WKB APPROXIMATION FOR A BARRIER WITH SLOPING SIDES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.10.

We've studied the WKB approximation in the cases where the potential is increasing and decreasing at a finite rate (that is, the potential has no step functions). We've applied this to the case of a potential well with sloping sides, such as the harmonic oscillator. You might think that, since we've worked out the behaviour of the WKB solutions at both increasing and decreasing turning points, that we could apply these solutions to the case of a potential barrier with sloping sides. However, there is one fly in the ointment here: in considering the potential well, we assumed that $E<V(x)$ out to infinity on both sides of the well, meaning that we could throw away the positive exponential term in the solution. With a potential barrier of finite width, we can't do this since $E<V(x)$ only within the barrier. We can, however, apply the same techniques to find a solution.

The starting point is the WKB functions for the three regions we're interested in. We'll take the barrier to be between x_1 on the left and x_2 on the right, so we have

$$\psi(x)\approx\begin{cases}\frac{1}{\sqrt{p(x)}}\left[Ae^{i\int_x^{x_1}p(x')dx'/\hbar}+Be^{-i\int_x^{x_1}p(x')dx'/\hbar}\right] & x<x_1\\ \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\int_{x_1}^{x}|p(x')|dx'/\hbar}+De^{-\int_{x_1}^{x}|p(x')|dx'/\hbar}\right] & x_1<x<x_2\\ \frac{1}{\sqrt{p(x)}}\left[Fe^{i\int_{x_2}^{x}p(x')dx'/\hbar}\right] & x>x_2\end{cases}\tag{1}$$

There's no negative exponential in the last term, since we're treating the usual scattering problem where a particle comes in from the left and is reflected and transmitted by the barrier. The key difference between the scattering problem and the potential well is that we can't set $C=0$ in the middle equation for the reason given above.

We'll consider first the turning point at $x=x_1$, where the potential is increasing. As before, we'll set $x_1=0$ temporarily to ease the notation a bit. Recall that we approximate the potential at the turning points by

$$V(x)\approx E+V'(0)x\tag{2}$$

and following the same procedure as before, we get the WKB function to the right of the left turning point (that is, for x slightly larger than 0) to be

$$\psi \approx \frac{1}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}}\left[Ce^{2(\alpha x)^{3/2}/3}+De^{-2(\alpha x)^{3/2}/3}\right] \tag{3}$$

where

$$\alpha \equiv \left(\frac{2mV'(0)}{\hbar^2}\right)^{1/3} \tag{4}$$

As before, we introduce a patching wave function ψ_p to span the turning point, and find that it satisfies Airy's equation

$$\frac{d^2\psi_p}{dz^2} = z\psi_p \tag{5}$$

where $z = \alpha x$. This has the general solution

$$\psi_p(z) = aAi(z) + bBi(z) \tag{6}$$

$$\psi_p(x) = aAi(\alpha x) + bBi(\alpha x) \tag{7}$$

The asymptotic forms of the Airy functions $Ai(z)$ and $Bi(z)$ are

$$Ai(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left[\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right] & z \ll 0 \\ \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-2z^{3/2}/3} & z \gg 0 \end{cases} \tag{8}$$

$$Bi(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}}\cos\left[\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right] & z \ll 0 \\ \frac{1}{\sqrt{\pi}z^{1/4}}e^{2z^{3/2}/3} & z \gg 0 \end{cases} \tag{9}$$

Restricting our attention to values of z that are large enough that we can use the asymptotic forms of the Airy functions (but still satisfy 2), we get

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(\alpha x)^{1/4}}\left[\frac{a}{2}e^{-2(\alpha x)^{3/2}/3}+be^{2(\alpha x)^{3/2}/3}\right] \tag{10}$$

This time we can't set $b = 0$, but by equating coefficients between 3 and 10 we find

$$a = \sqrt{\frac{4\pi}{\alpha\hbar}}D \tag{11}$$

$$b = \sqrt{\frac{\pi}{\alpha\hbar}}C \tag{12}$$

Now looking at the region just to the left of the left-hand turning point, the WKB function is

$$\psi \approx \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}}\left[Ae^{2i(-\alpha x)^{3/2}/3} + Be^{-2i(-\alpha x)^{3/2}/3}\right] \tag{13}$$

The patching function comes out to (this time using the asymptotic forms of the Airy functions for large negative x):

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}\left[a\sin\left(\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right) + b\cos\left(\frac{2}{3}(\alpha x)^{3/2} + \frac{\pi}{4}\right)\right] \tag{14}$$

$$= \frac{1}{2\sqrt{\pi}(-\alpha x)^{1/4}}\left[e^{i\pi/4}e^{2i(-\alpha x)^{3/2}/3}(b-ai) + e^{-i\pi/4}e^{-2i(-\alpha x)^{3/2}/3}(b+ai)\right] \tag{15}$$

