P443 WKB I
D.Rubin
February 18, 2008

Connection Formulae

The WKB approximation falls apart near a turning point. Then $E - V \rightarrow 0$ so $\frac{1}{\sqrt{p}} \rightarrow \infty$. And because the momentum goes to zero the wavelength gets very long and the approximation is only valid if the wavelength is short compared to the distance over which the potential changes. But if want to determine bound state energies, we need to be able to match wave functions at the turning points. The strategy to overcome this limitation of the WKB wave functions at the turning points is to

1. Linearize the potential at the turning point ($x = 0$). $V(x) = V(0) + x\frac{dV}{dx}$

2. Solve Schrodinger's equation exactly near the turning point for the linear potential There will be two cases to consider. One where $\frac{dV}{dx} > 0$ and the particle has positive kinetic energy to the left of the turning point ($x < 0$), and negative kinetic energy to the right ($x > 0$). The other case is when $\frac{dV}{dx} < 0$ and then there is negative kinetic energy to the left and positive to the right. We consider first $\frac{dV}{dx} > 0$.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V(0) + xV')\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V(0) - xV')\psi = -\frac{p^2}{\hbar^2}\psi$$

The turning point is at $x = 0$ and that is where $V(x) = E$. So $V(0) = E$ and we have

$$\frac{d^2\psi}{dx^2} = \alpha^3 x\psi$$

where $\alpha^3 = \frac{2m}{\hbar^2}V'$. Then if we define the dimensionless parameter $z = \alpha x$ we have

$$\frac{d^2\psi}{dz^2} = z\psi$$

which is Airy's equation and the general solution is

$$\psi_p = aAi(x) + bBi(x)$$

ψ_p is referred to as the patching wave function since its sole purpose is to patch together the WKB wave functions on each side of the turning point.

3. Determine the WKB wave function in the region of the linear potential. It will be different on each side of the turning point. To the left of the turning point for case one, the WKB wave function is

$$\psi_l(x) = \frac{A}{\sqrt{p}} e^{i\phi(x)} + \frac{B}{\sqrt{p}} e^{-i\phi(x)}$$

and

$$\phi(x) = \frac{1}{\hbar} \int_0^x p(x')dx' = \int_0^x \alpha^{\frac{3}{2}} (-x)^{\frac{1}{2}} dx' = -\frac{2}{3}(-\alpha x)^{\frac{3}{2}} \tag{1}$$

where

$$p(x) = \sqrt{2m(E-V)} \sim \sqrt{2m(-xV')} = \hbar\alpha^{\frac{3}{2}}(-x)^{\frac{1}{2}}$$

(Since we are to the left of the turning point $x < 0$ and the argument of the square root is positive.) The WKB wave function to the left of the turning point where the slope of the potential is positive is

$$\psi_l(x) = \frac{A}{\hbar^{\frac{1}{2}}(-\alpha^3 x)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} + \frac{B}{\hbar^{\frac{1}{2}}(-\alpha^3 x)^{\frac{1}{4}}} e^{i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} \tag{2}$$

or in terms of the parameter $z = \alpha x$

$$\psi_l(x) = \frac{A}{(\hbar\alpha)^{\frac{1}{2}}(-z)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-z)^{\frac{3}{2}}} + \frac{B}{(\hbar\alpha)^{\frac{1}{2}}(-z)^{\frac{1}{4}}} e^{i\frac{2}{3}(-z)^{\frac{3}{2}}} \tag{3}$$

To the right of the turning point, $(x > 0)$, and the WKB wave function is

$$\psi_r(x) = \frac{C}{\sqrt{|p|}} e^{\phi(x)} + \frac{D}{\sqrt{|p|}} e^{-\phi(x)}$$

and

$$\phi(x) = \frac{1}{\hbar} \int_0^x |p(x')|dx' = \frac{2}{3}(\alpha x)^{\frac{3}{2}} \tag{4}$$

and the WKB wave function to the right of the crossing point is

$$\psi_r(x) = \frac{C}{\hbar^{\frac{1}{2}}(\alpha^3 x)^{\frac{1}{4}}} e^{\frac{2}{3}(\alpha x)^{\frac{3}{2}}} + \frac{D}{\hbar^{\frac{1}{2}}(\alpha^3 x)^{\frac{1}{4}}} e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} \tag{5}$$

or in terms of the parameter z

$$\psi_r(x) = \frac{C}{(\hbar\alpha)^{\frac{1}{2}} z^{\frac{1}{4}}} e^{\frac{2}{3}z^{\frac{3}{2}}} + \frac{D}{(\hbar\alpha)^{\frac{1}{2}} z^{\frac{1}{4}}} e^{-\frac{2}{3}z^{\frac{3}{2}}} \tag{6}$$

