WKB APPROXIMATION OF DOUBLE-WELL POTENTIAL - WAVE FUNCTIONS

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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

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

where

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

The odd extension of 1 is thus

$$\psi(-x)=-\psi(x) \tag{3}$$

for $x\ge0$. For this case, we must have $\psi(0)=0$, so we have

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

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

$$\phi\equiv\frac{2}{\hbar}\int_{0}^{x_1}\left|p\left(x'\right)\right|dx'=\frac{1}{\hbar}\int_{-x_1}^{x_1}\left|p\left(x'\right)\right|dx' \tag{6}$$

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

$$\tan\theta = -2e^{\phi} \tag{7}$$

Since both ϕ and θ 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

$$\psi(-x) = \psi(x) \tag{8}$$

$$\psi'(0) = 0 \tag{9}$$

The latter condition gives us

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

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

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

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

Setting this to zero gives the other energy quantization condition

$$\tan\theta = 2e^{\phi} \tag{13}$$

so the combined conditions are

$$\boxed{\tan\theta = \pm 2e^{\phi}} \tag{14}$$

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

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

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

Now suppose we give the potential a specific formula:

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

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 $x > 0$:

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

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

We can now work out θ from 2 by first working out the integral using Maple

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

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

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

$$= \frac{\pi E}{\hbar\omega} \tag{22}$$

Using the approximation 16 we get

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

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 ψ_n^+ are slightly lower than those in the odd state ψ_n^-.

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

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

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

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

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

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

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

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

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

$$\frac{\omega e^{-\phi}}{\pi} = \frac{2\pi}{\tau} \tag{29}$$

$$\tau = \frac{2\pi^2 e^{\phi}}{\omega} \tag{30}$$

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

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

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

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

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

$$du = \sqrt{\frac{m\omega^2}{2E}}dx \tag{34}$$

The limits transform as

$$x = 0 \to u = -a\sqrt{\frac{m\omega^2}{2E}} \tag{35}$$

$$x = x_1 = -\sqrt{\frac{2E}{m\omega^2}} + a \to u = -1 \tag{36}$$

So

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

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

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

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

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

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

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

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

$$\approx \frac{2V_0}{\hbar\omega} = \frac{m\omega a^2}{\hbar} \tag{43}$$

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