

WKB APPROXIMATION: TURNING POINTS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.6.

We've seen that the WKB approximation for the wave function has the form

$$(1) \quad \psi(x) \approx \frac{1}{\sqrt{p(x)}} \left(B e^{i \int p dx / \hbar} + C e^{-i \int p dx / \hbar} \right)$$

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

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

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

$$(3) \quad \psi(x) \approx \frac{1}{\sqrt{|p|}} \left(D e^{-\frac{1}{\hbar} \int |p(x)| dx} + F e^{\frac{1}{\hbar} \int |p(x)| dx} \right)$$

If the region in which $E < V(x)$ extends out to $x \rightarrow \infty$, the positive exponential term must vanish, so we have $F = 0$ and

$$(4) \quad \psi(x) \approx \frac{1}{\sqrt{|p|}} D e^{-\frac{1}{\hbar} \int |p(x)| dx}$$

The WKB approximation was derived by approximating the differential equation

$$(5) \quad \frac{A''}{A} = (\phi')^2 - \frac{p^2}{\hbar^2}$$

by assuming that the LHS is very small compared to both terms on the RHS, in particular, that

$$(6) \quad \frac{A''}{A} \ll \frac{p^2(x)}{\hbar^2}$$

Now suppose we have a potential that increases at some finite rate (that is, there are no vertical walls as in the infinite square well). Then if the particle's energy is E , there is a point x_2 , say, where $E = V(x_2)$ and at this point $p(x_2) = 0$ so the condition 6 is not valid. Griffiths calls x_2 the turning point, and it's clear that the WKB approximation breaks down at turning points. We can see this from 1 and 4 as well, since if $p(x_2) = 0$, $\psi(x) \rightarrow \infty$ as $x \rightarrow x_2$, which can't be allowed since an infinite wave function cannot be normalized. Because of this problem, we can't satisfy the condition that the wave function must be continuous at the turning point.

The way around this is a bit of a fudge, but the way it works is as follows. If the potential varies continuously at the turning point (as all physical potential do), then for a small region around the turning point we can approximate the potential by its tangent line at $x = x_2$. (For convenience, we'll take $x_2 = 0$ in the argument that follows.) That is, around $x = 0$ we assume

$$(7) \quad V(x) \approx E + V'(0)x$$

With a linear potential, we have a situation similar to the problem we solved earlier, with a particle moving in the gravitational field at the Earth's surface. The Schrödinger equation is

$$(8) \quad -\frac{\hbar^2}{2m} \frac{d^2 \psi_p}{dx^2} + (E + V'(0)x) \psi_p = E \psi_p$$

where $\psi_p(x)$ is a 'patching' wave function that spans a small distance either side of the turning point. The idea is that *this* patching wave function *is* continuous across the turning point, and that we can make it continuous with one WKB wave function on one side and with the other WKB function on the other side of the turning point.

To make things definite, suppose the potential is increasing at $x = 0$, so that $V'(0) > 0$, $E > V(x)$ for $x < 0$ and $E < V(x)$ for $x > 0$. Then the WKB function 1 applies for $x < 0$ and the function 4 applies for $x > 0$. The idea is that we should be able to make $\psi_p(x)$ equal to 1 for some range of $x < 0$ and also make $\psi_p(x)$ equal to 4 for some range of $x > 0$.

It's important to understand that we're *not* going to make the wave functions match up right at $x = 0$. Rather, we will take a range of x on the $x < 0$ side of the turning point that is close enough to the turning point that we can still use 7 as an approximation for the potential (and thus that the patching wave function is still valid), but far enough from $x = 0$ that the WKB approximation is also valid. It's a bit of a leap of faith that such a region can actually be found, although in practice it turns out that in most cases it can be.

We must first find $\psi_p(x)$. We can rewrite 8 as

$$(9) \quad \frac{d^2 \psi_p}{dx^2} = \frac{2mV'(0)}{\hbar^2} x \psi_p$$

By defining

$$(10) \quad \alpha \equiv \left(\frac{2mV'(0)}{\hbar^2} \right)^{1/3}$$

$$(11) \quad z \equiv \alpha x$$

we end up with Airy's equation

$$(12) \quad \frac{d^2 \psi_p}{dz^2} = z \psi_p$$

As we saw earlier, this has the general solution

$$(13) \quad \psi_p(z) = aAi(z) + bBi(z)$$

$$(14) \quad \psi_p(x) = aAi(\alpha x) + bBi(\alpha x)$$

It is this function that we need to match up to 1 for $x < 0$ and to 4 for $x > 0$.

