

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

$$V(x) = f(t) \delta\left(x - \frac{a}{2} - \epsilon\right) \quad (1)$$

where $f(t)$ is a function that rises slowly from 0 to ∞ . 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 ∞ 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 ($n = 1$):

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

$$E_l = \frac{\pi^2 \hbar^2}{2m \left(\frac{a}{2} + \epsilon \right)^2} \quad (3)$$

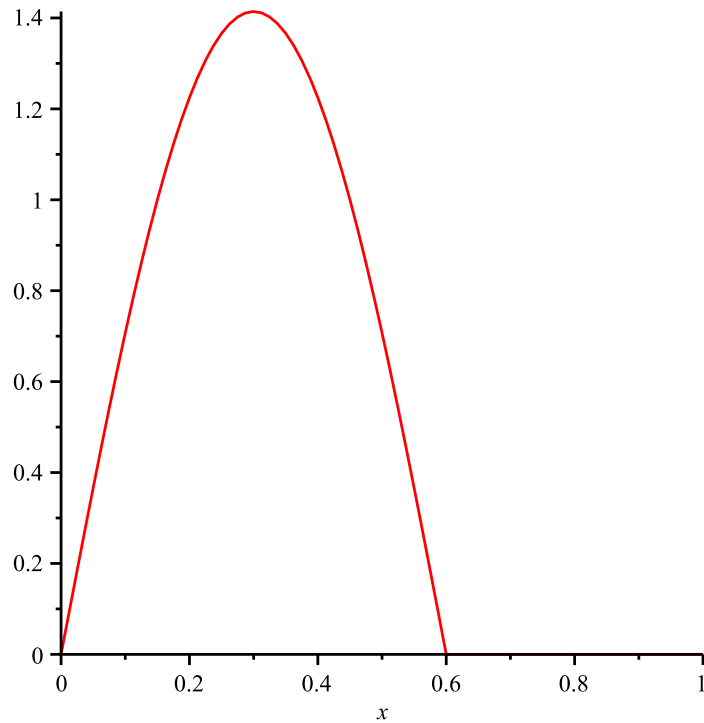
$$E_r = \frac{\pi^2 \hbar^2}{2m \left(\frac{a}{2} - \epsilon \right)^2} \quad (4)$$

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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

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{\frac{a}{2} + \epsilon}} \sin \frac{\pi}{\frac{a}{2} + \epsilon} x & 0 \leq x < \frac{a}{2} + \epsilon \\ 0 & \frac{a}{2} + \epsilon < x < a \end{cases} \quad (5)$$

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

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & 0 \leq x < \frac{a}{2} + \epsilon \\ Ce^{ikx} + De^{-ikx} & \frac{a}{2} + \epsilon < x \leq a \end{cases} \quad (6)$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad (7)$$

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

$$A = -B \quad (8)$$

$$C = -De^{-2ika} \quad (9)$$

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

$$A \left(e^{ik\left(\frac{a}{2}+\varepsilon\right)} - e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) = D \left(-e^{-2ika} e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) \quad (10)$$

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

$$-\frac{\hbar^2}{2m} \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \frac{d^2\psi}{dx^2} dx + f(t) \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \delta(x) \psi dx = E \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \psi dx \quad (11)$$

$$-\frac{\hbar^2}{2m} \frac{d\psi}{dx} \Big|_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} + f(t) \psi \left(\frac{a}{2} + \varepsilon \right) = E \int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} \psi dx \quad (12)$$

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

$$A \frac{2mf(t)}{\hbar^2} \left(e^{ik\left(\frac{a}{2}+\varepsilon\right)} - e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) = -ikD \left(e^{-2ika} e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) - ikA \left(e^{ik\left(\frac{a}{2}+\varepsilon\right)} + e^{-ik\left(\frac{a}{2}+\varepsilon\right)} \right) \quad (13)$$

If we now define

$$z \equiv ka \quad (14)$$

$$\delta \equiv \frac{2\varepsilon}{a} \quad (15)$$

$$k \left(\frac{a}{2} + \varepsilon \right) = \frac{1}{2}z(1 + \delta) \quad (16)$$

we get, transforming the complex exponentials to trig functions

$$A \frac{4imf(t)}{\hbar^2} \sin \left[\frac{1}{2}z(1 + \delta) \right] = -2ikDe^{-iz} \cos \left[\frac{1}{2}z(1 - \delta) \right] - 2ikA \cos \left[\frac{1}{2}z(1 + \delta) \right] \quad (17)$$

Multiplying through by a and defining

$$T \equiv \frac{maf(t)}{\hbar^2} \quad (18)$$

we get

$$2AT \sin \left[\frac{1}{2}z(1 + \delta) \right] = -zDe^{-iz} \cos \left[\frac{1}{2}z(1 - \delta) \right] - zA \cos \left[\frac{1}{2}z(1 + \delta) \right] \quad (19)$$

We can write 10 as

$$2iA \sin \left[\frac{1}{2}z(1 + \delta) \right] = 2ie^{-iz}D \sin \left[\frac{1}{2}z(1 - \delta) \right] \quad (20)$$

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

Substituting this into 19, multiplying through by $\sin \left[\frac{1}{2}z(1 + \delta) \right]$ and cancelling terms we get

$$2T \sin \left[\frac{1}{2}z(1 - \delta) \right] \sin \left[\frac{1}{2}z(1 + \delta) \right] = -z \left[\cos \left[\frac{1}{2}z(1 - \delta) \right] \sin \left[\frac{1}{2}z(1 + \delta) \right] + \sin \left[\frac{1}{2}z(1 - \delta) \right] \cos \left[\frac{1}{2}z(1 + \delta) \right] \right] \quad (22)$$

