WKB APPROXIMATION OF A DOUBLE POTENTIAL WELL: TURNING POINTS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.15a.

In this post, we'll start applying the WKB approximation to the problem of a double potential well, in which the potential is an even function with two minima, at $\pm x_0$ and a finite maximum V_0 at $x=0$. The potential will tend to $+\infty$ as $x\to\pm\infty$, and we'll be looking for bound states with a total energy $E<V_0$, so classically, the particle would be confined to one of the two wells. To make things definite, we'll look at the wave function in the right-hand well, where the turning points are at x_1 (where $V'(x_1)<0$) and x_2 (where $V'(x_2)>0$).

The situation at turning point x_2 is the same as with the single-well potential, so we get

$$\psi(x)\approx\begin{cases}\frac{2D}{\sqrt{p(x)}}\sin\left[\int_x^{x_2}p(x')\,dx'/\hbar+\frac{\pi}{4}\right] & x_1<x<x_2\\ \frac{D}{\sqrt{|p(x)|}}\exp\left[-\int_{x_2}^{x}|p(x')|\,dx'/\hbar\right] & x>x_2\end{cases} \tag{0.1}$$

where D is a normalization constant.

To get the wave function for $0<x<x_1$ we need to use the patching function to connect the WKB functions on either side of $x=x_1$. We've done a similar analysis for the downward sloping turning point in a single well potential, but in that case we assumed that $V(x)\to\infty$ as $x\to-\infty$ so we could throw away the positive exponential term in the wave function. In this case, we can't do that since the potential is finite to the left of $x=0$, at least up to the point where it decreases and goes below E in the left-hand well.

The plan is essentially the same as that used in analyzing the finite barrier with sloping sides. First, we linearize the potential near the point $x=x_1$, then we work out the patching function in the region $x>x_1$ and relate it to the WKB function in that region. Since we already know the WKB function for $x_1<x<x_2$, we make the WKB function from the left turning point match that given in 0.1. Finally, we use the patching function to find the WKB function for $0<x<x_1$.

As usual, we'll do the analysis by shifting x_1 to the origin. Then the WKB functions near $x=0$ are

$$\psi=\begin{cases}\frac{1}{\sqrt{|p|}}\left[Ge^{\int_x^0|p(x')|dx'/\hbar}+Fe^{-\int_x^0|p(x')|dx'/\hbar}\right] & x<0\\ \frac{1}{\sqrt{p}}\left[Be^{i\int_0^x p(x')dx'/\hbar}+Ce^{-i\int_0^x p(x')dx'/\hbar}\right] & x>0\end{cases} \tag{0.2}$$

Linearizing the potential, we have

$$V(x)\approx E+V'(0)x \tag{0.3}$$

As before, solving the Schrödinger equation for this linearized potential gives us the patching wave function ψ_p:

$$\psi_p(x) = aAi(\alpha x)+bBi(\alpha x) \tag{0.4}$$

$$\alpha \equiv \left(\frac{2mV'(0)}{\hbar^2}\right)^{1/3} \tag{0.5}$$

In the overlap region to the right of x_1, $x>0$ so

$$p(x)=\sqrt{2m(E-V(x))}=\hbar\sqrt{-\alpha^3 x} \tag{0.6}$$

Note that p is real, since $\alpha<0$ (due to $V'(0)<0$) and $x>0$. Therefore

$$\int_0^x p(x')\,dx'=\frac{2}{3}\hbar(-\alpha x)^{3/2} \tag{0.7}$$

and the WKB function from 0.2 for $x>0$ is

$$\psi(x)=\frac{1}{\sqrt{\hbar}(-\alpha)^{3/4}x^{1/4}}\left(Be^{iq}+Ce^{-iq}\right) \tag{0.8}$$

$$q\equiv\frac{1}{\hbar}\int_0^x p(x')\,dx'=\frac{2}{3}(-\alpha x)^{3/2} \tag{0.9}$$

Now for the patching function ψ_p for $x>0$ from 0.4, we see that the argument is negative since $\alpha<0$, so we can apply the large negative asymptotic forms for the Airy functions:

$$Ai(z)\sim\begin{cases}\frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left[\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right] & z\ll 0\\ \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-2z^{3/2}/3} & z\gg 0\end{cases} \tag{0.10}$$

$$Bi(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] & z \ll 0 \\ \frac{1}{\sqrt{\pi} z^{1/4}} e^{2z^{3/2}/3} & z \gg 0 \end{cases} \tag{0.11}$$