Comparing coefficients gives

$$b - ai = \sqrt{\frac{4\pi}{\alpha\hbar}}Ae^{-i\pi/4} \tag{16}$$

$$b + ai = \sqrt{\frac{4\pi}{\alpha\hbar}}Be^{i\pi/4} \tag{17}$$

Solving for a and b and comparing with 11 and 12 we get

$$C = Ae^{-i\pi/4} + Be^{i\pi/4} \tag{18}$$

$$D = \frac{1}{2i}\left(-Ae^{-i\pi/4} + Be^{i\pi/4}\right) \tag{19}$$

$$A = e^{i\pi/4}\left(\frac{C}{2} - iD\right) \tag{20}$$

$$B = e^{-i\pi/4}\left(\frac{C}{2} + iD\right) \tag{21}$$

That relates the WKB functions to the left and right of the left hand turning point at $x = x_1$. Now we need to repeat the calculation for the turning point at $x = x_2$, where the potential is decreasing. First, we need to rewrite the WKB functions so that the middle equation in 1 is in terms of x_2 rather than x_1. We can do this by noting that an integral from x_1 to x is the sum of integrals from x_1 to x_2 and then from x_2 to x. When we considered the WKB approximation in tunneling we saw that the transmission coefficient was approximately

$$T \equiv \frac{|F|^2}{|A|^2} \approx e^{-2\gamma} = e^{-2\int_{x_1}^{x_2}|p(x)|dx/\hbar} \tag{22}$$

We can therefore rewrite the WKB functions at the turning point in terms of γ to get, for the region just to the left of $x = x_2$ (again, we can reposition x_2 to zero to make things easier):

$$\psi(x) \approx \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\left(\int_{x_1}^{x_2}+\int_{x_2}^{x}\right)|p(x')|dx'/\hbar} + De^{-\left(\int_{x_1}^{x_2}+\int_{x_2}^{x}\right)|p(x')|dx'/\hbar}\right] \tag{23}$$

$$= \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\left(\int_{x_1}^{0}+\int_{0}^{x}\right)|p(x')|dx'/\hbar} + De^{-\left(\int_{x_1}^{0}+\int_{0}^{x}\right)|p(x')|dx'/\hbar}\right] \tag{24}$$

$$= \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}}\left[Ce^{\gamma}e^{-2(-\alpha x)^{3/2}/3} + De^{-\gamma}e^{2(-\alpha x)^{3/2}/3}\right] \tag{25}$$

where the $-x$ in the denominator in the last line is because $x < 0$.

For the patching function in this region we have

$$\alpha \equiv \left(\frac{2m|V'(0)|}{\hbar^2}\right)^{1/3} \tag{26}$$

$$z \equiv -\alpha x \tag{27}$$

so the asymptotic form of the Airy functions for large positive z (since $x < 0$) can be used to get

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}\left[\frac{c}{2}e^{-2(-\alpha x)^{3/2}/3} + de^{2(-\alpha x)^{3/2}/3}\right] \tag{28}$$

Comparing coefficients between ψ and ψ_p we get

$$c = \sqrt{\frac{4\pi}{\alpha\hbar}}Ce^{\gamma} \tag{29}$$

$$d = \sqrt{\frac{\pi}{\alpha\hbar}}De^{-\gamma} \tag{30}$$

Looking now at the region just to the right of x_2 we get for the WKB function

$$\psi(x) \approx \frac{1}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}}\left[Fe^{2i(\alpha x)^{3/2}/3}\right] \tag{31}$$

Using the asymptotic forms of the Airy functions for large negative z we get

$$\psi_p(x) \approx \frac{1}{\sqrt{\pi}(\alpha x)^{1/4}}\left[c\sin\left(\frac{2}{3}(\alpha x)^{3/2}+\frac{\pi}{4}\right)+d\cos\left(\frac{2}{3}(\alpha x)^{3/2}+\frac{\pi}{4}\right)\right] \tag{32}$$

$$= \frac{1}{2\sqrt{\pi}(\alpha x)^{1/4}}\left[e^{i\pi/4}e^{2i(\alpha x)^{3/2}/3}(d-ci)+e^{-i\pi/4}e^{-2i(\alpha x)^{3/2}/3}(d+ci)\right] \tag{33}$$

Comparing coefficients:

$$d+ci=0 \tag{34}$$

$$= \sqrt{\frac{4\pi}{\alpha\hbar}}\left(\frac{D}{2}e^{-\gamma}+iCe^{\gamma}\right) \tag{35}$$

$$D=-2ie^{2\gamma}C \tag{36}$$

$$d-ci=\sqrt{\frac{4\pi}{\alpha\hbar}}Fe^{-i\pi/4} \tag{37}$$

$$= \sqrt{\frac{4\pi}{\alpha\hbar}}\left(\frac{D}{2}e^{-\gamma}-iCe^{\gamma}\right) \tag{38}$$

$$F=e^{i\pi/4}\left(\frac{D}{2}e^{-\gamma}-iCe^{\gamma}\right) \tag{39}$$

$$= -2Cie^{\gamma}e^{i\pi/4} \tag{40}$$

We've thus managed to express D and F in terms of C. We can find the transmission coefficient by using 20 to get

$$A = e^{i\pi/4}\left(\frac{C}{2} - iD\right) \tag{41}$$

$$= e^{i\pi/4}C\left(\frac{1}{2} - 2e^{2\gamma}\right) \tag{42}$$

$$T = \frac{|F|^2}{|A|^2} \tag{43}$$

$$= \frac{4e^{2\gamma}}{\left(\frac{1}{2} - 2e^{2\gamma}\right)^2} \tag{44}$$

$$= \frac{e^{-2\gamma}}{\left(\frac{e^{-2\gamma}}{4} - 1\right)^2} \tag{45}$$

For a wide or high barrier, γ gets very large, so the denominator tends to 1, and we get

$$T \approx e^{-2\gamma} \tag{46}$$

which agrees with our earlier result 22 which was derived by ignoring the effects at the turning points. (Well, actually, it wasn't 'derived' as such; it was more of a plausibility argument.)

PINGBACKS

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