WKB APPROXIMATION AT A TURNING POINT WITH DECREASING POTENTIAL

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.9.

In the last post, we worked out the WKB approximation on either side of a turning point where the potential is increasing. We can do the same analysis for a turning point where the potential is decreasing. The calculations are almost exactly the same as in the first case.

The wave function has the form

$$\psi(x)\approx\frac{1}{\sqrt{p(x)}}\left(Be^{i\int p\,dx/\hbar}+Ce^{-i\int p\,dx/\hbar}\right) \tag{1}$$

if the particle's energy $E>V(x)$, where

$$p(x)=\sqrt{2m(E-V(x))} \tag{2}$$

is the momentum of the particle. In the tunneling case, where $E<V(x)$, the WKB approximation gives

$$\psi(x)\approx\frac{1}{\sqrt{|p|}}\left(De^{-\frac{1}{\hbar}\int|p(x)|dx}+Fe^{\frac{1}{\hbar}\int|p(x)|dx}\right) \tag{3}$$

In the decreasing potential case, we have $E<V(x)$ for $x<x_1$ and $E>V(x)$ for $x>x_1$. As before, we'll move the turning point so that $x_1=0$ and shift if back after the analysis. In this case, the limits on the integrals above give the results

$$\psi(x)=\begin{cases}\frac{1}{\sqrt{|p|}}\left(De^{-\frac{1}{\hbar}\int_x^0|p(x')|dx'}+Fe^{\frac{1}{\hbar}\int_x^0|p(x')|dx'}\right) & x<0\\ \frac{1}{\sqrt{p(x)}}\left(Be^{i\int_0^x p(x')\,dx'/\hbar}+Ce^{-i\int_0^x p(x')\,dx'/\hbar}\right) & x>0\end{cases} \tag{4}$$

As the integrand for $x<0$ is non-negative, we must have $F=0$ to keep ψ finite as $x\to-\infty$, so we have

$$\psi(x)=\begin{cases}\frac{1}{\sqrt{|p|}}\left(De^{-\frac{1}{\hbar}\int_x^0|p(x')|dx'}\right) & x<0\\ \frac{1}{\sqrt{p(x)}}\left(Be^{i\int_0^x p(x')\,dx'/\hbar}+Ce^{-i\int_0^x p(x')\,dx'/\hbar}\right) & x>0\end{cases} \tag{5}$$

As before, we assume that around $x=0$

$$V(x)\approx E+V'(0)x \tag{6}$$

where now $V'(0)<0$ since the potential is decreasing. We now define the patching function ψ_p that satisfies the Schrödinger equation with this approximate potential near $x=0$.

$$\frac{d^2\psi_p}{dx^2} = \frac{2mV'(0)}{\hbar^2}x\psi_p \tag{7}$$

$$= -\frac{2m|V'(0)|}{\hbar^2}x\psi_p \tag{8}$$

By defining

$$\alpha \equiv \left(\frac{2m|V'(0)|}{\hbar^2}\right)^{1/3} \tag{9}$$

$$z \equiv -\alpha x \tag{10}$$

we end up with Airy's equation

$$\frac{d^2\psi_p}{dz^2}=z\psi_p \tag{11}$$

As we saw earlier, this has the general solution

$$\psi_p(z) = aAi(z)+bBi(z) \tag{12}$$

$$\psi_p(x) = aAi(-\alpha x)+bBi(-\alpha x) \tag{13}$$

It is this function that we need to match up to 5.

To do this, we make a further assumption that the overlap regions (where we're trying to match the WKB functions with ψ_p) are far enough from $x=0$ that we can use the asymptotic forms of the Airy functions. These forms are

$$Ai(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] & z \ll 0 \\ \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-2z^{3/2}/3} & z \gg 0 \end{cases} \tag{14}$$

$$Bi(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] & z \ll 0 \\ \frac{1}{\sqrt{\pi}z^{1/4}} e^{2z^{3/2}/3} & z \gg 0 \end{cases} \tag{15}$$

The forms can't be used if we get too close to $x = 0$, but the hope is that there is still some range of x where both the WKB wave function and ψ_p are reasonable approximations to the true wave function. Under this assumption, we have from 13 for $z = -\alpha x \gg 0$, or $x \ll 0$:

$$\psi_p(x) = \frac{a}{2\sqrt{\pi}z^{1/4}} e^{-2z^{3/2}/3} + \frac{b}{\sqrt{\pi}z^{1/4}} e^{2z^{3/2}/3} \tag{16}$$

$$= \frac{a}{2\sqrt{\pi}(-\alpha x)^{1/4}} e^{-2(-\alpha x)^{3/2}/3} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} e^{2(-\alpha x)^{3/2}/3} \tag{17}$$