4. Now we want to use the patching wave function to connect the WKB wave to the left of the turning point with the WKB wave function to the right. We use the large negatve z asymtotic form of the Airy functions

$$\left.\begin{aligned} Ai(z) &\sim \tfrac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \sin\left[\tfrac{2}{3}(-z)^{\frac{3}{2}} + \tfrac{\pi}{4}\right] = \tfrac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \tfrac{1}{2i}\left[e^{i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{i\frac{\pi}{4}} - e^{-i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{-i\frac{\pi}{4}}\right] \\ Bi(z) &\sim \tfrac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \cos\left[\tfrac{2}{3}(-z)^{\frac{3}{2}} + \tfrac{\pi}{4}\right] = \tfrac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \tfrac{1}{2}\left[e^{i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{i\frac{\pi}{4}} + e^{-i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{-i\frac{\pi}{4}}\right] \end{aligned}\right\} z \ll 0$$

Then setting

$$\psi_l(z) = aAi(z) + bBi(z)$$

we have

$$\begin{aligned} \psi_l(x) &= \tfrac{A}{(\hbar\alpha)^{\frac{1}{2}}(-z)^{\frac{1}{4}}} e^{-i\frac{2}{3}(-z)^{\frac{3}{2}}} + \tfrac{B}{(\hbar\alpha)^{\frac{1}{2}}(-z)^{\frac{1}{4}}} e^{i\frac{2}{3}(-z)^{\frac{3}{2}}} \\ &= \tfrac{1}{2\sqrt{\pi}(-z)^{\frac{1}{4}}}\left[(b - ia)e^{i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{i\frac{\pi}{4}} + (b + ia)e^{-i\frac{2}{3}(-z)^{\frac{3}{2}}} e^{-i\frac{\pi}{4}}\right] \end{aligned}$$

Evidently

$$\frac{B}{(\hbar\alpha)^{1/2}} = \frac{b - ia}{2\sqrt{\pi}} e^{i\frac{\pi}{4}} \quad \text{and} \quad \frac{A}{(\hbar\alpha)^{1/2}} = \frac{b + ia}{2\sqrt{\pi}} e^{-i\frac{\pi}{4}}$$

Solving for a and b in terms of A and B we have that

$$b = \sqrt{\frac{\pi}{\hbar\alpha}}(Ae^{i\pi/4} + Be^{-i\pi/4}) \quad \text{and} \quad a = \sqrt{\frac{\pi}{\hbar\alpha}}(Ae^{-i\pi/4} + Be^{i\pi/4}) \tag{7}$$

and that takes care of matching the WKB wave function to the left of the turing point to the patching wave function.

Now let's do the same thing to the right of the turning point. Here we use the large positive z asymtotic form of the Airy functions. Namely

$$\left.\begin{aligned} Ai(z) &\sim \tfrac{1}{2\sqrt{\pi}(z)^{1/4}} e^{-\frac{2}{3}z^{\frac{3}{2}}} \\ Bi(z) &\sim \tfrac{1}{\sqrt{\pi}(z)^{1/4}} e^{\frac{2}{3}z^{\frac{3}{2}}} \end{aligned}\right\} z \gg 0$$

Setting

$$\psi_r(z) = aAi(z) + bBi(z)$$

we have

$$\frac{C}{(\hbar\alpha)^{\frac{1}{2}} z^{\frac{1}{4}}} e^{\frac{2}{3}z^{\frac{3}{2}}} + \frac{D}{(\hbar\alpha)^{\frac{1}{2}} z^{\frac{1}{4}}} e^{-\frac{2}{3}z^{\frac{3}{2}}} = a\frac{1}{2\sqrt{\pi}(z)^{1/4}} e^{-\frac{2}{3}z^{\frac{3}{2}}} + b\frac{1}{\sqrt{\pi}(z)^{1/4}} e^{\frac{2}{3}z^{\frac{3}{2}}}$$

from which we see that

$$a = \sqrt{\frac{4\pi}{\hbar\alpha}} D \quad \text{and} \quad b = \sqrt{\frac{\pi}{\hbar\alpha}} C \tag{8}$$

Finally we equate equations 7 and 8 to eliminate a and b yielding the connection formulae

$$\sqrt{\frac{4\pi}{\hbar\alpha}} D = \sqrt{\frac{\pi}{\hbar\alpha}} (Ae^{-i\pi/4} + Be^{i\pi/4}) \tag{9}$$

and

$$\sqrt{\frac{\pi}{\hbar\alpha}} C = \sqrt{\frac{\pi}{\hbar\alpha}} (Ae^{i\pi/4} + Be^{-i\pi/4}) \tag{10}$$

In summary, for a barrier to the right, the connection formulae are

$$\text{barrier to right} \begin{cases} D = \frac{1}{2}(Ae^{-i\pi/4} + Be^{i\pi/4}) \quad & C = Ae^{i\pi/4} + Be^{-i\pi/4} \\ \\ A = De^{i\pi/4} + \frac{1}{2}Ce^{-i\pi/4} \quad & B = De^{-i\pi/4} + \frac{1}{2}Ce^{i\pi/4} \end{cases}$$