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

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

$$(16) \quad Bi(z) \sim \begin{cases} \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos \left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4} \right] & z \ll 0 \\ \frac{1}{\sqrt{\pi}z^{1/4}} e^{2z^{3/2}/3} & z \gg 0 \end{cases}$$

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 14 for $z = \alpha x \gg 0$:

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

$$(18) \quad = \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} e^{-2(\alpha x)^{3/2}/3} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} e^{2(\alpha x)^{3/2}/3}$$

With the potential 7, the WKB function 4 is

$$(19) \quad p(x) = \sqrt{2m(E - V(x))}$$

$$(20) \quad = \sqrt{-2mV'(0)x}$$

$$(21) \quad \psi(x) = \frac{1}{\sqrt{|p|}} D e^{-\frac{1}{\hbar} \int_0^x |p(x')| dx'}$$

$$(22) \quad \int_0^x |p(x')| dx' = \int_0^x |p(x')| dx'$$

$$(23) \quad = \sqrt{2mV'(0)} \int_0^x \sqrt{x'} dx'$$

$$(24) \quad = \sqrt{2mV'(0)} \frac{2}{3} x^{3/2}$$

$$(25) \quad = \frac{2}{3} \hbar (\alpha x)^{3/2}$$

$$(26) \quad p(x) = \sqrt{-2mV'(0)x}$$

$$(27) \quad = \hbar \alpha^{3/2} \sqrt{-x}$$

$$(28) \quad \psi(x) = \frac{D}{\sqrt{\hbar \alpha^{3/4} x^{1/4}}} e^{-2(\alpha x)^{3/2}/3}$$

Matching this up with 18, we see that $b = 0$ and

$$(29) \quad \frac{a}{2\sqrt{\pi} \alpha^{1/4}} = \frac{D}{\sqrt{\hbar} \alpha^{3/4}}$$

$$(30) \quad a = 2\sqrt{\frac{\pi}{\hbar}} D$$

The patching function must therefore have the form

$$(31) \quad \psi_p(x) = 2\sqrt{\frac{\pi}{\hbar}} D e^{-2(\alpha x)^{3/2}/3}$$

for $\alpha x \gg 0$.

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

$$(32) \quad \psi_p(x) = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}} \sin \left[\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4} \right]$$

For the WKB function, we start with 1

$$(33) \quad p(x) = \sqrt{-2mV'(0)x}$$

$$(34) \quad = \hbar\alpha^{3/2}\sqrt{-x}$$

$$(35) \quad \int_x^0 p(x) dx = \frac{2}{3}\hbar\alpha^{3/2}(-x)^{3/2}$$

$$(36) \quad \psi(x) = \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}} \left(Be^{2i(-\alpha x)^{3/2}/3} + Ce^{-2i(-\alpha x)^{3/2}/3} \right)$$

We can now compare this with 32 by writing the sine in terms of exponentials

$$(37) \quad \psi_p(x) = \frac{a}{2i\sqrt{\pi}(-\alpha x)^{1/4}} \left[e^{i\left[\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right]} - e^{-i\left[\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right]} \right]$$

Comparing terms, we have

$$(38) \quad \frac{B}{\sqrt{\hbar}\alpha^{3/4}} = \frac{ae^{i\pi/4}}{2i\sqrt{\pi}\alpha^{1/4}}$$

$$(39) \quad B = \frac{ae^{i\pi/4}\sqrt{\hbar}\alpha}{2i\sqrt{\pi}}$$

$$(40) \quad = -ie^{i\pi/4}D$$

$$(41) \quad \frac{C}{\sqrt{\hbar}\alpha^{3/4}} = -\frac{ae^{-i\pi/4}}{2i\sqrt{\pi}\alpha^{1/4}}$$

