

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

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 10.8.

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

$$(0.1) \quad V(x) = f(t) \delta\left(x - \frac{a}{2} - \varepsilon\right)$$

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  $t \rightarrow \infty$ . [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  $\frac{a}{2} + \varepsilon$  and one well of width  $\frac{a}{2} - \varepsilon$ . The wave functions in both wells must be zero at their boundaries, so we get for the ground state ( $n = 1$ ):

$$(0.2) \quad \psi(x) = \begin{cases} A \sin \frac{\pi}{\frac{a}{2} + \varepsilon} x & 0 \leq x < \frac{a}{2} + \varepsilon \\ A \sin \left[ \frac{\pi}{\frac{a}{2} - \varepsilon} \left( x - \frac{a}{2} - \varepsilon \right) \right] & \frac{a}{2} + \varepsilon < x < a \end{cases}$$

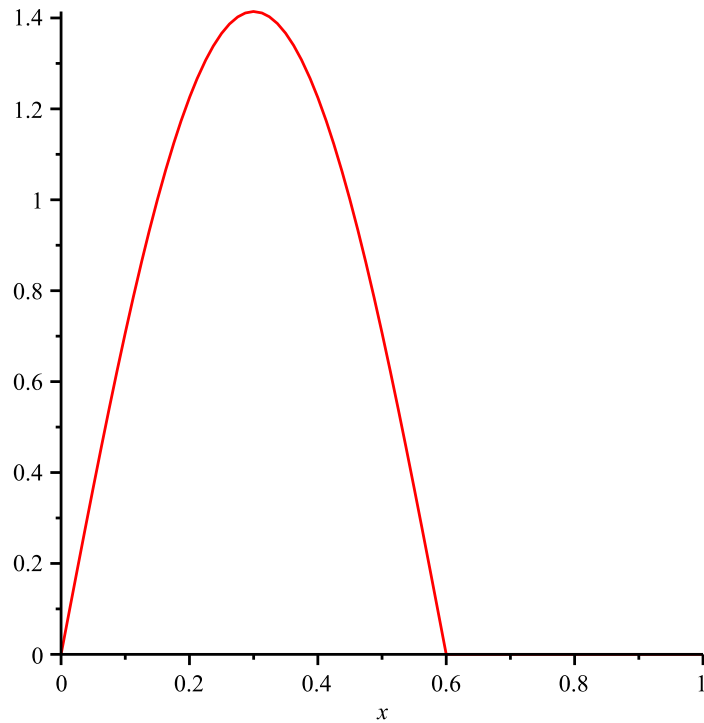
$$(0.3) \quad E_l = \frac{\pi^2 \hbar^2}{2m \left( \frac{a}{2} + \varepsilon \right)^2}$$

$$(0.4) \quad E_r = \frac{\pi^2 \hbar^2}{2m \left( \frac{a}{2} - \varepsilon \right)^2}$$

Thus  $E_l < E_r$ , so the ground state confines the particle to the left well. The wave function for the ground state is

$$(0.5) \quad \psi(x) = \begin{cases} \sqrt{\frac{2}{\frac{a}{2} + \epsilon}} \sin \frac{\pi}{\frac{a}{2} + \epsilon} x & 0 \leq x < \frac{a}{2} + \epsilon \\ 0 & \frac{a}{2} + \epsilon < x < a \end{cases}$$

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

$$(0.6) \quad \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & 0 \leq x < \frac{a}{2} + \epsilon \\ Ce^{ikx} + De^{-ikx} & \frac{a}{2} + \epsilon < x \leq a \end{cases}$$

where

$$(0.7) \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

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

$$(0.8) \quad A = -B$$

$$(0.9) \quad C = -De^{-2ika}$$

The wave function must be continuous at the barrier, so we get

$$(0.10) \quad A \left( e^{ik\left(\frac{a}{2}+\varepsilon\right)} - e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) = D \left( -e^{-2ika} e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right)$$

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

$$(0.11) \quad -\frac{\hbar^2}{2m} \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \frac{d^2\psi}{dx^2} dx + f(t) \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \delta(x) \psi dx = E \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \psi dx$$

$$(0.12) \quad -\frac{\hbar^2}{2m} \frac{d\psi}{dx} \Big|_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} + f(t) \psi \left( \frac{a}{2} + \varepsilon \right) = E \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \psi dx$$