Note that in the connection formulae, there is no mention of the linearized potential, the parameter α, V' or Airy functions. The linearization procedure served only as a mechanism to relate the constants A and B to the left of the turning point with the constants C and D to the right of the turning point. Having established that relationship, which by the way is good for any arbitrary potential, (as long as it is not too nonlinear), we no longer need the patching wave function. Now we know how to deal with a turning point to the right (namely with $V' > 0$). We need an equivalent set of relations to deal with turning points to the left ($V' < 0$) and they can be derived by a similar procedure. The derivations are nearly identical. The only difference is that the phase integrals change sign. Equation 1 will become

$$\phi(x) = \frac{1}{\hbar}\int_0^x p(x')dx' = \int_0^x \alpha^{\frac{3}{2}}(-x)^{\frac{1}{2}}dx' = \frac{2}{3}(-\alpha x)^{\frac{3}{2}} \tag{11}$$

and equation 4 will become

$$\phi(x) = \frac{1}{\hbar}\int_0^x |p(x')|dx' = -\frac{2}{3}(\alpha x)^{\frac{3}{2}} \tag{12}$$

The result is that we interchange A for B and C for D. The connection formulae for a barrier to the left are given here for reference.

$$\text{barrier to left}\begin{cases} D = Ae^{-i\pi/4} + Be^{i\pi/4} & C = \frac{1}{2}(Ae^{i\pi/4} + Be^{-i\pi/4}) \\ \\ A = \frac{1}{2}De^{i\pi/4} + Ce^{-i\pi/4} & B = \frac{1}{2}De^{-i\pi/4} + Ce^{i\pi/4} \end{cases}$$

5. Now that we know how to match WKB wave functions at the turning points we can derive the quantization condition. Suppose that we are trying to determine the energy of a bound state. Imagine something like the harmonic oscillator potential with $V' < 0$ at the left turning point ($x = x_1$) and $V' > 0$ at the right turning point ($x = x_2$). Then the region $x < x_1$ is classically forbidden, (we refer to it as region I) and

$$\psi_I(x) = \frac{C}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int_{x_1}^x |p(x')|dx'} + \frac{D}{\sqrt{|p|}}e^{-\frac{1}{\hbar}\int_{x_1}^x |p(x')|dx'} \tag{13}$$

In region II the WKB wave function for $x > x_1$ is

$$\psi_{II}(x) = \frac{A}{\sqrt{p}}e^{\frac{i}{\hbar}\int_{x_1}^x p(x')dx'} + \frac{B}{\sqrt{p}}e^{\frac{-i}{\hbar}\int_{x_1}^x p(x')dx'} \tag{14}$$

In order that $\psi_I(x)$ be finite for $x \ll 0$, it must be that $D = 0$. Then connection formulae for a barrier to the left yield

$$0 = Ae^{-i\pi/4} + Be^{i\pi/4}, \rightarrow A = -iB, \quad A = Ce^{-i\pi/4}, \quad B = Ce^{i\pi/4} \tag{15}$$

And using Equation 15 to substitute for A and B, Equation 14 becomes

$$\psi_{II}(x) = \frac{C}{\sqrt{p}}e^{\frac{i}{\hbar}\int_{x_1}^x p(x')dx' - i\pi/4} + \frac{C}{\sqrt{p}}e^{\frac{-i}{\hbar}\int_{x_1}^x p(x')dx' + i\pi/4} \tag{16}$$

Next we have to connect WKB wave functions for region II and III at $x = x_2$. In order to apply the connection formulae for a barrier to the right we need to have the wave function in the form

$$\psi = \frac{A'}{\sqrt{p}}e^{\frac{i}{\hbar}\int_{x_2}^x p(x')dx'} + \frac{B'}{\sqrt{p}}e^{\frac{-i}{\hbar}\int_{x_2}^x p(x')dx'} \tag{17}$$

We can write Equation 16 in the same form as follows

$$\psi_{II}(x) = \frac{C}{\sqrt{p}} e^{\frac{i}{\hbar}(\int_{x_1}^{x_2} p(x')dx' + \int_{x_2}^{x} p(x')dx' - i\pi/4)} + \frac{C}{\sqrt{p}} e^{\frac{-i}{\hbar}(\int_{x_1}^{x_2} p(x')dx' + \int_{x_2}^{x} p(x')dx' - i\pi/4)}$$

Comparing the previous equation with 17 we have that

$$Ce^{i(\theta-\pi/4)} = A', \quad Ce^{-i(\theta-\pi/4)} = B'$$

where

$$\theta = \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')dx'$$

Now we can use the connection formulae for a barrier to the right to connect ψ_{II} with ψ_{III}.

$$\psi_{III}(x) = \frac{C'}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx'} + \frac{D'}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx'} \tag{18}$$

We know that $C' = 0$ since C' is the coefficient of the exponentially growing term for the WKB wave function in region III. The connection formulae for a barrier to the right give

$$C' = A'e^{i\pi/4} + B'e^{-i\pi/4} = Ce^{i(\theta-\pi/4)}e^{i\pi/4} + Ce^{-i(\theta-\pi/4)}e^{-i\pi/4} = 2C\cos\theta$$

But $C' = 0$ so

$$\cos\theta = 0, \Rightarrow \theta = (n + \frac{1}{2})\pi \tag{19}$$

and

$$\int_{x_1}^{x_2} p(x)dx = \hbar\pi(n + \frac{1}{2}) \tag{20}$$

Equation 20 determines the allowed energies of the system.