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

$$V(x) = f(t)\,\delta\left(x - \frac{a}{2} - \varepsilon\right) \tag{1}$$

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 $t \to \infty$. [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 ∞ 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 ($n = 1$):

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

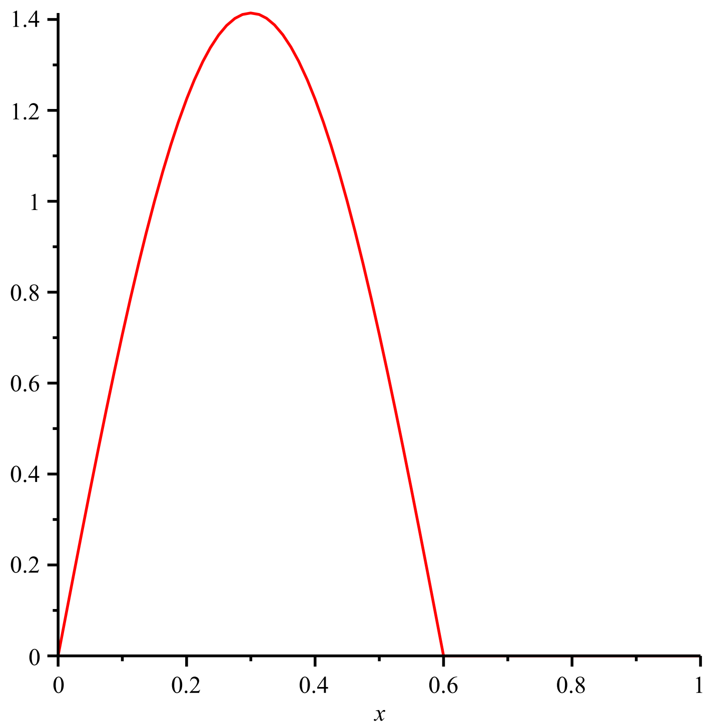
$$E_l = \frac{\pi^2\hbar^2}{2m\left(\frac{a}{2}+\varepsilon\right)^2} \tag{3}$$

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

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

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

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

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

where

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

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

$$A = -B \tag{8}$$
$$C = -De^{-2ika} \tag{9}$$

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

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

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

$$-\frac{\hbar^2}{2m}\int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta}\frac{d^2\psi}{dx^2}dx + f(t)\int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta}\delta(x)\psi dx = E\int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta}\psi dx \tag{11}$$
$$-\frac{\hbar^2}{2m}\left.\frac{d\psi}{dx}\right|_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta} + f(t)\,\psi\left(\frac{a}{2}+\varepsilon\right) = E\int_{\frac{a}{2}+\varepsilon-\beta}^{\frac{a}{2}+\varepsilon+\beta}\psi dx \tag{12}$$

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

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

If we now define

$$z \equiv ka \tag{14}$$
$$\delta \equiv \frac{2\varepsilon}{a} \tag{15}$$
$$k\left(\frac{a}{2}+\varepsilon\right) = \frac{1}{2}z(1+\delta) \tag{16}$$

we get, transforming the complex exponentials to trig functions

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

Multiplying through by a and defining

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

we get

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

We can write 10 as

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

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

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

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

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

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

The LHS can be transformed using

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

$$=\cos z\delta-\cos z \tag{26}$$

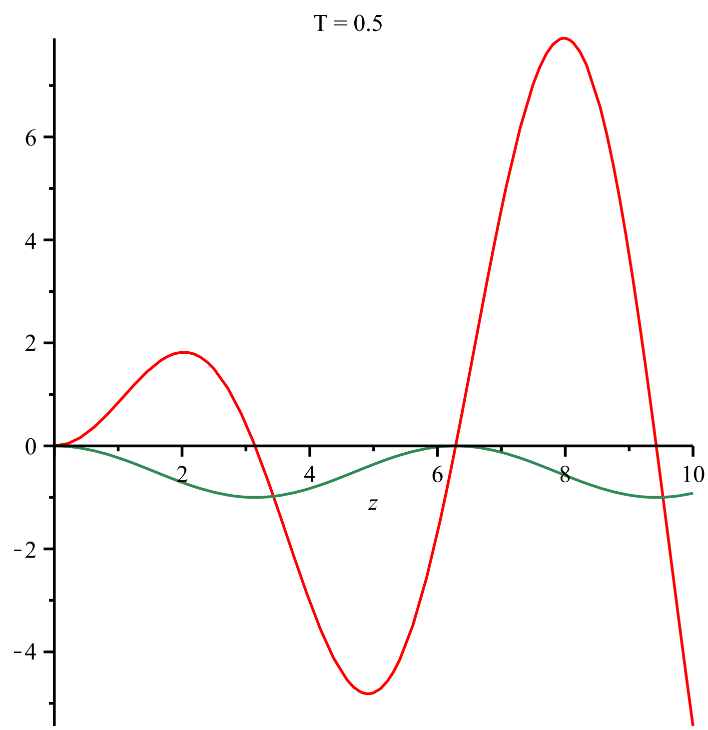
Putting it together we get the transcendental equation for the ground state energy

