HYBRID INFINITE-FINITE SQUARE WELL

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.40.

As a sort of hybrid of the finite and infinite square wells, suppose we have the potential

$$V(x)=\begin{cases}\infty & x<0\\ -\frac{32\hbar^{2}}{ma^{2}} & 0\le x\le a\\ 0 & x>a\end{cases} \tag{0.1}$$

We can look for bound states ($E<0$) for this potential. From our analysis of the infinite and finite square wells, we can write down the wave function's general form:

$$\psi(x)=\begin{cases}0 & x<0\\ A\cos(lx)+B\sin(lx) & 0\le x\le a\\ Ce^{-\kappa x} & x>a\end{cases} \tag{0.2}$$

Here, $l\equiv\sqrt{2m\left(E+32\hbar^{2}/ma^{2}\right)}/\hbar$ and $\kappa\equiv\sqrt{-2mE}/\hbar$. Note that for a bound state, $E<0$.

Using the continuity of ψ at $x=0$:

$$\psi(0) = 0 \tag{0.3}$$
$$A = 0 \tag{0.4}$$

At $x=a$: continuity of ψ gives

$$B\sin(la)=Ce^{-\kappa a} \tag{0.5}$$

Continuity of ψ' gives

$$lB\cos(la)=-\kappa Ce^{-\kappa a} \tag{0.6}$$

Combining the last two gives

$$\tan(la) = -\frac{l}{\kappa} \tag{0.7}$$

We can now define the auxiliary variables

$$z \equiv la \tag{0.8}$$

$$z_0 \equiv \frac{a}{\hbar}\sqrt{2m\frac{32\hbar^2}{ma^2}} \tag{0.9}$$

$$= 8 \tag{0.10}$$

Also,

$$\left(l^2+\kappa^2\right)\hbar^2 = 2m\frac{32\hbar^2}{ma^2} \tag{0.11}$$

$$= \left(\frac{\hbar}{a}z_0\right)^2 \tag{0.12}$$

$$z_0^2 = \left(l^2+\kappa^2\right)a^2 \tag{0.13}$$

$$= z^2+\kappa^2a^2 \tag{0.14}$$

$$\kappa a = \sqrt{z_0^2-z^2} \tag{0.15}$$

$$= \sqrt{64-z^2} \tag{0.16}$$

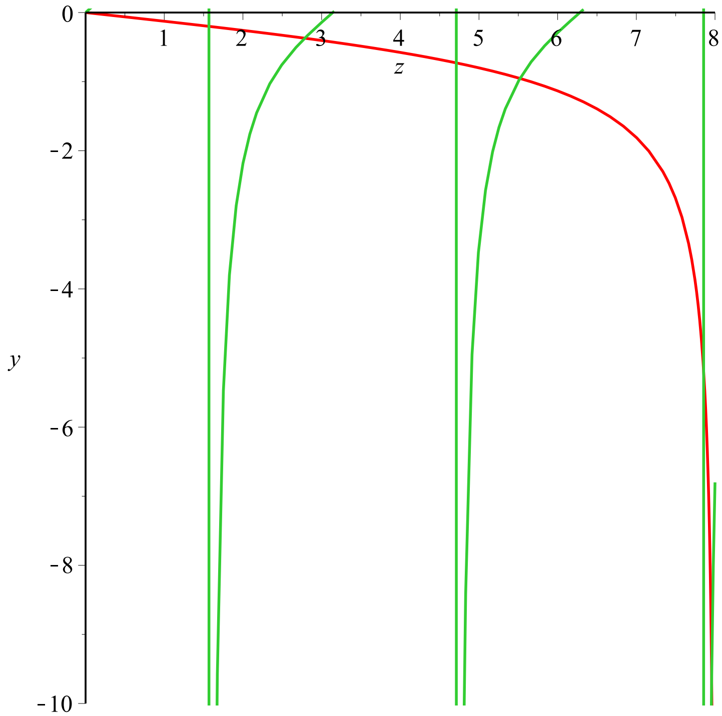
The equation to be solved for z is therefore:

$$\tan(z) = -\frac{la}{\kappa a} \tag{0.17}$$

$$= \frac{-z}{\sqrt{64-z^2}} \tag{0.18}$$

$$= -\frac{1}{\sqrt{64/z^2-1}} \tag{0.19}$$

This is a transcendental equation which can be solved graphically or numerically. The graph looks like this, with $\tan(z)$ in green and $-\frac{1}{\sqrt{64/z^2-1}}$ in red:



[The vertical green lines are the asymptotes of $\tan z$; I couldn't find a way to get Maple not to draw them.]

As can be seen from the graphical solution, there are 3 bound states. We can solve the equation numerically (using Maple's 'fsolve', for example) to find the three solutions and corresponding energies.

From small to large z, we get

$$z_1 = 2.785902114 \tag{0.20}$$
$$E_1 = -28.119\frac{\hbar^2}{ma^2} \tag{0.21}$$
$$z_2 = 5.521446430 \tag{0.22}$$
$$E_2 = -16.757\frac{\hbar^2}{ma^2} \tag{0.23}$$
$$z_3 = 7.957321494 \tag{0.24}$$
$$E_3 = -0.3405\frac{\hbar^2}{ma^2} \tag{0.25}$$

For the highest energy, we can find the probability that the particle is outside the box (that is, its position is outside the range $[0,a]$).

From the boundary conditions, we find

$$C=\frac{\sin(la)}{e^{-\kappa a}}B \tag{0.26}$$

so the integral of the square modulus of the wave function over its entire range is

$$\left[\int_0^a \sin^2(lx)dx+\frac{\sin^2(la)}{e^{-2\kappa a}}\int_a^\infty e^{-2\kappa x}dx\right]B^2 \tag{0.27}$$

The probability of the particle being outside the box is therefore the second term in the above expression divided by the entire expression:

$$p_3=\frac{B^2\frac{\sin^2(la)}{e^{-2\kappa a}}\int_a^\infty e^{-2\kappa x}dx}{\left[\int_0^a \sin^2(lx)dx+\frac{\sin^2(la)}{e^{-2\kappa a}}\int_a^\infty e^{-2\kappa x}dx\right]B^2} \tag{0.28}$$

Using the value of $z=7.957321494$ given above, we can get values for l and κ in terms of a. Plugging these into the above expression and evaluating (using Maple) gives

$$p_3=0.5420 \tag{0.29}$$

Note that this answer is very sensitive to the value of z. Even a minor rounding error will cause a significant difference in the value of p. For example, rounding z to 7.96 gives $p=0.550$.

It's interesting that for this barely bound state, the probability of the particle being outside the box is actually greater than that for being inside.

We can do similar calculations for the other two energies, and find:

$$p_2 = 0.0702 \tag{0.30}$$

$$p_1 = 0.0143 \tag{0.31}$$

Since these energies are lower, the probability of being found outside the well is much smaller, as we would expect.

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