

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 $x \rightarrow \pm\infty$, 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 $V(x) \rightarrow \infty$ as $x \rightarrow -\infty$ 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 $0 < x < x_1$.

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

$$\psi = \begin{cases} \frac{1}{\sqrt{|p|}} \left[G e^{\int_x^0 |p(x')| dx' / \hbar} + F e^{-\int_x^0 |p(x')| dx' / \hbar} \right] & x < 0 \\ \frac{1}{\sqrt{p}} \left[B e^{i \int_0^x p(x') dx' / \hbar} + C e^{-i \int_0^x p(x') dx' / \hbar} \right] & x > 0 \end{cases} \quad (2)$$

Linearizing the potential, we have

$$V(x) \approx E + V'(0)x \quad (3)$$

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

$$\psi_p(x) = aAi(\alpha x) + bBi(\alpha x) \quad (4)$$

$$\alpha \equiv \left(\frac{2mV'(0)}{\hbar^2} \right)^{1/3} \quad (5)$$

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

$$p(x) = \sqrt{2m(E - V(x))} = \hbar \sqrt{-\alpha^3 x} \quad (6)$$

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

$$\int_0^x p(x') dx' = \frac{2}{3} \hbar (-\alpha x)^{3/2} \quad (7)$$

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

$$\psi(x) = \frac{1}{\sqrt{\hbar} (-\alpha)^{3/4} x^{1/4}} (B e^{iq} + C e^{-iq}) \quad (8)$$

$$q \equiv \frac{1}{\hbar} \int_0^x p(x') dx' = \frac{2}{3} (-\alpha x)^{3/2} \quad (9)$$

Now for the patching function ψ_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:

$$Ai(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin \left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4} \right] & z \ll 0 \\ \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-2z^{3/2}/3} & z \gg 0 \end{cases} \quad (10)$$

$$Bi(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos \left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4} \right] & z \ll 0 \\ \frac{1}{\sqrt{\pi}z^{1/4}} e^{2z^{3/2}/3} & z \gg 0 \end{cases} \quad (11)$$

This gives us

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

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

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

$$a = i \sqrt{\frac{\pi}{-\hbar\alpha}} \left(B e^{-i\pi/4} - C e^{i\pi/4} \right) \quad (14)$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}} \left(B e^{-i\pi/4} + C e^{i\pi/4} \right) \quad (15)$$

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

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

Applying this to 1 we get

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

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

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

where

$$\theta \equiv \frac{1}{\hbar} \int_{x_1}^{x_2} p(x') dx' \quad (20)$$

This function must be the same as 8 so we can get the constants B and C in terms of D :

$$B = -\frac{D}{i}e^{-i\theta-i\pi/4} \quad (21)$$

$$C = \frac{D}{i}e^{i\theta+i\pi/4} \quad (22)$$

We can insert these into 14 and 15 to get

$$a = -\sqrt{\frac{\pi}{-\hbar\alpha}}D \left(e^{-i\theta-i\pi/2} + e^{i\theta+i\pi/2} \right) \quad (23)$$

$$= -2\sqrt{\frac{\pi}{-\hbar\alpha}}D \cos\left(\theta + \frac{\pi}{2}\right) \quad (24)$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D \sin\theta \quad (25)$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}}\frac{D}{i} \left(-e^{-i\theta-i\pi/2} + e^{i\theta+i\pi/2} \right) \quad (26)$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D \sin\left(\theta + \frac{\pi}{2}\right) \quad (27)$$

$$= 2\sqrt{\frac{\pi}{-\hbar\alpha}}D \cos\theta \quad (28)$$

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 6

$$|p(x)| = \left| \hbar\sqrt{-\alpha^3 x} \right| = \hbar\sqrt{\alpha^3 x} \quad (29)$$

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

$$\int_x^0 |p(x')| dx' = \int_0^{-x} p(x') dx' = \hbar q \quad (30)$$

Therefore, from 2 with $x < 0$ we get

$$\psi(x) = \frac{1}{\sqrt{\hbar}(-\alpha)^{3/4}(-x)^{1/4}} (Ge^q + Fe^{-q}) \quad (31)$$

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

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(\alpha x)^{1/4}} \left(\frac{a}{2}e^{-q} + be^q \right) \quad (32)$$

Comparing coefficients with the WKB form:

$$\frac{a}{2} = \sqrt{\frac{\pi}{-\hbar\alpha}} F \quad (33)$$

$$b = \sqrt{\frac{\pi}{-\hbar\alpha}} G \quad (34)$$

Using 25 and 28 we can write F and G in terms of D :

$$F = D \sin \theta \quad (35)$$

$$G = 2D \cos \theta \quad (36)$$

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

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

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

PINGBACKS

Pingback: WKB approximation of double-well potential: wave functions