WKB APPROXIMATION OF A DOUBLE POTENTIAL WELL:
TURNING POINTS

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Post date: 26 Jul 2014.

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

$$\psi(x) \approx \begin{cases} 
\frac{2D}{\sqrt{p(x)}} \sin \left[ \int_{x}^{x_2} p(x') \, dx'/\hbar + \frac{\pi}{4} \right] & x_1 < x < x_2 \\
\frac{D}{\sqrt{|p(x)|}} \exp \left[ - \int_{x_2}^{x} |p(x')| \, dx'/\hbar \right] & x > x_2 
\end{cases} \quad (1)$$

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 (1). Finally, we use the patching function to find the WKB function for $0 < x < x_1$. 

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

$$
\psi = \begin{cases} 
\frac{1}{\sqrt{|p|}} \left[ Ge^{\int_{x_0}^0 p(x') dx'/\hbar} + Fe^{-\int_{x_0}^0 p(x') dx'/\hbar} \right] & x < 0 \\
\frac{1}{\sqrt{p}} \left[ Be^{i \int_0^x p(x') dx'/\hbar} + Ce^{-i \int_0^x p(x') dx'/\hbar} \right] & x > 0
\end{cases}
$$

(2)

Linearizing the potential, we have

$$
V(x) \approx E + V'(0)x
$$

(3)

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

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

(4)

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

(5)

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

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

(6)

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

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

(7)

and the WKB function from (2) for $x > 0$ is

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

(8)

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

(9)

Now for the patching function $\psi_p$ for $x > 0$ from (4) we see that the argument is negative since $\alpha < 0$, so we can apply the large negative asymptotic forms for the Airy functions:

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

(10)

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

(11)
This gives us

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}} \left[ a \sin \left( q + \frac{\pi}{4} \right) + b \cos \left( q + \frac{\pi}{4} \right) \right]$$  \hspace{1cm} (12)$$

$$= \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}} \left[ \frac{a}{2i} \left( e^{iq+i\pi/4} - e^{-iq-i\pi/4} \right) + \frac{b}{2} \left( e^{iq+i\pi/4} + e^{-iq-i\pi/4} \right) \right]$$  \hspace{1cm} (13)$$

Equating coefficients of $e^{\pm iq}$ in this equation and the WKB function 8 we get

$$a = i \sqrt{\frac{\pi}{-\hbar \alpha}} \left( Be^{-i\pi/4} - Ce^{i\pi/4} \right)$$  \hspace{1cm} (14)$$

$$b = \sqrt{\frac{\pi}{-\hbar \alpha}} \left( Be^{-i\pi/4} + Ce^{i\pi/4} \right)$$  \hspace{1cm} (15)$$

The WKB function 8 must be the same as 1 in the region $x_1 < x < x_2$. To use this fact, we note that

$$\int_x^{x_2} p(x') dx' = \int_{x_1}^{x_2} p(x') dx' - \int_{x_1}^x p(x') dx'$$  \hspace{1cm} (16)$$

Applying this to 1 we get

$$\psi(x) \approx \frac{2D}{\sqrt{p(x)}} \sin \left[ \frac{1}{\hbar} \int_{x_1}^{x_2} p(x') dx' - \frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \frac{\pi}{4} \right]$$  \hspace{1cm} (17)$$

$$= \frac{2D}{\sqrt{p(x)}} \sin \left( \theta - q + \frac{\pi}{4} \right)$$  \hspace{1cm} (18)$$

$$= \frac{2D}{\sqrt{p(x)}} \frac{1}{2i} \left( e^{i\theta - iq + i\pi/4} - e^{-i\theta + iq - i\pi/4} \right)$$  \hspace{1cm} (19)$$

where

$$\theta = \frac{1}{\hbar} \int_{x_1}^{x_2} p(x') dx'$$  \hspace{1cm} (20)$$

This function must be the same as 8 so we can get the constants $B$ and $C$ in terms of $D$:
\[ B = -\frac{D}{i} e^{-i\vartheta - i\pi/4} \]  
\[ C = \frac{D}{i} e^{i\vartheta + i\pi/4} \]  

We can insert these into Eqs. 14 and 15 to get

\[ a = -\sqrt{\frac{\pi}{-\hbar \alpha}} D \left( e^{-i\vartheta - i\pi/2} + e^{i\vartheta + i\pi/2} \right) \]  
\[ = -2 \sqrt{\frac{\pi}{-\hbar \alpha}} D \cos \left( \theta + \frac{\pi}{2} \right) \]  
\[ = 2 \sqrt{\frac{\pi}{-\hbar \alpha}} D \sin \theta \]  
\[ b = \sqrt{\frac{\pi}{-\hbar \alpha}} D \left( -e^{-i\vartheta - i\pi/2} + e^{i\vartheta + i\pi/2} \right) \]  
\[ = 2 \sqrt{\frac{\pi}{-\hbar \alpha}} D \sin \left( \theta + \frac{\pi}{2} \right) \]  
\[ = 2 \sqrt{\frac{\pi}{-\hbar \alpha}} D \cos \theta \]  

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 Eq. 6

\[ |p(x)| = |\hbar \sqrt{-\alpha^3 x}| = \hbar \sqrt{\alpha^3 x} \]  

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

\[ \int_{x}^{0} |p(x')| \, dx' = \int_{0}^{-x} p(x') \, dx' = \hbar q \]  

Therefore, from Eq. 2 with \( x < 0 \) we get

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

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

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

Comparing coefficients with the WKB form:
Using (25) and (28) we can write $F$ and $G$ in terms of $D$:

\[
F = D \sin \theta \tag{35}
\]
\[
G = 2D \cos \theta \tag{36}
\]

Substituting back into the first of (2) and restoring the turning point from $x = 0$ to $x = x_1$ we get for $0 < x < x_1$:

\[
\psi(x) \approx \frac{D}{\sqrt{|p(x)|}} \left[ 2 \cos \theta e^{\int_{x_1}^{x} |p(x')| dx'/\hbar} + \sin \theta e^{-\int_{x_1}^{x} |p(x')| dx'/\hbar} \right] \tag{37}
\]

This, together with (1) gives us the complete WKB wave function for $x > 0$. 

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