

## WKB APPROXIMATION OF DOUBLE-WELL POTENTIAL: WAVE FUNCTIONS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.15b-f.

Continuing our application of the WKB approximation to the problem of a double potential well, we can now look at determining the allowed energies for bound states. Since the potential  $V(x)$  is even, the wave function is a linear combination of even and odd functions. We worked out the WKB wave functions for  $x > 0$  and they are

$$(1) \quad \psi(x) \approx \begin{cases} \frac{D}{\sqrt{|p(x)|}} \left[ 2 \cos \theta e^{\int_x^{x_1} |p(x')| dx' / \hbar} + \sin \theta e^{-\int_x^{x_1} |p(x')| dx' / \hbar} \right] & 0 \leq x < x_1 \\ \frac{2D}{\sqrt{p(x)}} \sin \left[ \int_x^{x_2} p(x') dx' / \hbar + \frac{\pi}{4} \right] & x_1 < x < x_2 \\ \frac{D}{\sqrt{|p(x)|}} \exp \left[ -\int_{x_2}^x |p(x')| dx' / \hbar \right] & x > x_2 \end{cases}$$

where

$$(2) \quad \theta \equiv \frac{1}{\hbar} \int_{x_1}^{x_2} p(x') dx'$$

The odd extension of 1 is thus

$$(3) \quad \psi(-x) = -\psi(x)$$

for  $x \geq 0$ . For this case, we must have  $\psi(0) = 0$ , so we have

$$(4) \quad \psi(0) = \frac{D}{\sqrt{|p(0)|}} \left[ 2 \cos \theta e^{\int_0^{x_1} |p(x')| dx' / \hbar} + \sin \theta e^{-\int_0^{x_1} |p(x')| dx' / \hbar} \right]$$

$$(5) \quad = \frac{D}{\sqrt{|p(0)|}} e^{-\int_0^{x_1} |p(x')| dx' / \hbar} \left[ 2 \cos \theta e^{\phi} + \sin \theta \right]$$

$$(6) \quad \phi \equiv \frac{2}{\hbar} \int_0^{x_1} |p(x')| dx' = \frac{1}{\hbar} \int_{-x_1}^{x_1} |p(x')| dx'$$

where the last line follows from the fact that if  $V(x)$  is even, then  $p(x) = \sqrt{2m(E - V(x))}$  is also even. Setting 5 to zero gives the condition

$$(7) \quad \tan \theta = -2e^\phi$$

Since both  $\phi$  and  $\theta$  depend on  $p(x)$ , they both contain the energy  $E$ , so this condition imposes constraints on  $E$ .

For the even extension of the WKB function, we have

$$(8) \quad \psi(-x) = \psi(x)$$

$$(9) \quad \psi'(0) = 0$$

The latter condition gives us

$$(10) \quad \psi'(x) = -\frac{1}{2} \frac{D}{|p(x)|} p'(x) \psi(x) + \frac{D}{\hbar} \sqrt{|p(x)|} \left[ -2 \cos \theta e^{\int_{x_1}^{x_1} |p(x')| dx' / \hbar} + \sin \theta e^{-\int_{x_1}^{x_1} |p(x')| dx' / \hbar} \right]$$

Because  $p(x)$  is even,  $p'(0) = 0$  so

$$(11) \quad \psi'(0) = \frac{D}{\hbar} \sqrt{|p(0)|} \left[ -2 \cos \theta e^{\int_0^{x_1} |p(x')| dx' / \hbar} + \sin \theta e^{-\int_0^{x_1} |p(x')| dx' / \hbar} \right]$$

$$(12) \quad = \frac{D}{\hbar} \sqrt{|p(0)|} e^{-\int_0^{x_1} |p(x')| dx' / \hbar} \left[ -2 \cos \theta e^\phi + \sin \theta \right]$$

