HARMONIC OSCILLATOR EXCITED STATES - NUMERICAL SOLUTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.55.

In the last post, we looked at calculating the ground state energy of the harmonic oscillator numerically, using the 'wag the dog' method. In this post, we'll look at calculating the first three excited states in the same way.

In the analytic solution, we arrived at the following differential equation

$$\frac{d^2\psi}{dy^2}=(y^2-\varepsilon)\psi \tag{1}$$

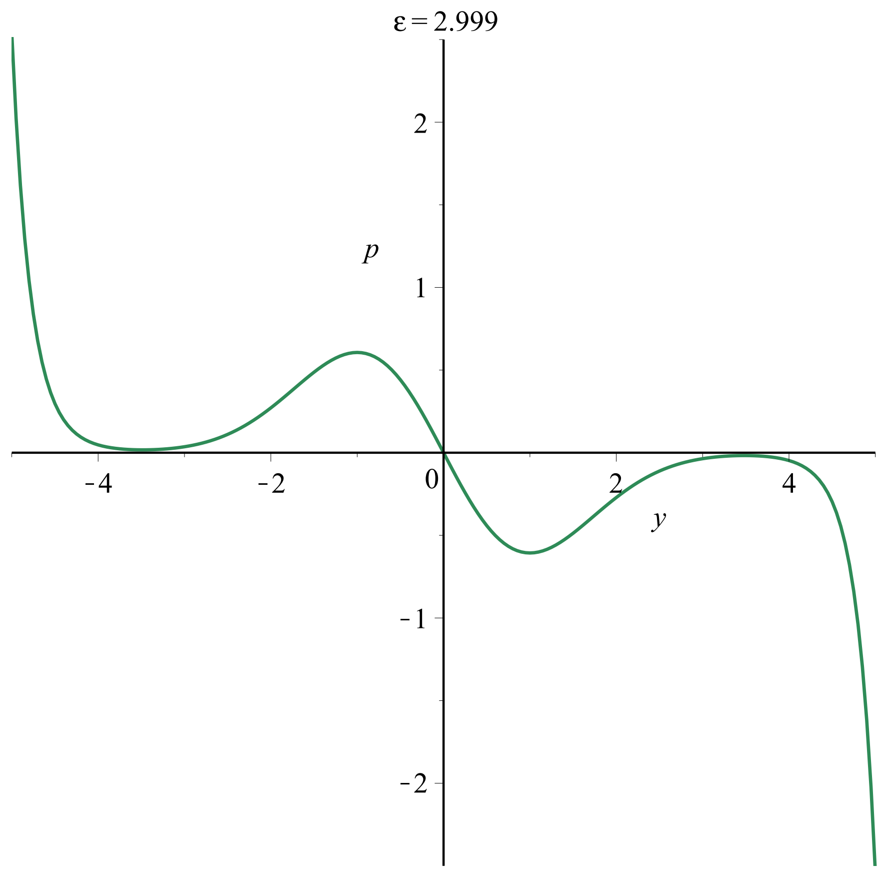
where we've used dimensionless parameters

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{2}$$

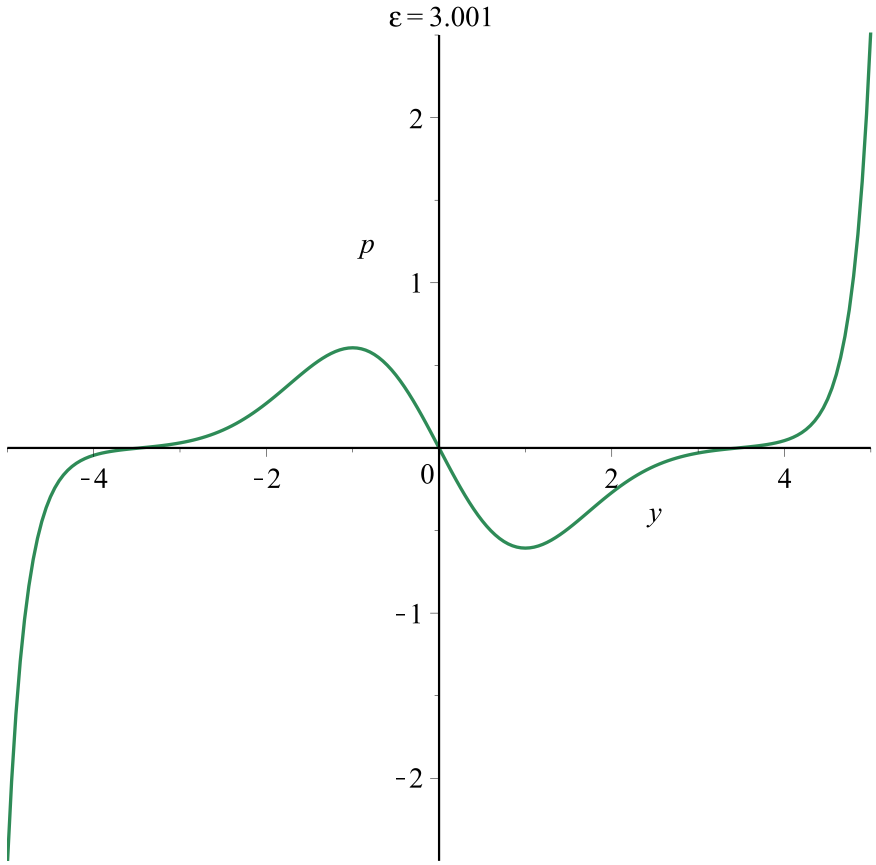
$$\varepsilon \equiv \frac{2E}{\hbar\omega} \tag{3}$$

