FINITE SQUARE WELL - NUMERICAL SOLUTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.56 (supplementary).

We've looked at calculating the ground state energy and first three excited states of the harmonic oscillator, and the infinite square well, numerically, using the 'wag the dog' method. Those were special cases, in that we had an exact analytic solution. In the finite square well, however, we had to resort to a numerical or graphical solution to obtain the energies, so it's interesting to apply the wag the dog method to this case.

The finite square well potential is

$$V(x)=\begin{cases}0 & x<-a\\ -V_{0} & -a\le x\le a\\ 0 & x>a\end{cases} \tag{1}$$

For bound states, $-V_0<E<0$ and we expect a sinusoidal wave function within the well, with exponential decay on either side of the well. Using the same variable substitution as before ($\xi=x/a$), we can rewrite the Schrödinger equation as

$$\frac{d^{2}\psi}{d\xi^{2}}-P\psi=-K\psi \tag{2}$$

where

$$P(x) \equiv \frac{2ma^{2}V(x)}{\hbar^{2}} \tag{3}$$

$$K \equiv \frac{2ma^{2}E}{\hbar^{2}} \tag{4}$$

We can apply the same technique in Maple to solve the Schrödinger equation numerically, but since the potential is a piecewise function (consisting of three discontinuous sections), we need a way of specifying this function in Maple. We can do this using the 'piecewise' keyword:

$$P := x -> piecewise(x <= -1,\ 0,\ -1 < x \ and\ x < 1,\ -1,\ 1 <= x,\ 0) \quad (5)$$

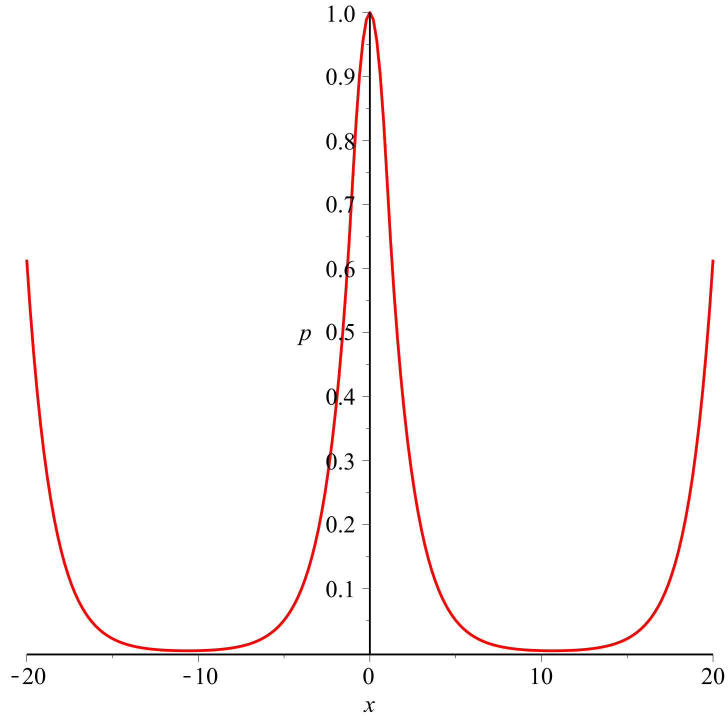
This defines $P(x)$ with a value of $P_0 = -1$ within the well and zero outside the well.

With this definition, we apply the same Maple code as in the harmonic oscillator and infinite square well cases. We need a couple of boundary conditions to get started. Since the potential is even, we can look for even and odd solutions. For the even case, we have $\psi'(0) = 0$ and $\psi(0) \neq 0$, so we can set $\psi(0) = 1$. This time we don't have an analytic solution to guide us to a starting value for K, so we have to make a guess and try to narrow it down from there. Since the bound state energy is negative, we do know that $K < 0$, so we can make a start with $K = -1$. We'll discover that the solution takes off to $+\infty$ on both sides, so we vary K in both directions to see what effect this has. Decreasing K (making it more negative) increases the rate at which the solution diverges, so we increase K instead. Eventually we will discover a value of K at which the tails of the solution flip over, so they now diverge to $-\infty$. The correct solution must lie between the two values where we observed the flip, so we can narrow things down from there.