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

$$(0.13) \quad A \frac{2mf(t)}{\hbar^2} \left( e^{ik\left(\frac{a}{2}+\varepsilon\right)} - e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) = -ikD \left( e^{-2ika} e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) - ikA \left( e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right)$$

If we now define

$$(0.14) \quad z \equiv ka$$

$$(0.15) \quad \delta \equiv \frac{2\varepsilon}{a}$$

$$(0.16) \quad k \left( \frac{a}{2} + \varepsilon \right) = \frac{1}{2}z(1 + \delta)$$

we get, transforming the complex exponentials to trig functions

$$(0.17) \quad A \frac{4imf(t)}{\hbar^2} \sin \left[ \frac{1}{2}z(1 + \delta) \right] = -2ikDe^{-iz} \cos \left[ \frac{1}{2}z(1 - \delta) \right] - 2ikA \cos \left[ \frac{1}{2}z(1 + \delta) \right]$$

Multiplying through by  $a$  and defining

$$(0.18) \quad T \equiv \frac{maf(t)}{\hbar^2}$$

we get

$$(0.19) \quad 2AT \sin \left[ \frac{1}{2}z(1 + \delta) \right] = -zDe^{-iz} \cos \left[ \frac{1}{2}z(1 - \delta) \right] - zA \cos \left[ \frac{1}{2}z(1 + \delta) \right]$$

We can write 0.10 as

$$(0.20) \quad 2iA \sin \left[ \frac{1}{2}z(1 + \delta) \right] = 2ie^{-iz}D \sin \left[ \frac{1}{2}z(1 - \delta) \right]$$

$$(0.21) \quad A = e^{-iz}D \frac{\sin \left[ \frac{1}{2}z(1 - \delta) \right]}{\sin \left[ \frac{1}{2}z(1 + \delta) \right]}$$

Substituting this into 0.19, multiplying through by  $\sin \left[ \frac{1}{2}z(1 + \delta) \right]$  and cancelling terms we get

$$(0.22) \quad 2T \sin \left[ \frac{1}{2}z(1 - \delta) \right] \sin \left[ \frac{1}{2}z(1 + \delta) \right] = -z \left[ \cos \left[ \frac{1}{2}z(1 - \delta) \right] \sin \left[ \frac{1}{2}z(1 + \delta) \right] + \sin \left[ \frac{1}{2}z(1 - \delta) \right] \cos \left[ \frac{1}{2}z(1 + \delta) \right] \right]$$

$$(0.23) \quad = -z \sin \left[ \frac{1}{2}z(1 - \delta) + \frac{1}{2}z(1 + \delta) \right]$$

$$(0.24) \quad = -z \sin z$$

The LHS can be transformed using

$$(0.25) \quad 2 \sin \left[ \frac{1}{2}z(1 - \delta) \right] \sin \left[ \frac{1}{2}z(1 + \delta) \right] = \cos \left[ \frac{1}{2}z(1 - \delta) - \frac{1}{2}z(1 + \delta) \right] - \cos \left[ \frac{1}{2}z(1 - \delta) + \frac{1}{2}z(1 + \delta) \right]$$

$$(0.26) \quad = \cos z\delta - \cos z$$

Putting it together we get the transcendental equation for the ground state energy

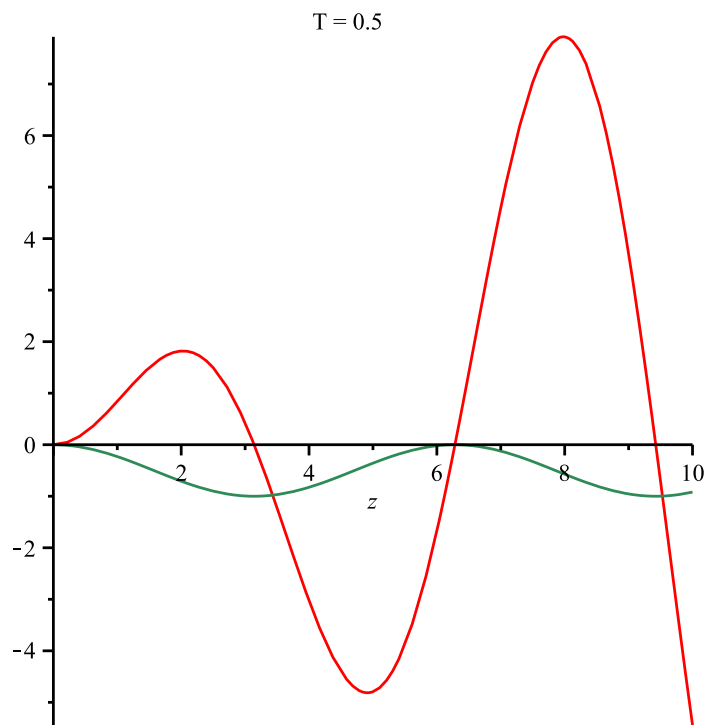
$$(0.27) \quad z \sin z = T (\cos z - \cos z\delta)$$