This gives us

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}} \left[a \sin\left(q + \frac{\pi}{4}\right) + b \cos\left(q + \frac{\pi}{4}\right)\right] \tag{0.12}$$

$$= \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}} \left[\frac{a}{2i}\left(e^{iq+i\pi/4} - e^{-iq-i\pi/4}\right) + \frac{b}{2}\left(e^{iq+i\pi/4} + e^{-iq-i\pi/4}\right)\right] \tag{0.13}$$

Equating coefficients of $e^{\pm iq}$ in this equation and the WKB function 0.8 we get

$$a = i\sqrt{\frac{\pi}{-\hbar\alpha}}\left(Be^{-i\pi/4} - Ce^{i\pi/4}\right) \tag{0.14}$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}}\left(Be^{-i\pi/4} + Ce^{i\pi/4}\right) \tag{0.15}$$

The WKB function 0.8 must be the same as 0.1 in the region $x_1 < x < x_2$. To use this fact, we note that

$$\int_x^{x_2} p(x')\,dx' = \int_{x_1}^{x_2} p(x')\,dx' - \int_{x_1}^{x} p(x')\,dx' \tag{0.16}$$

Applying this to 0.1 we get

$$\psi(x) \approx \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' - \frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4}\right] \tag{0.17}$$

$$= \frac{2D}{\sqrt{p(x)}} \sin\left(\theta - q + \frac{\pi}{4}\right) \tag{0.18}$$

$$= \frac{2D}{\sqrt{p(x)}} \frac{1}{2i}\left(e^{i\theta - iq + i\pi/4} - e^{-i\theta + iq - i\pi/4}\right) \tag{0.19}$$

where

$$\theta \equiv \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' \tag{0.20}$$

This function must be the same as 0.8 so we can get the constants B and C in terms of D:

$$B = -\frac{D}{i}e^{-i\theta-i\pi/4} \tag{0.21}$$

$$C = \frac{D}{i}e^{i\theta+i\pi/4} \tag{0.22}$$

We can insert these into 0.14 and 0.15 to get

$$a = -\sqrt{\frac{\pi}{-\hbar\alpha}}D\left(e^{-i\theta-i\pi/2}+e^{i\theta+i\pi/2}\right) \tag{0.23}$$

$$= -2\sqrt{\frac{\pi}{-\hbar\alpha}}D\cos\left(\theta+\frac{\pi}{2}\right) \tag{0.24}$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D\sin\theta \tag{0.25}$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}}\frac{D}{i}\left(-e^{-i\theta-i\pi/2}+e^{i\theta+i\pi/2}\right) \tag{0.26}$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D\sin\left(\theta+\frac{\pi}{2}\right) \tag{0.27}$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D\cos\theta \tag{0.28}$$

Now we can look at the other side of the turning point, where $x < x_1$ (or $x < 0$ in our calculations). First, we note that, from 0.6

$$|p(x)| = \left|\hbar\sqrt{-\alpha^3 x}\right| = \hbar\sqrt{\alpha^3 x} \tag{0.29}$$

since $\alpha < 0$ and $x < 0$. Also, since $|p(x)|$ is an even function and $x < 0$

$$\int_x^0 \left|p\left(x'\right)\right| dx' = \int_0^{-x} p\left(x'\right) dx' = \hbar q \tag{0.30}$$

Therefore, from 0.2 with $x < 0$ we get

$$\psi(x) = \frac{1}{\sqrt{\hbar}(-\alpha)^{3/4}(-x)^{1/4}}\left(Ge^{q}+Fe^{-q}\right) \tag{0.31}$$

Using the same patching function as before but now taking its large positive asymptotic form (since $\alpha < 0$ and $x < 0$, so $\alpha x > 0$), we get

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(\alpha x)^{1/4}}\left(\frac{a}{2}e^{-q} + be^{q}\right) \tag{0.32}$$

Comparing coefficients with the WKB form:

$$\frac{a}{2} = \sqrt{\frac{\pi}{-\hbar\alpha}}F \tag{0.33}$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}}G \tag{0.34}$$

Using 0.25 and 0.28 we can write F and G in terms of D:

$$F = D\sin\theta \tag{0.35}$$

$$G = 2D\cos\theta \tag{0.36}$$

Substituting back into the first of 0.2 and restoring the turning point from $x = 0$ to $x = x_1$ we get for $0 < x < x_1$:

$$\psi(x) \approx \frac{D}{\sqrt{|p(x)|}}\left[2\cos\theta e^{\int_x^{x_1}|p(x')|dx'/\hbar} + \sin\theta e^{-\int_x^{x_1}|p(x')|dx'/\hbar}\right] \tag{0.37}$$

This, together with 0.1, gives us the complete WKB wave function for $x > 0$.

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