Quantum Double Well

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Consider the potential

$$V = \begin{cases} \infty & |x| > a+b \\ 0 & a < |x| < a+b \\ V_0 & |x| < a \end{cases}$$

We study the symmetric and antisymmetric wave functions in the 3 regions.

1 Symmetric

For even parity, we have

$$\begin{aligned} \psi_I &= \psi_{III} \\ &= A \sin k (a+b-x) \\ \psi_{II} &= C \cosh \kappa x \end{aligned}$$

where

$$\begin{aligned} \kappa &= \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \\ k &= \sqrt{\frac{2mE}{\hbar^2}} \end{aligned}$$

We need only the boundary conditions for $x > 0$ since the wave function is symmetric.

$$\begin{aligned} \psi_{III}(a+b) &= 0 \\ \psi_{III}(a) &= \psi_{II}(a) \\ \psi'_{III}(a) &= \psi'_{II}(a) \end{aligned}$$

Substituting,

$$\begin{aligned} A \sin kb &= B \cosh \kappa a \\ -Ak \cos kb &= B\kappa \sinh \kappa a \end{aligned}$$

Now solve. Taking the ratio of the last two,

$$\begin{aligned} \kappa \tanh \kappa a &= -k \frac{\cos kb}{\sin kb} \\ \kappa \tanh \kappa a &= -\frac{k}{\tan kb} \\ \tanh \kappa a \tan kb &= -\frac{k}{\kappa} \end{aligned}$$

2 Antisymmetric

For odd parity, we have

$$\begin{aligned}\psi_I &= \psi_{III} \\ &= A\sin k(a+b-x) \\ \psi_{II} &= C\sinh \kappa x\end{aligned}$$

We need only the boundary conditions for $x > 0$ since the wave function is antisymmetric.

$$\begin{aligned}\psi_{III}(a+b) &= 0 \\ \psi_{III}(a) &= \psi_{II}(a) \\ \psi'_{III}(a) &= \psi'_{II}(a)\end{aligned}$$

Substituting,

$$\begin{aligned}A\sin kb &= C\sinh \kappa a \\ -Ak\cos kb &= C\kappa\cosh \kappa a\end{aligned}$$

Taking the ratio,

$$\begin{aligned}\frac{1}{\kappa}\tanh \kappa a &= -\frac{1}{k}\tan kb \\ \frac{k}{\kappa} &= -\frac{\tan kb}{\tanh \kappa a}\end{aligned}$$

3 Approximation of the energies

We have the two solutions,

$$\begin{aligned}\frac{k_S}{\kappa_S} &= -\tan k_S b \tanh \kappa_S a \\ \frac{k_A}{\kappa_a} &= -\frac{\tan k_A b}{\tanh \kappa_A a}\end{aligned}$$

where

$$\begin{aligned}\kappa_{S,A} &= \sqrt{\frac{2m(V_0 - E_{S,A})}{\hbar^2}} \\ k_{S,A} &= \sqrt{\frac{2mE_{S,A}}{\hbar^2}}\end{aligned}$$

We have

$$\begin{aligned}-\frac{k_S}{\kappa_S\tan k_S b} &= \tanh \kappa_S a \\ -\frac{k_A}{\kappa_a\tan k_A b} &= \frac{1}{\tanh \kappa_A a}\end{aligned}$$

for the two cases.

On the right side we have the hyperbolic tangent,

$$\begin{aligned}\tanh \kappa a &= \frac{e^{\kappa a} - e^{-\kappa a}}{e^{\kappa a} + e^{-\kappa a}} \\ &= \frac{1 - e^{-2\kappa a}}{1 + e^{-2\kappa a}}\end{aligned}$$

$$\begin{aligned}
&= 1-2e^{-2\kappa a} \\
&= 1-2e^{-2\sqrt{\frac{2m(V_0-E)}{\hbar^2}}a} \\
&= 1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}\left(1-\frac{E}{V_0}\right)}} \\
&= 1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}\left(1-\frac{E}{2V_0}\right)} \\
&= 1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}\left(-\frac{E}{2V_0}\right)} \\
&= 1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\left(1+\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right)
\end{aligned}$$

Now focus on the left sides, which both take the form

$$-\frac{k}{\kappa\tan kb}$$

Notice that for large κa, this ratio must be close to 1.