The energy is

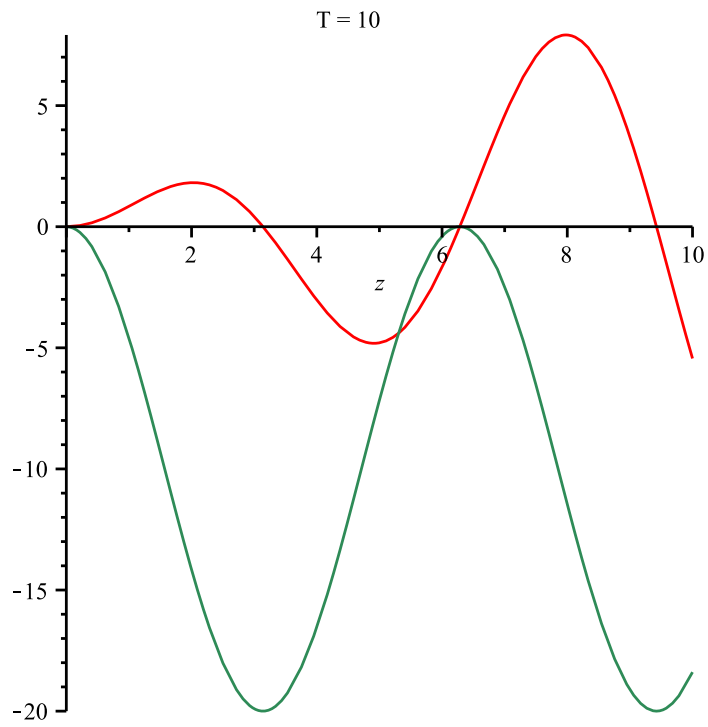
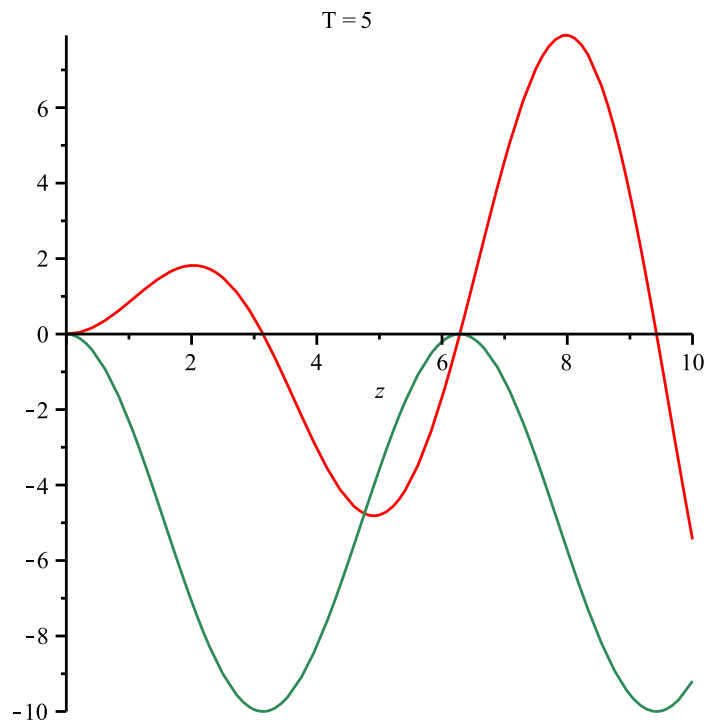
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$$(0.28) \quad E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 z^2}{2ma^2}$$

We can solve 0.27 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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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  $\frac{\hbar^2\pi^2}{2ma^2}$  up to  $\frac{4\hbar^2\pi^2}{2ma^2}$ . 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  $\delta = 0.01$ :

$T$	$z$
1	3.673
5	4.760
20	5.720
100	6.135
1000	6.215

PINGBACKS

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