INFINITE SQUARE WELL WITH DELTA FUNCTION BARRIER

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.44.

An interesting potential is one where we combine an infinite square well with a delta function barrier. That is,

$$V(x) = \begin{cases} \infty & x < -a \\ \alpha\delta(x) & -a < x < a \\ \infty & x > a \end{cases} \tag{0.1}$$

Outside the square well, $\psi(x) = 0$. Inside the well, we have two distinct regions, one on each side of the delta function.Inside the well, away from the delta function, the general solution is

$$\psi_1(x) = A\sin kx + B\cos kx \qquad -a < x < 0 \tag{0.2}$$

$$\psi_2(x) = C\sin kx + D\cos kx \qquad 0 < x < a \tag{0.3}$$

where $k = \sqrt{2mE}/\hbar$.

Since the potential is even, we can consider odd and even solutions separately. If we take the even solutions first, we have

$$\psi_1(x) = A\sin kx + B\cos kx \tag{0.4}$$

$$\psi_2(x) = -A\sin kx + B\cos kx \tag{0.5}$$

Continuity of the wave function at $x = \pm a$ gives the condition (the same condition at both points):

$$-A\sin ka + B\cos ka = 0 \tag{0.6}$$

$$\tan ka = \frac{B}{A} \tag{0.7}$$

The wave function is automatically continuous at $x = 0$. However, we can use the same condition on the derivative of the wave function at this point that we used in analyzing the delta function well. That is

$$\left[\frac{d\psi}{dx}\bigg|_{x\downarrow 0}-\frac{d\psi}{dx}\bigg|_{x\uparrow 0}\right]=\frac{2m\alpha}{\hbar^2}\psi(0) \tag{0.8}$$

Working out the derivatives, we get

$$-kA\cos kx-kB\sin kx|_{x\downarrow 0}-\left(kA\cos kx-kB\sin kx|_{x\uparrow 0}\right)=\frac{2m\alpha}{\hbar^2}B \tag{0.9}$$

$$-2kA=\frac{2m\alpha}{\hbar^2}B \tag{0.10}$$

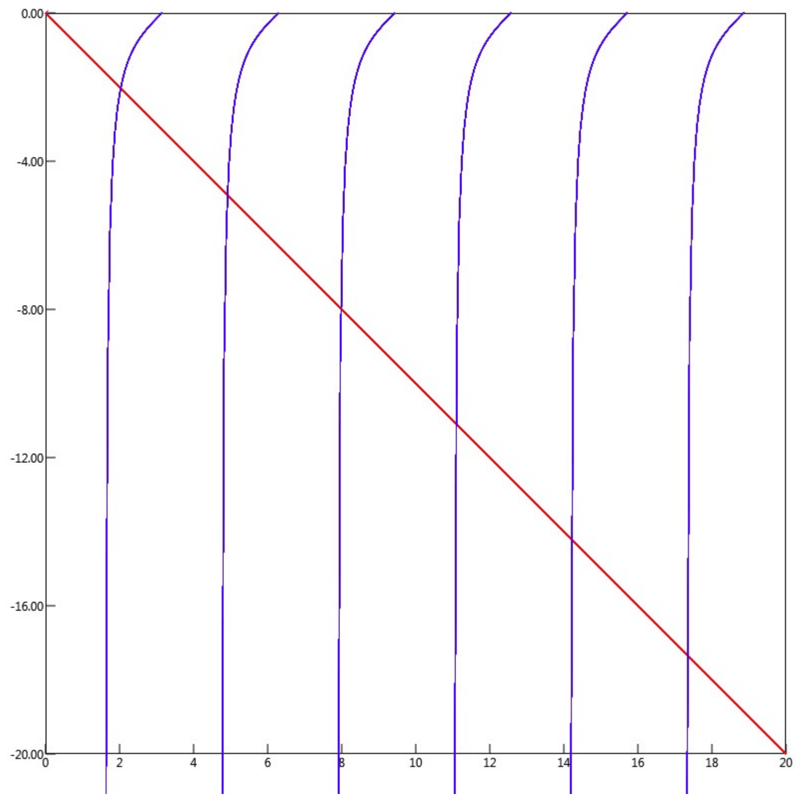
Substituting $B=A\tan ka$ from above, we get

$$-\frac{\hbar^2}{m\alpha a}ka=\tan ka \tag{0.11}$$

or, substituting $z\equiv ka$

$$-\frac{\hbar^2}{m\alpha a}z=\tan z \tag{0.12}$$

This is a transcendental equation in z and can be solved graphically or numerically, once we've chosen a value for $\hbar^2/m\alpha a$. If we take this to be 1, for example, a plot shows the intersections of $y=-z$ and $y=\tan z$ within a range of z. Since the left side is a straight line, and the tangent is periodic, there are an infinite number of solutions.