First,

$$\begin{aligned}
\frac{k}{\kappa} &= \frac{\sqrt{\frac{2mE}{\hbar^2}}}{\sqrt{\frac{2m(V_0-E)}{\hbar^2}}} \\
&= \sqrt{\frac{E}{V_0-E}} \\
&= \sqrt{\frac{E}{V_0}\frac{1}{1-\frac{E}{V_0}}} \\
&= \sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)
\end{aligned}$$

Since we know that there will be slightly more than one lobe of the sine in the right well, the wavelength for either case will be slightly greater than $2b$. Then

$$\begin{aligned}
\lambda &> 2b \\
k &= \frac{2\pi}{\lambda} \\
k &< \frac{\pi}{b}
\end{aligned}$$

so we can set

$$kb = \pi - \varepsilon$$

The tangent becomes

$$\begin{aligned}
\tan kb &= \tan(\pi-\varepsilon) \\
&= \frac{\sin(\pi-\varepsilon)}{\cos(\pi-\varepsilon)} \\
&= -\frac{\sin\varepsilon}{\cos\varepsilon} \\
&= -\tan\varepsilon
\end{aligned}$$

We would like to express this in terms of $\frac{E}{V_0}$, but it is not possible:

$$\begin{aligned}
\varepsilon &= \pi - kb \\
&= \pi - \sqrt{\frac{2mb^2E}{\hbar^2}}
\end{aligned}$$

and the small ratio depends only on b, while V_0 may be varied independently. So there really are two independent small parameters. Let

$$\begin{aligned}
\sqrt{\frac{2mb^2E_0}{\hbar^2}} &= \pi \\
\varepsilon &= \pi - \sqrt{\frac{2mb^2\left(E_0+\Delta\right)}{\hbar^2}} \\
&= \pi - \sqrt{\pi^2 + \frac{2mb^2\Delta}{\hbar^2}} \\
&= \pi - \pi\sqrt{1+\frac{2mb^2\Delta}{\pi^2\hbar^2}} \\
&= -\frac{mb^2\Delta}{\pi\hbar^2}
\end{aligned}$$

Put it all together:

$$\begin{aligned}
-\frac{k_S}{\kappa_S \tan k_S b} &= \tanh \kappa_S a \\
\sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right) &= \tan\varepsilon\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right) \\
\tan\varepsilon &= \frac{\sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)}{1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)} \\
\tan\varepsilon &= \sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right)
\end{aligned}$$

Expanding in $\frac{E}{V}$,

$$\begin{aligned}
\tan\varepsilon_S &= \sqrt{\frac{E}{V_0}}\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E}{V_0}\left(\frac{1}{2}+e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)+e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)^2\right) \\
\tan\varepsilon_S &= \sqrt{\frac{E}{V_0}}\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E}{V_0}\left(\frac{1}{2}+e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)
\end{aligned}$$

Compare the antisymmetric case:

$$\begin{aligned}
-\frac{k_A}{\kappa_a \tan k_A b} &= \frac{1}{\tanh \kappa_A a} \\
\tan\varepsilon_A &= \sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right) \\
\tan\varepsilon_A &= \sqrt{\frac{E}{V_0}}\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E}{V_0}\left(\frac{1}{2}-e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)
\end{aligned}$$

Therefore, we need to compare:

$$\tan\varepsilon_S = \sqrt{\frac{E_S}{V_0}}\left(1+\frac{E_S}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E_S}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)$$

$$\tan\varepsilon_A = \sqrt{\frac{E_A}{V_0}}\left(1+\frac{E_A}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-\frac{E_A}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)$$

Now, for sufficiently large V_0

$$2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}} \gg \frac{E_S}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)$$

and we can drop the latter. The point is, it is $2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}$ that creates the first difference between the two expressions.