Setting this to zero gives the other energy quantization condition

$$(13) \quad \tan \theta = 2e^\phi$$

so the combined conditions are

$$(14) \quad \boxed{\tan \theta = \pm 2e^\phi}$$

If the central part of the potential (between  $x = -x_1$  and  $x = +x_1$ ) is high and/or broad then from 6,  $\phi$  will become large, since  $p(x)$  depends on  $V(x)$ . In that case we see from 14 that  $\tan \theta \rightarrow \pm\infty$  so  $\theta \rightarrow (n + \frac{1}{2}) \frac{\pi}{2}$  for some integer  $n$ . Rewriting 14 we get

$$(15) \quad \theta = \operatorname{arccot} \left( \pm \frac{1}{2} e^{-\phi} \right)$$

$$(16) \quad = \left( n + \frac{1}{2} \right) \pi \mp \frac{1}{2} e^{-\phi} + \mathcal{O} \left( e^{-3\phi} \right)$$

Now suppose we give the potential a specific formula:

$$(17) \quad V(x) = \begin{cases} \frac{1}{2} m \omega^2 (x+a)^2 & x < 0 \\ \frac{1}{2} m \omega^2 (x-a)^2 & x > 0 \end{cases}$$

That is, we're dealing with two linked harmonic oscillator potentials. The turning points are found from the condition  $p(x) = 0$  and are, for  $x > 0$ :

$$(18) \quad x_1 = -\sqrt{\frac{2E}{m\omega^2}} + a$$

$$(19) \quad x_2 = \sqrt{\frac{2E}{m\omega^2}} + a$$

We can now work out  $\theta$  from 2 by first working out the integral using Maple

$$(20) \quad \frac{1}{\hbar} \int p(x) dx = -\frac{m^{3/2} \omega^2}{2\hbar} (a-x) \left( -x^2 + 2ax + \frac{2E}{m\omega^2} - a^2 \right)^{1/2} - \frac{E}{\hbar\omega} \sin^{-1} \left( \sqrt{\frac{m\omega^2}{2E}} (a-x) \right)$$

The first term is zero at both  $x_1$  and  $x_2$ , and the argument of the arcsine is  $-1$  at  $x_2$  and  $+1$  at  $x_1$  so

$$(21) \quad \theta = \frac{1}{\hbar} \int_{x_1}^{x_2} p(x) dx$$

$$(22) \quad = \frac{\pi E}{\hbar\omega}$$

Using the approximation 16 we get

$$(23) \quad E_n^\pm \approx \left( n + \frac{1}{2} \right) \hbar\omega \mp \frac{\hbar\omega}{2\pi} e^{-\phi}$$

The  $+$  energy is for the even wave function, and corresponds to the minus sign on the RHS, so the energies of particles in the even state  $\psi_n^+$  are slightly lower than those in the odd state  $\psi_n^-$ .

We can get a full time-dependent (approximate) wave function for a particle that starts out in some linear combination of  $\psi_n^+$  and  $\psi_n^-$  by using the usual technique. Suppose we start the particle out in the following state:

$$(24) \quad \Psi(x, 0) = \frac{1}{\sqrt{2}} (\psi_n^+ + \psi_n^-)$$

This particle is entirely within the well in the region  $x > 0$ , since for  $x < 0$ ,  $\psi_n^+(x) = -\psi_n^-(x)$  and for  $x > 0$ ,  $\psi_n^+(x) = \psi_n^-(x)$  so the total wave function is zero for  $x < 0$ . Then the full time-dependent wave function is, using 23

$$(25) \quad \Psi(x, t) = \frac{1}{\sqrt{2}} \left( \psi_n^+ e^{-iE_n^+ t/\hbar} + \psi_n^- e^{-iE_n^- t/\hbar} \right)$$

$$(26) \quad = \frac{1}{\sqrt{2}} e^{-i(n+\frac{1}{2})\omega t} \left( \psi_n^+ e^{i\omega t e^{-\phi}/2\pi} + \psi_n^- e^{-i\omega t e^{-\phi}/2\pi} \right)$$