$$z\sin z=T\left(\cos z-\cos z\delta\right) \tag{27}$$

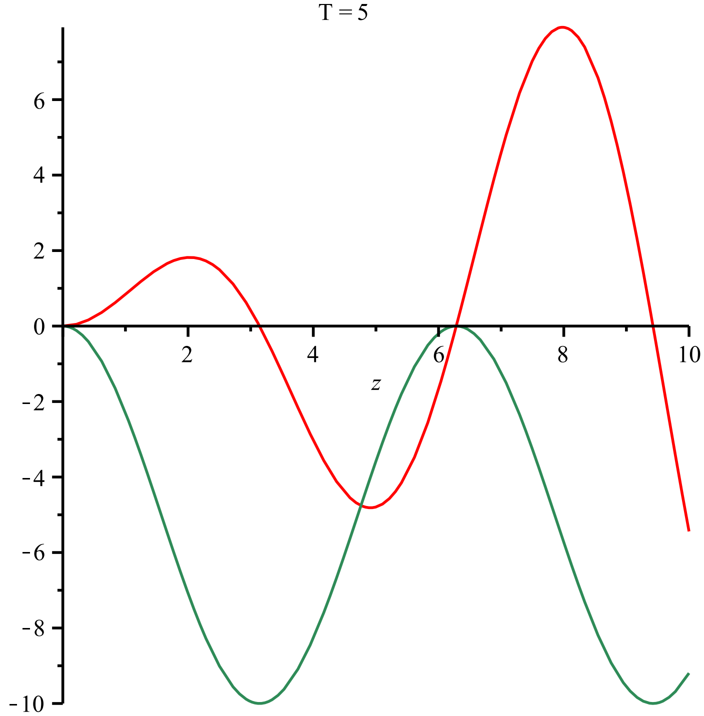
The energy is

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 z^2}{2ma^2} \tag{28}$$

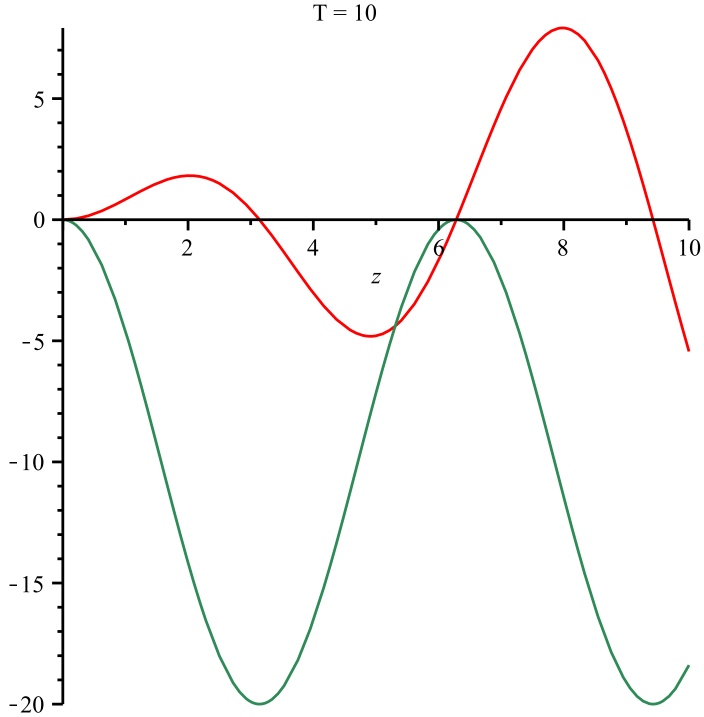
We can solve 27 graphically or numerically. For $\delta = 0$, here are plots of $z \sin z$ (red) and $T(\cos z - 1)$ (green) for 3 values of T:



T = 5



T = 10



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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