Then

$$\begin{aligned}
\tan\varepsilon_S &= \sqrt{\frac{E_S}{V_0}}\left(1+\frac{E_S}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
\tan\varepsilon_A &= \sqrt{\frac{E_A}{V_0}}\left(1+\frac{E_A}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)
\end{aligned}$$

where to lowest order,

$$\begin{aligned}
\tan\varepsilon_S &= -\frac{mb^2\Delta_S}{\pi\hbar^2}\\
\tan\varepsilon_A &= -\frac{mb^2\Delta_A}{\pi\hbar^2}
\end{aligned}$$

We may also write

$$\begin{aligned}
E_S &= E_0+\Delta_S\\
E_A &= E_0+\Delta_A
\end{aligned}$$

Therefore,

$$\begin{aligned}
-\frac{mb^2\Delta_S}{\pi\hbar^2} &= \sqrt{\frac{E_0+\Delta_S}{V_0}}\left(1+\frac{E_0+\Delta_S}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
&= \sqrt{\frac{E_0}{V_0}}\sqrt{1+\frac{\Delta_S}{E_0}}\left(1+\frac{E_0}{2V_0}\left(1+\frac{\Delta_S}{E_0}\right)+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
&= \sqrt{\frac{E_0}{V_0}}\left(\left(1+\frac{\Delta_S}{2E_0}\right)+\frac{E_0}{2V_0}\left(1+\frac{\Delta_S}{2E_0}\right)\left(1+\frac{\Delta_S}{E_0}\right)+\left(1+\frac{\Delta_S}{2E_0}\right)2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
&= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{\Delta_S}{2E_0}+\frac{E_0}{2V_0}+\frac{\Delta_S}{E_0}\frac{E_0}{2V_0}+\frac{\Delta_S}{2E_0}\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_S}{E_0}e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
&= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_S}{E_0}\left(\frac{1}{2}+\frac{3E_0}{4V_0}+e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\right)\\
&= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_S}{2E_0}\right)\\
-\frac{mb^2\Delta_A}{\pi\hbar^2} &= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_A}{2E_0}\right)
\end{aligned}$$

Collecting Δ terms,

$$
\begin{aligned}
-\Delta_S\left(\frac{mb^2}{\pi\hbar^2}+\frac{1}{2E_0}\sqrt{\frac{E_0}{V_0}}\right) &= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
-\Delta_A\left(\frac{mb^2}{\pi\hbar^2}+\frac{1}{2E_0}\sqrt{\frac{E_0}{V_0}}\right) &= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)
\end{aligned}
$$

or, since

$$E_0=\frac{\pi^2\hbar^2}{2mb^2}$$

we have

$$
\begin{aligned}
-\frac{\pi\Delta_S}{2E_0}\left(1+\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right) &= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
-\frac{\pi\Delta_A}{2E_0}\left(1+\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right) &= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)
\end{aligned}
$$

and therefore,

$$
\begin{aligned}
-\frac{\pi\Delta_S}{2E_0} &= \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
-\frac{\pi\Delta_A}{2E_0} &= \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)
\end{aligned}
$$

Now define

$$
\begin{aligned}
\frac{\pi\Delta}{2E_0} &= \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}\right)\\
&= \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}+\frac{E_0}{2V_0}+\ldots\right)\\
&= \sqrt{\frac{E_0}{V_0}}+\ldots
\end{aligned}
$$

Then, keeping only the lowest order,

$$
\begin{aligned}
\Delta_S &= -(\Delta+\ldots)\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\ldots\right)\\
\Delta_A &= -(\Delta+\ldots)\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\ldots\right)
\end{aligned}
$$

There are small corrections to both Δ and to the exponential terms, but they are small by comparison. By taking V_0 as large as we like, we can make those corrections as small as we like. So the final energy difference is

$$
\begin{aligned}
E_A-E_S &= (E_0+\Delta_A)-(E_0+\Delta_S)\\
&= \Delta_A-\Delta_S\\
&= -\Delta\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)+\Delta\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)\\
&= 4\Delta e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\\
&= \frac{8}{\pi}E_0\sqrt{\frac{E_0}{V_0}}e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}
\end{aligned}
$$

where E_0 is the ground state energy of the corresponding infinite square well.