Note that since both k and a are real and positive, we're interested only in values of $z > 0$, so that's what is shown in the plot.

The odd solutions are easier. In this case

$$\psi_1(x) = A\sin kx + B\cos kx \tag{0.13}$$

$$\psi_2(x) = A\sin kx - B\cos kx \tag{0.14}$$

Continuity at $x = 0$ requires $B = -B$, so $B = 0$. In this case, the derivative is also automatically continuous across $x = 0$, so gives us no information. The only other boundary condition we can use is at $x = \pm a$, from which we get

$$A\sin ka = 0 \tag{0.15}$$

$$ka = n\pi \tag{0.16}$$

This is the same condition as in the square well without the delta function, and we can write

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{0.17}$$
$$= \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2} \tag{0.18}$$

We've written the energies in the latter form since the well's width is $2a$, so we can see that the odd solutions give only the even-numbered energy levels. Thus it is only the odd-numbered energy levels (arising from the even wave functions) that get modified due to the delta function. The odd wave functions are not affected by the delta function since they are zero at $x = 0$.

It's worth looking at the asymptotic behaviour of the even solutions as α gets very small or very large.

For $\alpha \to 0$, from 0.12, we must have $\tan z \to \infty$, which means

$$z = ka = \frac{(2n+1)\pi}{2} \tag{0.19}$$
$$E = \frac{(2n+1)^2\pi^2\hbar^2}{2m(2a)^2} \tag{0.20}$$

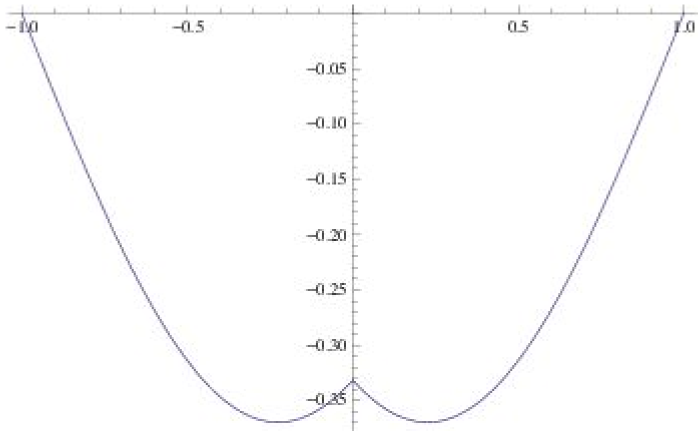
Thus we reclaim the odd numbered energy levels when the delta function disappears.

At the other extreme, if $\alpha \to \infty$, we must have $\tan z = 0$, which happens when

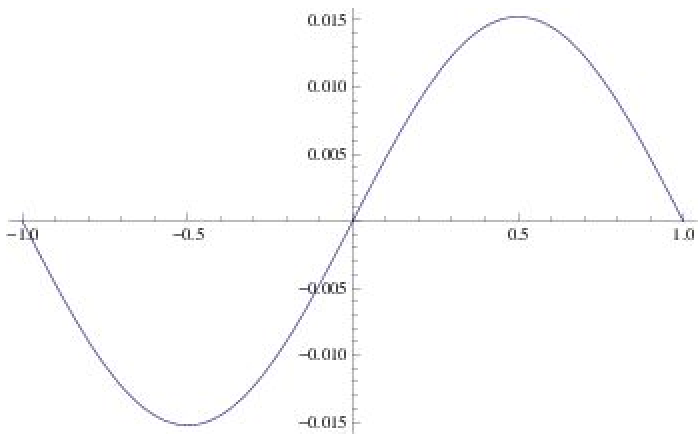
$$z = ka = n\pi \tag{0.21}$$
$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{0.22}$$

These are the same energy levels as in the square well of width a, thus it seems that making the delta function infinitely strong separates the well into two individual wells of half the width.

