > V$ is separated from a WKB region with $E < V$ by a simple crossing of $V(x)$ and E that can be described over a sufficiently wide range of x by

$$V(x) - E \approx g(x - a), \qquad g = dV/dx|_{x=a}. \tag{2}$$

Based on our previous study of the linear potential, we know that the most general solution of the Schrödinger equation within a region described by Eq. (2) is $\psi(x) = C_A \mathrm{Ai}(s) + C_B \mathrm{Bi}(s)$, where $s = (x - a)/l$ and $l = (\hbar^2/2m|g|)^{1/3} \operatorname{sgn} g$.

Let us temporarily specialize to the case $g > 0$. Since $k(x)^2 = -s/l^2$, it follows that $k'(x) = (dk/ds)(ds/dx) = -1/\sqrt{-s}\, l^2$, and the WKB condition $|k'(x)| \ll |k(x)|^2$ becomes $|s|^{3/2} \gg \frac{1}{2}$. Provided that the potential can be taken to be linear at least within some region $|s| < \alpha$, where $\alpha \gg 1$ ($\alpha = 5$, say), then the WKB wave functions valid for $|s| \geq \alpha$ can be patched together using Airy functions for $|s| \leq \alpha$.

For $0 < s < \alpha$, $\int_a^x \kappa(x')dx' = \int_0^s \sqrt{s}\, ds = 2s^{3/2} \equiv \sigma$, so the WKB wave function can be written as linear combinations of

$$\kappa(x)^{-1/2} \exp\left[-\int_a^x \kappa(x')dx'\right] = \sqrt{l} s^{-1/4} e^{-\sigma} = \lim_{s \gg 1} 2\sqrt{\pi l}\, \mathrm{Ai}(s) \tag{3}$$

and

$$\kappa(x)^{-1/2} \exp\left[\int_a^x \kappa(x')dx'\right] = \sqrt{l} s^{-1/4} e^{\sigma} = \lim_{s \gg 1} \sqrt{\pi l}\, \mathrm{Bi}(s). \tag{4}$$

For $-\alpha < s < 0$, $\int_x^a k(x')dx' = \int_0^{|s|} \sqrt{|s|}\, d|s| = 2|s|^{3/2} \equiv \sigma$, so

$$k(x)^{-1/2} \cos\left[\int_x^a k(x')dx' - \pi/4\right] = \sqrt{l}|s|^{-1/4} \cos(\sigma - \pi/4) = \lim_{s \ll -1} \sqrt{\pi l}\, \mathrm{Ai}(s) \tag{5}$$

and

$$k(x)^{-1/2} \sin\left[\int_x^a k(x')dx' - \pi/4\right] = \sqrt{l}|s|^{-1/4} \sin(\sigma - \pi/4) = \lim_{s \ll -1} -\sqrt{\pi l}\, \mathrm{Bi}(s). \tag{6}$$

Matching the coefficients of each Airy function between $s < 0$ and $s > 0$, we obtain the **connection formulae**, which link WKB wave functions across a classical turning point located at $x = a$:

$$C\psi_-(x) \quad \longrightarrow \quad 2C\sqrt{\pi|l|}Ai\left(\frac{x-a}{l}\right) \quad \longrightarrow \quad 2C\psi_c(x) \tag{7}$$

$$-D\psi_+(x) \quad \longleftarrow \quad D\sqrt{\pi|l|}Bi\left(\frac{x-a}{l}\right) \quad \longleftarrow \quad D\psi_s(x) \tag{8}$$

where

$$\psi_\pm(x) = \kappa(x)^{-1/2}\exp\left[\pm\int \kappa(x')dx'\right], \qquad l = \left(\frac{\hbar^2}{2m|g|}\right)^{1/3}\operatorname{sgn} g, \quad g = \left.\frac{dV}{dx}\right|_{x=a}, \tag{9}$$

$$\psi_c(x) = k(x)^{-1/2}\cos\left[\int k(x')dx' - \frac{\pi}{4}\right], \qquad \psi_s(x) = k(x)^{-1/2}\sin\left[\int k(x')dx' - \frac{\pi}{4}\right]. \tag{10}$$

Each integration is carried out from $\min(x,a)$ to $\max(x,a)$, so the integral has a non-negative value which grows with $|x-a|$; hence, $|\psi_+|$ increases ($|\psi_-|$ decreases) on moving away from the turning point. With this convention, Eqs. (7)–(10) apply irrespective of the sign of g.

Directionality: The connection formulae given above are exact only in the limit $\epsilon \to 0^+$, where $\epsilon = \sqrt{\hbar^2/(2ml_0^2V_0)}$ is the small parameter entering the WKB treatment of the potential $V(x) = V_0 w(x/l_0)$. For finite ϵ, errors arising from use of the connection formulae will be minimized if Eqs. (7) and (8) are applied in the direction of the arrows:

1. If the wave function is proportional to ψ_c in the classically allowed region, one *cannot* deduce that the wave function on the other side of the turning point is strictly proportional to ψ_-; only that the coefficient of ψ_+ is subleading in ϵ. Neglect of a ψ_+ component with even a very small coefficient could have severe consequences, because this component grows exponentially away from the turning point, and at sufficiently large distances must overshadow the exponentially shrinking ψ_- component.

   However, if $V(x) > E$ for all x on one side of the turning point, say $x > a$, the requirement that $\psi(x) \to 0$ for $x \to \infty$ ensures that the coefficient of ψ_+ is identically zero. Then the WKB solution for $x < a$ is well-predicted by Eq. (1). The effect of finite ϵ is at worst to introduce an error in the phase of the oscillatory solution.

2. Equation (8) is needed only in problems involving tunneling through a finite-width barrier, inside which the WKB wave function can have have nonzero coefficients of both ψ_+ and ψ_-. If we use Eq. (8) in the reverse direction, then in the classically allowed region we neglect a subleading ψ_s component, possibly leading to a large error in the phase of the oscillatory wave function. Application of Eq. (8) in the direction shown results in neglect of a subleading ψ_- component in the forbidden region, which has minimal consequences since ψ_- decays exponentially away from the turning point.

   Equation (8) can usefully be generalized to

   $$D\sin\phi\,\psi_+(x) \quad \longleftarrow \quad \frac{D}{\sqrt{k(x)}}\cos\left[\int k(x')dx' - \frac{\pi}{4} + \phi\right], \tag{11}$$

   which is valid so long as $\sin\phi$ is not approximately zero.