$$(42) \quad C = -\frac{ae^{-i\pi/4}\sqrt{\hbar}\alpha}{2i\sqrt{\pi}}$$

$$(43) \quad = ie^{-i\pi/4}D$$

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 $x < 0$:

$$(44) \quad \psi(x) \cong \frac{-iD}{\sqrt{p(x)}} \left(e^{i(\int p dx/\hbar + \pi/4)} - e^{-i(\int p dx/\hbar + \pi/4)} \right)$$

$$(45) \quad = \frac{2D}{\sqrt{p(x)}} \frac{1}{2i} \left(e^{i(\int p dx/\hbar + \pi/4)} - e^{-i(\int p dx/\hbar + \pi/4)} \right)$$

$$(46) \quad = \frac{2D}{\sqrt{p(x)}} \sin \left[\int_x^0 p dx'/\hbar + \pi/4 \right]$$

And for $x > 0$

$$(47) \quad \psi(x) \cong \frac{D}{\sqrt{|p(x)|}} \exp \left[- \int_0^x |p(x')| dx'/\hbar \right]$$

If the turning point is at the general location of x_2 , we can just replace the 0 in the limits of the integrals by x_2 .

As an example, we can revisit the case of the particle moving under gravity at the Earth's surface. The potential has a vertical wall at $x = 0$ and for a particle of energy E , there is a turning point at

$$(48) \quad x_2 = \frac{E}{mg}$$

The potential can then be written as

$$(49) \quad p(x) = \sqrt{2m(E - mgx)}$$

$$(50) \quad = m\sqrt{2g(x_2 - x)}$$

We can get the allowed energy levels from the boundary condition that $\psi(0) = 0$. From 46 (replacing the 0 in the limit by x_2) we have

$$(51) \quad \psi(0) = \frac{2D}{\sqrt{p(x)}} \sin \left[\int_0^{x_2} p dx'/\hbar + \pi/4 \right] = 0$$

$$(52) \quad \int_0^{x_2} p dx'/\hbar + \pi/4 = n\pi$$

$$(53) \quad \int_0^{x_2} p dx' = \left(n - \frac{1}{4} \right) \pi \hbar$$

Doing the integral, we get

$$(54) \quad m\sqrt{2g} \int_0^{x_2} \sqrt{x_2 - x'} dx' = \left(n - \frac{1}{4}\right) \pi \hbar$$

$$(55) \quad \frac{m\sqrt{g}}{3} (2x_2)^{3/2} = \left(n - \frac{1}{4}\right) \pi \hbar$$

$$(56) \quad \frac{m\sqrt{g}}{3} \left(2\frac{E_n}{mg}\right)^{3/2} = \left(n - \frac{1}{4}\right) \pi \hbar$$

$$(57) \quad E_n = \frac{1}{8} (6\pi\hbar g (4n - 1))^{2/3} m^{1/3}$$

Using values from the previous problem ($g = 9.8 \text{ m s}^{-2}$ and a mass of 0.1 kg), we get the WKB estimate of the first four energy levels:

$$(58) \quad E_1 = 8.738 \times 10^{-23} \text{ J}$$

$$(59) \quad E_2 = 1.537 \times 10^{-22} \text{ J}$$

$$(60) \quad E_3 = 2.078 \times 10^{-22} \text{ J}$$

$$(61) \quad E_4 = 2.555 \times 10^{-22} \text{ J}$$

Comparing with the exact results shows the WKB values are quite good in this case:

$$(62) \quad E_1 = 8.805 \times 10^{-23} \text{ J}$$

$$(63) \quad E_2 = 1.539 \times 10^{-22} \text{ J}$$

$$(64) \quad E_3 = 2.079 \times 10^{-22} \text{ J}$$

$$(65) \quad E_4 = 2.556 \times 10^{-22} \text{ J}$$

From the previous problem, we can find the average height of the particle for a given energy level:

$$(66) \quad \langle x_n \rangle = \frac{2E_n}{3mg}$$

If we want $\langle x_n \rangle = 1 \text{ m}$, then

$$(67) \quad \frac{1}{12g} (6\pi\hbar g (4n - 1))^{2/3} m^{-2/3} = 1$$

$$(68) \quad n = 1.6366 \times 10^{33}$$

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