INFINITE SQUARE WELL WITH VARIABLE DELTA FUNCTION BARRIER: GROUND STATE ENERGY

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Here’s another example of the adiabatic theorem. This time, we have an infinite square well in which a delta function barrier is inserted slowly at a position that is slightly off centre, so that for \( 0 < x < a \) we have the potential

\[
V(x) = f(t) \delta \left( x - \frac{a}{2} - \epsilon \right)
\]  

where \( f(t) \) is a function that rises slowly from 0 to \( \infty \). The adiabatic theorem says that the system will remain in the ground state of the time-varying hamiltonian.

First, we’ll look at what the state is when the barrier has attained infinite strength, so that \( t \to \infty \). [OK, the delta function itself is always infinite at a single point, but it can have a constant ‘strength’ factor multiplying it. We’ve looked at the case of the infinite square well with a constant delta function barrier and we’ve seen that increasing the strength factor to \( \infty \) effectively divides the well into two wells that are isolated from each other, while a finite strength barrier does allow the wave function to communicate across the barrier.]

For an infinitely strong delta function barrier then, we have one well of width \( \frac{a}{2} + \epsilon \) and one well of width \( \frac{a}{2} - \epsilon \). The wave functions in both wells must be zero at their boundaries, so we get for the ground state (\( n = 1 \)):

\[
\psi(x) = \begin{cases} 
A \sin \left( \frac{\pi}{2 \epsilon} x \right) & 0 \leq x < \frac{a}{2} + \epsilon \\
A \sin \left[ \frac{\pi}{2 - \epsilon} (x - \frac{a}{2} - \epsilon) \right] & \frac{a}{2} + \epsilon < x < a
\end{cases}
\]  

\[
E_I = \frac{\pi^2 \hbar^2}{2m \left( \frac{a}{2} + \epsilon \right)^2} 
\]  

\[
E_R = \frac{\pi^2 \hbar^2}{2m \left( \frac{a}{2} - \epsilon \right)^2} 
\]
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Thus $E_l < E_r$ so the ground state confines the particle to the left well. The wave function for the ground state is

$$
\psi(x) = \begin{cases} 
\sqrt{\frac{2}{\pi(\sqrt{a^2+\epsilon})}} \sin \frac{\pi}{\sqrt{a^2+\epsilon}} x & 0 \leq x < \frac{a}{2} + \epsilon \\
0 & \frac{a}{2} + \epsilon < x < a 
\end{cases}
$$

(5)

The plot looks like this:

Now for the general case where $f(t)$ is finite. In this case we can write the wave functions as

$$
\psi(x) = \begin{cases} 
A e^{ikx} + Be^{-ikx} & 0 \leq x < \frac{a}{2} + \epsilon \\
C e^{ikx} + De^{-ikx} & \frac{a}{2} + \epsilon < x \leq a 
\end{cases}
$$

(6)

where

$$
k \equiv \frac{\sqrt{2mE}}{\hbar}
$$

(7)

The barriers at $x = 0$ and $x = a$ are still infinite so the wave function must be zero there, giving
The wave function must be continuous at the barrier, so we get

\[ A \left( e^{ik(\frac{a}{2}+\epsilon)} - e^{-ik(\frac{a}{2}+\epsilon)} \right) = D \left( -e^{-2ika}e^{ik(\frac{a}{2}+\epsilon)} + e^{-ik(\frac{a}{2}+\epsilon)} \right) \]  

(10)

Finally, we can analyze the derivative at the barrier in the same way we did for the delta function well and we get

\[ \frac{\hbar^2}{2m} \int_{\frac{a}{2}+\epsilon-\beta}^{\frac{a}{2}+\epsilon+\beta} \frac{d^2\psi}{dx^2} dx + f(t) \int_{\frac{a}{2}+\epsilon-\beta}^{\frac{a}{2}+\epsilon+\beta} \delta(x) \psi dx = E \int_{\frac{a}{2}+\epsilon-\beta}^{\frac{a}{2}+\epsilon+\beta} \psi dx \]  

(11)

\[ \frac{\hbar^2}{2m} \frac{d\psi}{dx} \bigg|_{\frac{a}{2}+\epsilon-\beta}^{\frac{a}{2}+\epsilon+\beta} + f(t) \psi \left( \frac{a}{2} + \epsilon \right) = E \int_{\frac{a}{2}+\epsilon-\beta}^{\frac{a}{2}+\epsilon+\beta} \psi dx \]  

(12)