With the potential 6, the WKB function 5 for $x < 0$ is

$$p(x) = \sqrt{2m(E - V(x))} \tag{18}$$

$$= \sqrt{-2mV'(0)x} \tag{19}$$

$$= \hbar\sqrt{x}\alpha^{3/2} \tag{20}$$

$$\psi(x) = \frac{1}{\sqrt{|p|}} De^{-\frac{1}{\hbar}\int_x^0 |p(x')|dx'} \tag{21}$$

$$\int_0^x |p(x')|\,dx' = \sqrt{-2mV'(0)} \int_x^0 \sqrt{-x'}dx' \tag{22}$$

$$= \sqrt{2m|V'(0)|}\frac{2}{3}(-x)^{3/2} \tag{23}$$

$$= \frac{2}{3}\hbar(-\alpha x)^{3/2} \tag{24}$$

$$\psi(x) = \frac{D}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}} e^{-2(-\alpha x)^{3/2}/3} \tag{25}$$

Matching this up with 17, we see that $b = 0$ and

$$\frac{a}{2\sqrt{\pi}\alpha^{1/4}} = \frac{D}{\sqrt{\hbar}\alpha^{3/4}} \tag{26}$$

$$a = 2\sqrt{\frac{\pi}{\hbar\alpha}}D \tag{27}$$

The patching function must therefore have the form

$$\psi_p(x) = 2\sqrt{\frac{\pi}{\hbar\alpha}}De^{-2(-\alpha x)^{3/2}/3} \tag{28}$$

for $\alpha x \ll 0$.

We can do the same calculation for the overlap region for $x > 0$, where $E > V(x)$. Since $x > 0$, $z = -\alpha x < 0$ and we can use the asymptotic form of $Ai(x)$ for large negative x and we get

$$\psi_p(x) = \frac{a}{\sqrt{\pi}(\alpha x)^{1/4}}\sin\left[\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right] \tag{29}$$

For the WKB function, we start with 5

$$p(x) = \sqrt{-2mV'(0)x} \tag{30}$$

$$= \hbar\alpha^{3/2}\sqrt{x} \tag{31}$$

$$\int_0^x p(x')\,dx' = \frac{2}{3}\hbar(\alpha x)^{3/2} \tag{32}$$

$$\psi(x) = \frac{1}{\sqrt{\hbar}\alpha^{3/4}(x)^{1/4}}\left(Be^{2i(\alpha x)^{3/2}/3} + Ce^{-2i(\alpha x)^{3/2}/3}\right) \tag{33}$$

We can now compare this with 29 by writing the sine in terms of exponentials

$$\psi_p(x) = \frac{a}{2i\sqrt{\pi}(\alpha x)^{1/4}}\left[e^{i\left[\frac{2}{3}(\alpha x)^{3/2}+\frac{\pi}{4}\right]} - e^{-i\left[\frac{2}{3}(\alpha x)^{3/2}+\frac{\pi}{4}\right]}\right] \tag{34}$$

Comparing terms, we have

$$\frac{B}{\sqrt{\hbar}\alpha^{3/4}} = \frac{ae^{i\pi/4}}{2i\sqrt{\pi}\alpha^{1/4}} \tag{35}$$

$$B = \frac{ae^{i\pi/4}\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} \tag{36}$$

$$= -ie^{i\pi/4}D \tag{37}$$

$$\frac{C}{\sqrt{\hbar}\alpha^{3/4}} = -\frac{ae^{-i\pi/4}}{2i\sqrt{\pi}\alpha^{1/4}} \tag{38}$$

$$C = -\frac{ae^{-i\pi/4}\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} \tag{39}$$

$$= ie^{-i\pi/4}D \tag{40}$$

We now have the constants B and C, belonging to the WKB wave function for $x>0$, in terms of the constant D belonging to the WKB function for $x<0$, which is what we were after. Note that the WKB functions are still valid only for values of x that maintain a respectable distance from the turning point; all we have done is connected the approximations on either side of the turning point. The final form of the WKB function is, for $x>0$:

$$\psi(x) \cong \frac{-iD}{\sqrt{p(x)}}\left(e^{i\left(\int p\,dx/\hbar+\pi/4\right)} - e^{-i\left(\int p\,dx/\hbar+\pi/4\right)}\right) \tag{41}$$

$$= \frac{2D}{\sqrt{p(x)}}\frac{1}{2i}\left(e^{i\left(\int p\,dx/\hbar+\pi/4\right)} - e^{-i\left(\int p\,dx/\hbar+\pi/4\right)}\right) \tag{42}$$

$$= \frac{2D}{\sqrt{p(x)}}\sin\left[\int_0^x p\,dx'/\hbar + \pi/4\right] \tag{43}$$

And for $x<0$

$$\psi(x) \cong \frac{D}{\sqrt{|p(x)|}}\exp\left[-\int_x^0 \left|p\left(x'\right)\right|\,dx'/\hbar\right] \tag{44}$$

If the turning point is at the general location of x_1, we can just replace the 0 in the limits of the integrals by x_1. The only difference between the cases of increasing and decreasing potentials is that the limits of integration are reversed.

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