INFINITE SQUARE WELL - NUMERICAL SOLUTION

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Post date: 29 Aug 2012.

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

We've looked at calculating the ground state energy and first three excited states of the harmonic oscillator numerically, using the 'wag the dog' method. In this post, we'll apply this method to the infinite square well.

The Schrödinger equation in this case reduces to

$$\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi \tag{1}$$

for $0\le x\le a$, for some constant a. In order to make this a dimensionless system, we can introduce the auxiliary variable

$$\xi\equiv\frac{x}{a} \tag{2}$$

Then the equation becomes

$$\frac{d^2\psi}{d\xi^2}=-K\psi \tag{3}$$

where

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

is also dimensionless. In these coordinates, the well extends over the range $0\le\xi\le1$.

Because the potential is infinite outside the well, we can't get any boundary conditions on the derivative ψ'. However, we do know that for an acceptable solution, $\psi(0)=\psi(1)=0$ since the wave function must be continuous at the boundaries. However, if we try a numerical solution with these boundary conditions, the result is simply $\psi(\xi)=0$, which isn't much use.

We can instead impose a value for $\psi'(0)$ to force the solution away from this zero-everywhere case. If we do that, the condition we want to look for is $\psi(1)=0$, so we can adjust K until that condition is satisfied. Since in this case we're looking for the value of ψ at a specific point, we don't need to look at the graphs; we can just get Maple to calculate the solution at $\psi(1)$ and try to make it zero. (We can, of course, check the graph once we've found this solution in order to see if it's the right function.)

Analytically, we know that the energy levels in the infinite square well are

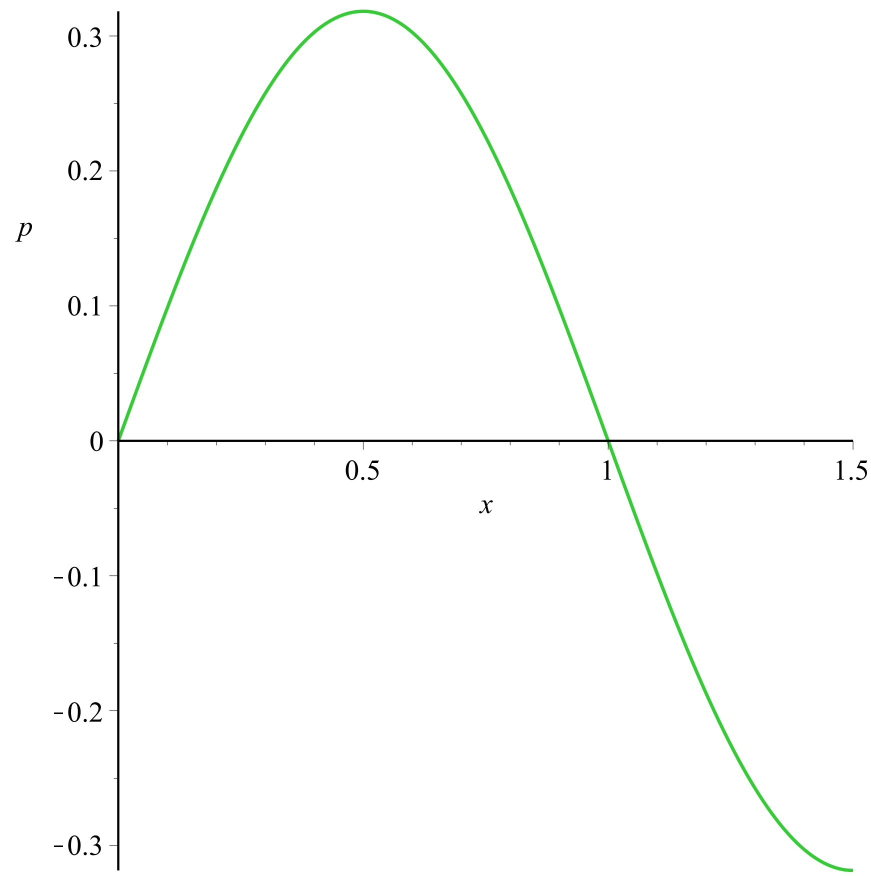
$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{5}$$

In the ground state, $n = 1$ so $K = \pi^2$. We can start off with $K = 9$ and see how it goes.

K	$\psi(1)$
9	0.04704
9.5	0.01926
10	-0.00654
9.75	0.00611
9.875	-0.00027
9.870	-0.00002
9.8695	5.3×10^{-6}

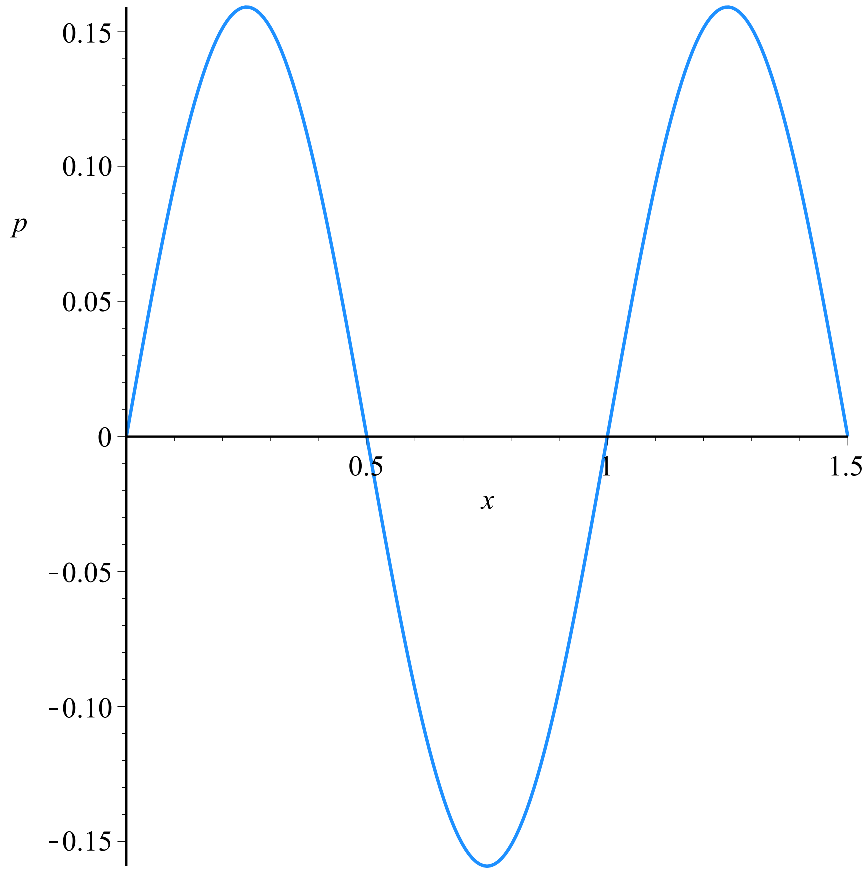
For comparison, $\pi^2 = 9.869604404\ldots$

The graph of ψ for this value of K is this:



It is the familiar sine curve that we know is the correct solution.

We can repeat the process for higher energy levels. For $n = 2$, the correct value of K is $4\pi^2 = 39.47841762$. Starting with $K = 39$ and tweaking the value until we get the same accuracy as in the ground state above, we get $K = 39.478$. The graph in this case is:



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