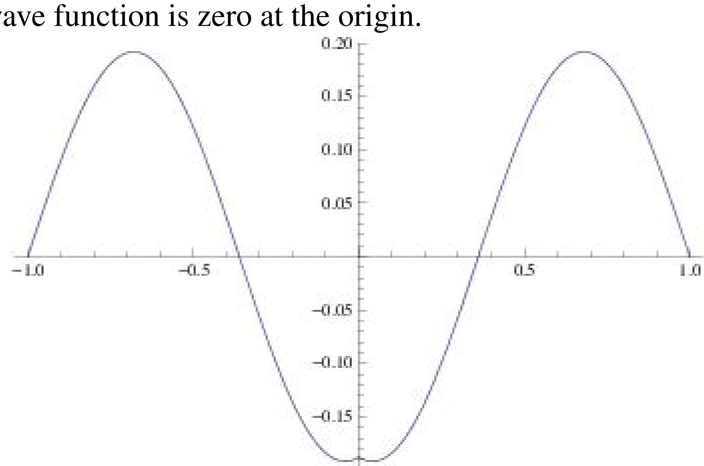
Here are a few plots of the wave functions for various energies, courtesy of KCErb (see link in comments below).



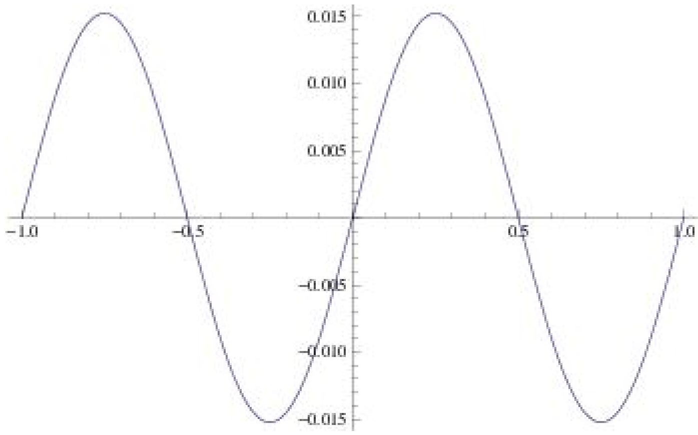
Lowest even energy state. Note the discontinuity of the derivative at $x = 0$.



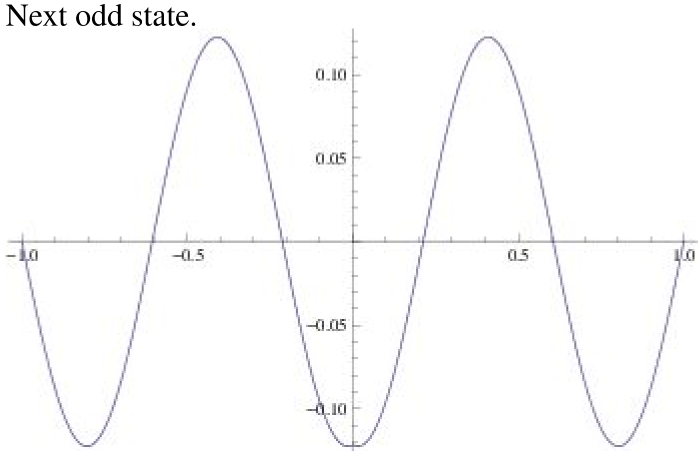
Lowest odd energy state. Here the delta function has no effect, since the wave function is zero at the origin.



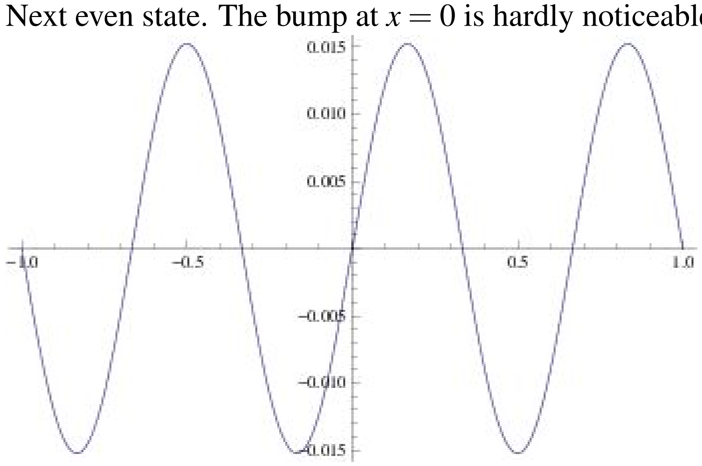
Next even state. There's a slight bump at $x = 0$.



Next odd state.



Next even state. The bump at $x = 0$ is hardly noticeable now.



And another odd state.

PINGBACKS

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