WKB APPROXIMATION - ANALYSIS OF THE OVERLAP REGION NEAR A TURNING POINT

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog and include the title or URL of this post in your comment.

Post date: 17 October 2021.

We've looked at the WKB approximation at the points called turning points where the particle's total energy is close to the potential energy. A fundamental problem with WKB is that it breaks down at turning points, so we can't connect the functions on either side by requiring that they are continuous at the turning point itself. We connected the WKB wave functions on either side of a turning point by defining a patching function ψ_p which is a solution of the Schrödinger equation for a linearized potential of the form

$$V(x) \approx E + V'(0)\,x \tag{1}$$

where the turning point occurs at $x = 0$. In order to apply boundary conditions we assumed that there was a region on either side of the turning point where we were sufficiently far from $x = 0$ for WKB to be a good approximation, yet close enough to $x = 0$ that 1 is a good approximation to the potential. Here we'll examine the harmonic oscillator to see if this assumption is valid.

We'll look specifically at the turning point x_2, where the potential is increasing, so $V'(x_2) > 0$. Using the exact potential:

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{2}$$

we can find x_2:

$$E_n = \frac{1}{2}m\omega^2 x_2^2 \tag{3}$$

$$x_2 = \frac{1}{\omega}\sqrt{\frac{2E_n}{m}} \tag{4}$$

$$= \sqrt{\frac{(2n-1)\hbar}{m\omega}} \tag{5}$$

where we've used the formula for the energy levels of the harmonic oscillator

$$E_n = \left(n - \frac{1}{2}\right)\hbar\omega \tag{6}$$

with $n = 1, 2, 3, \ldots$

The linearized potential for a point $x = x_2 + d$ is

$$\begin{aligned} V_{lin} &= E_n + m\omega^2 x_2 d & (7)\\ &= \left(n - \frac{1}{2}\right)\hbar\omega + \sqrt{(2n-1)\hbar m\omega^3}d & (8) \end{aligned}$$

and the exact potential at the same point is

$$\begin{aligned} V(x_2 + d) &= \frac{1}{2}m\omega^2 (x_2 + d)^2 & (9)\\ &= \frac{1}{2}m\omega^2 \left(\sqrt{\frac{(2n-1)\hbar}{m\omega}} + d\right)^2 & (10) \end{aligned}$$

Suppose we want to find the largest value of d such that the difference between the exact and linearized potentials is within 1%, that is

$$\frac{V(x_2 + d) - V_{lin}(x_2 + d)}{V(x_2 + d)} = 0.01 \tag{11}$$

Solving for d (which requires solving a quadratic equation) we get

$$d = 0.1\sqrt{\frac{(2n-1)\hbar}{m\omega}} \tag{12}$$

Thus the larger the energy level n, the further we can go from the turning point x_2 and still have a good approximation using the linearized potential.

The patching wave function in this region is given by the Airy function $Ai(z) = Ai(\alpha(x - x_2)) = Ai(\alpha d)$. From an analysis of the Airy functions, it is known that the asymptotic form for large z is within 1% of the true value provided $z = \alpha d > 5$. From our earlier analysis, we have

$$\begin{aligned} \alpha &= \left(\frac{2m}{\hbar^2}V'(x_2)\right)^{1/3} & (13)\\ &= \left(\frac{2m}{\hbar^2}\sqrt{(2n-1)\hbar m\omega^3}\right)^{1/3} & (14) \end{aligned}$$

Therefore

$$\alpha d = 0.1\left(\frac{2m}{\hbar^2}\sqrt{(2n-1)\hbar m\omega^3}\right)^{1/3}\sqrt{\frac{(2n-1)\hbar}{m\omega}} \tag{15}$$

$$= 0.1\,(2)^{1/3}\,(2n-1)^{2/3} \tag{16}$$

Requiring $\alpha d > 5$ results in $n > 125.5$, so the smallest value of n for which the asymptotic form of the Airy function $Ai(\alpha d)$ is accurate to within 1% is $n = 126$ (assuming that the ground state is given by $n = 1$). Thus for large n, an overlap region in which both the linearized potential and the asymptotic form of the Airy function are valid does indeed exist.

In some cases (as we saw with the harmonic oscillator) however, WKB does actually give good results for smaller n.