The integral on the RHS goes to zero as \( \beta \to 0 \) since \( \psi \) is finite, so

\[ A \frac{mf(t)}{\hbar^2} \left( e^{ik(\frac{a}{2}+\epsilon)} - e^{-ik(\frac{a}{2}+\epsilon)} \right) = -ikD \left( e^{-2ika}e^{ik(\frac{a}{2}+\epsilon)} + e^{-ik(\frac{a}{2}+\epsilon)} \right) - \]

\[ ikA \left( e^{ik(\frac{a}{2}+\epsilon)} + e^{-ik(\frac{a}{2}+\epsilon)} \right) \]  

(13)

If we now define

\[ z \equiv ka \]  

(14)

\[ \delta \equiv \frac{2\epsilon}{a} \]  

(15)

\[ k \left( \frac{a}{2} + \epsilon \right) = \frac{1}{2} z (1 + \delta) \]  

(16)

we get, transforming the complex exponentials to trig functions

\[ A \frac{4imf(t)}{\hbar^2} \sin \left[ \frac{1}{2} z (1 + \delta) \right] = -2ikDe^{-iz} \cos \left[ \frac{1}{2} z (1 - \delta) \right] - 2ikA \cos \left[ \frac{1}{2} z (1 + \delta) \right] \]  

(17)

Multiplying through by \( a \) and defining

\[ T \equiv \frac{maf(t)}{\hbar^2} \]  

(18)

we get
We can write Eq. 10 as
\[2iA \sin \left( \frac{1}{2} z (1 + \delta) \right) = 2ie^{-iz} D \sin \left( \frac{1}{2} z (1 - \delta) \right)\]  
(20)

\[A = e^{-iz} D \frac{\sin \left( \frac{1}{2} z (1 - \delta) \right)}{\sin \left( \frac{1}{2} z (1 + \delta) \right)}\]  
(21)

Substituting this into Eq. 19, multiplying through by \(\sin \left( \frac{1}{2} z (1 + \delta) \right)\) and cancelling terms we get
\[2T \sin \left( \frac{1}{2} z (1 - \delta) \right) \sin \left( \frac{1}{2} z (1 + \delta) \right) = -z \left[ \cos \left( \frac{1}{2} z (1 - \delta) \right) \sin \left( \frac{1}{2} z (1 + \delta) \right) + \sin \left( \frac{1}{2} z (1 - \delta) \right) \cos \left( \frac{1}{2} z (1 + \delta) \right) \right]\]  
(22)

\[= -z \sin \left( \frac{1}{2} z (1 - \delta) + \frac{1}{2} z (1 + \delta) \right)\]  
(23)

\[= -z \sin z\]  
(24)

The LHS can be transformed using
\[2 \sin \left( \frac{1}{2} z (1 - \delta) \right) \sin \left( \frac{1}{2} z (1 + \delta) \right) = \cos \left( \frac{1}{2} z (1 - \delta) - \frac{1}{2} z (1 + \delta) \right) - \cos \left( \frac{1}{2} z (1 - \delta) + \frac{1}{2} z (1 + \delta) \right)\]  
(25)

\[= \cos z \delta - \cos z\]  
(26)

Putting it together we get the transcendental equation for the ground state energy
\[z \sin z = T \left( \cos z - \cos z \delta \right)\]  
(27)

The energy is
\[E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 z^2}{2ma^2}\]  
(28)

We can solve Eq. 27 graphically or numerically. For \(\delta = 0\), here are plots of \(z \sin z\) (red) and \(T (\cos z - 1)\) (green) for 3 values of \(T\):
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T = 0.5

T = 5
Discounting the trivial solutions at $z = 0$ and $z = 2\pi$ which are valid for all $T$, we see that the intersection point moves from $z = \pi$ out to $z = 2\pi$ as $T$ increases. This is equivalent to the energy moving from $\frac{h^2 \pi^2}{2ma^2}$ up to $\frac{4h^2 \pi^2}{2ma^2}$. The first energy is that of a well of width $a$ while the second energy is that of a well of width $\frac{a}{2}$, which is what we’d expect. As the barrier gets stronger, the ground state energy approaches that of a well of half the width of the original.

Using Maple’s `fsolve` command we can work out some other values of $z$ for $\delta = 0.01$:

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<thead>
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<th>$T$</th>
<th>$z$</th>
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<tbody>
<tr>
<td>1</td>
<td>3.673</td>
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<tr>
<td>5</td>
<td>4.760</td>
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<td>5.720</td>
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<td>100</td>
<td>6.135</td>
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<td>1000</td>
<td>6.215</td>
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