The probability density is  $|\Psi(x, t)|^2$ , which can be calculated fairly easily since  $\psi_n^+$  and  $\psi_n^-$  are both real functions, as we can see from 1. We get

$$(27) \quad |\Psi(x, t)|^2 = \frac{1}{2} \left[ |\psi_n^+|^2 + |\psi_n^-|^2 + \psi_n^+ \psi_n^- \left( e^{i\omega t e^{-\phi}/\pi} + e^{-i\omega t e^{-\phi}/\pi} \right) \right]$$

$$(28) \quad = \frac{1}{2} \left( |\psi_n^+|^2 + |\psi_n^-|^2 \right) + \psi_n^+ \psi_n^- \cos \frac{\omega t e^{-\phi}}{\pi}$$

If  $x > 0$ ,  $\psi_n^+ \psi_n^- = |\psi_n^+|^2$  while if  $x < 0$ ,  $\psi_n^+ \psi_n^- = -|\psi_n^+|^2$  so as time progresses, the probability that the particle is one well or the other oscillates between the two wells, with a period given by

$$(29) \quad \frac{\omega e^{-\phi}}{\pi} = \frac{2\pi}{\tau}$$

$$(30) \quad \tau = \frac{2\pi^2 e^{\phi}}{\omega}$$

Finally, we can calculate  $\phi$  for the double harmonic oscillator potential, using 6. We get

$$(31) \quad \phi = \frac{2}{\hbar} \int_0^{x_1} \sqrt{2m \left( \frac{1}{2} m \omega^2 (x-a)^2 - E \right)} dx$$

$$(32) \quad = \frac{2\sqrt{2mE}}{\hbar} \int_0^{x_1} \sqrt{\left( \frac{m\omega^2}{2E} (x-a)^2 - 1 \right)} dx$$

To transform this to a form that Maple can handle, we use the substitution

$$(33) \quad u = \sqrt{\frac{m\omega^2}{2E}}(x-a)$$

$$(34) \quad du = \sqrt{\frac{m\omega^2}{2E}}dx$$

The limits transform as

$$(35) \quad x = 0 \rightarrow u = -a\sqrt{\frac{m\omega^2}{2E}}$$

$$(36) \quad x = x_1 = -\sqrt{\frac{2E}{m\omega^2}} + a \rightarrow u = -1$$

So

$$(37) \quad \phi = \frac{2\sqrt{2mE}}{\hbar} \sqrt{\frac{2E}{m\omega^2}} \int_{-a\sqrt{\frac{m\omega^2}{2E}}}^{-1} \sqrt{u^2-1} du$$

$$(38) \quad = \frac{4E}{\hbar\omega} \int_1^{a\sqrt{\frac{m\omega^2}{2E}}} \sqrt{u^2-1} du$$

where the last step uses the fact that the integrand is even. Since  $V(0) = \frac{1}{2}m\omega^2 a^2 \equiv V_0$  we can write this as

$$(39) \quad \phi = \frac{4E}{\hbar\omega} \int_1^{a\sqrt{V_0/E}} \sqrt{u^2-1} du$$

$$(40) \quad = \frac{2E}{\hbar\omega} \left( u\sqrt{u^2-1} - \ln(u + \sqrt{u^2-1}) \right) \Big|_1^{\sqrt{V_0/E}}$$

$$(41) \quad = \frac{2E}{\hbar\omega} \left[ \sqrt{\frac{V_0}{E}} \sqrt{\frac{V_0}{E}-1} - \ln \left( \sqrt{\frac{V_0}{E}} + \sqrt{\frac{V_0}{E}-1} \right) \right]$$

For a high central barrier,  $V_0 \gg E$  and we can approximate this by

$$(42) \quad \phi \approx \frac{2E}{\hbar\omega} \left[ \frac{V_0}{E} - \ln \left( 2\sqrt{\frac{V_0}{E}} \right) \right]$$

$$(43) \quad \approx \frac{2V_0}{\hbar\omega} = \frac{m\omega a^2}{\hbar}$$

where we've dropped the logarithm term as it's much smaller than  $V_0/E$ .