After a number of iterations, we can arrive at a value of

$$K = -0.4537545832 \quad (6)$$

The solution at this point looks like this:



We see that the solution still diverges, but this is the slowest divergence rate I could manage before getting bored with determining extra significant figures.

We can check the result by comparing it with the analysis we did earlier for even solutions. We saw there that the energies were determined by solving the transendental equation

$$\tan z=\sqrt{\frac{z_0^2}{z^2}-1} \tag{7}$$

where

$$z_0^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{8}$$

$$= P_0 \tag{9}$$

and

$$z^2 = \frac{2ma^2(E+V_0)}{\hbar^2} \tag{10}$$
$$= K+P_0 \tag{11}$$

Thus if we have found a solution, then we should find that

$$\tan\left(\sqrt{K+P_0}\right)-\sqrt{\frac{P_0}{K+P_0}-1}=0 \tag{12}$$

Plugging in $P_0=1$ and $K=-0.4537545832$, we find

$$\tan\sqrt{(1-0.4537545832)}-\sqrt{\frac{1}{1-0.4537545832}-1}=-4.3614\times10^{-6} \tag{13}$$

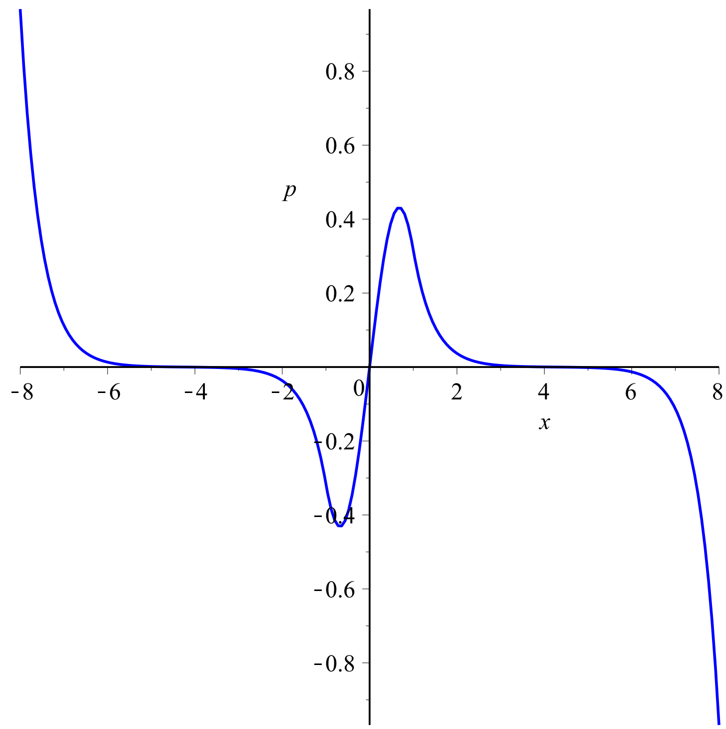
so the solution isn't too bad.

We can try to determine a solution for an odd wave function as well. Since we know from the analysis earlier that there are no bound odd states if the well is too shallow, we'll increase the depth of the well to $P_0=10$ to make sure there is at least one bound state. This time, since we're looking for an odd solution, we have $\psi(0)=0$ and $\psi'(0)=1$ (the value of $\psi'(0)$ can be any non-zero value). Starting with $K=-10$ we do the usual tweaking, and I arrived at

$$K=-4.624192830474 \tag{14}$$

before tedium got the better of me. (Obviously, in a more sophisticated setup, we could write a program in Maple to automate the process, but we'll leave that for another day.)

The wave function looks like this:



The transcendental equation that we arrived at in the odd case is

$$\tan z = -\left(\frac{z_0^2}{z^2}-1\right)^{-1/2} \tag{15}$$

or in terms of our variables here

$$\tan\left(\sqrt{K+P_0}\right)+\left(\frac{P_0}{K+P_0}-1\right)^{-1/2}=0 \tag{16}$$

Plugging in values for P_0 and K, we get

$$\tan\left(\sqrt{10-4.624192830474}\right)+\left(\frac{10}{10-4.624192830474}-1\right)^{-1/2}=8.58\times 10^{-7} \tag{17}$$

so again we've got a reasonable solution.