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

$$= -z \sin z \quad (24)$$

The LHS can be transformed using

$$2 \sin \left[\frac{1}{2}z(1 - \delta) \right] \sin \left[\frac{1}{2}z(1 + \delta) \right] = \cos \left[\frac{1}{2}z(1 - \delta) - \frac{1}{2}z(1 + \delta) \right] - \cos \left[\frac{1}{2}z(1 - \delta) + \frac{1}{2}z(1 + \delta) \right] \quad (25)$$

$$= \cos z \delta - \cos z \quad (26)$$

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

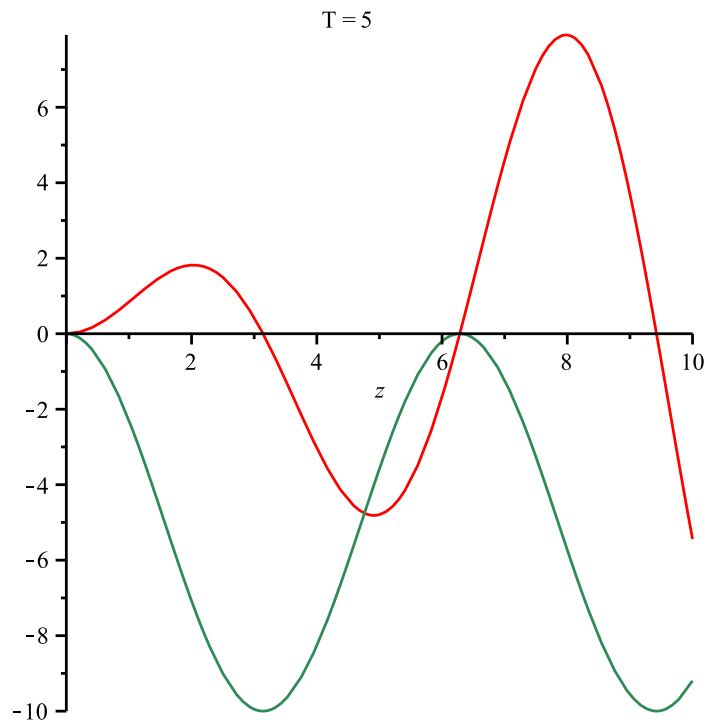
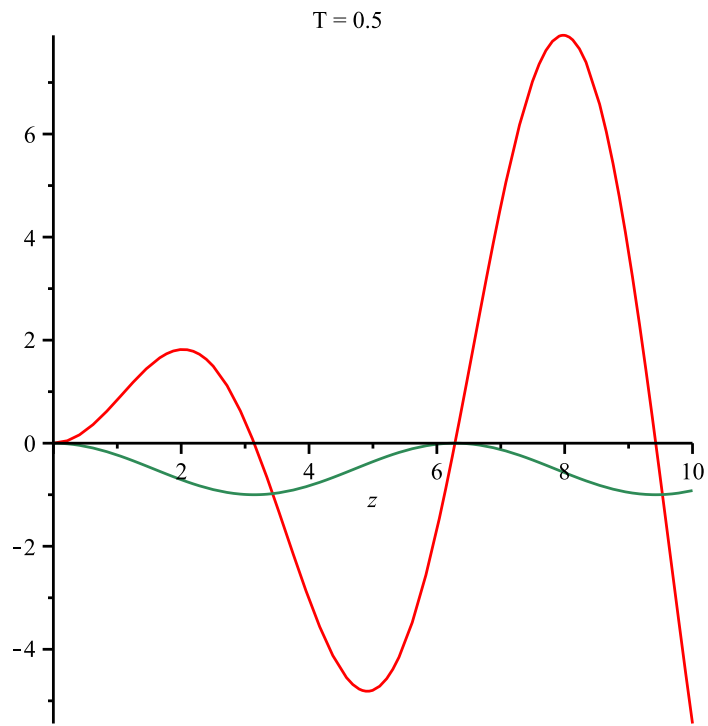
$$z \sin z = T (\cos z - \cos z \delta) \quad (27)$$

The energy is

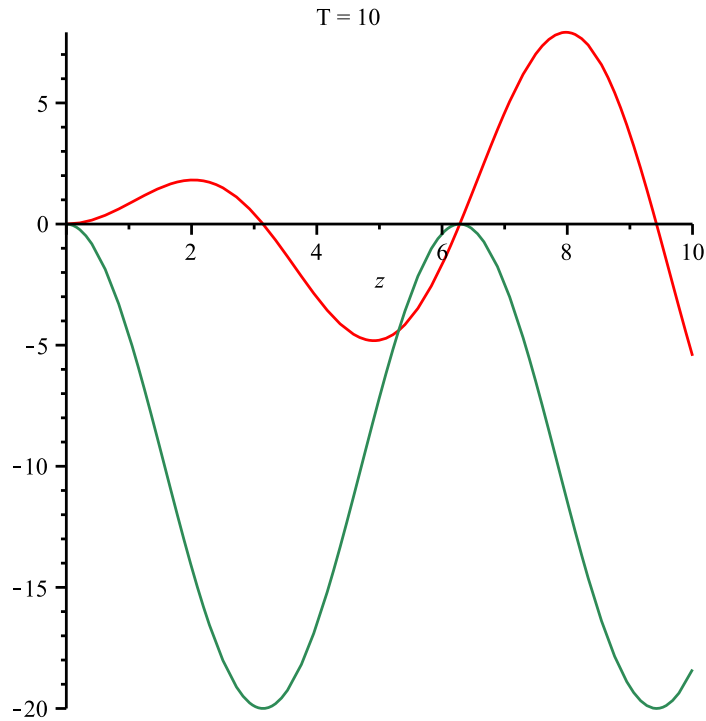
$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 z^2}{2ma^2} \quad (28)$$

We can solve 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

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