The ground state occurs when $\varepsilon=1$ and the next three excited states occur when $\varepsilon=3,5,7$ respectively. We know this, of course, only because we've solved the problem analytically, but for the purposes of numerical solution, we will show what happens if we take ε slightly less and greater than the correct values in each case. We'll use the same Maple code as in the previous post.

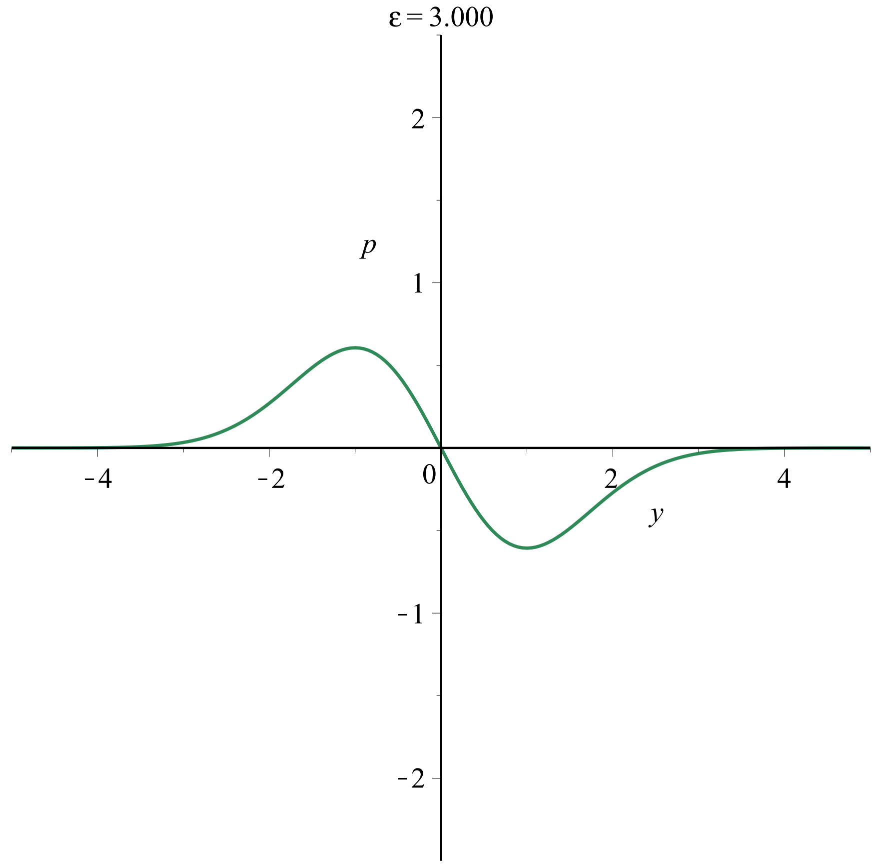
The solutions for $\varepsilon=3,7$ are odd, so as we saw in the last post, we'll need to take $\psi(0)=0$ and $\psi'(0)\neq 0$. Just for fun, we'll take $\psi'(0)=-1$. With $\varepsilon=2.999$, we get



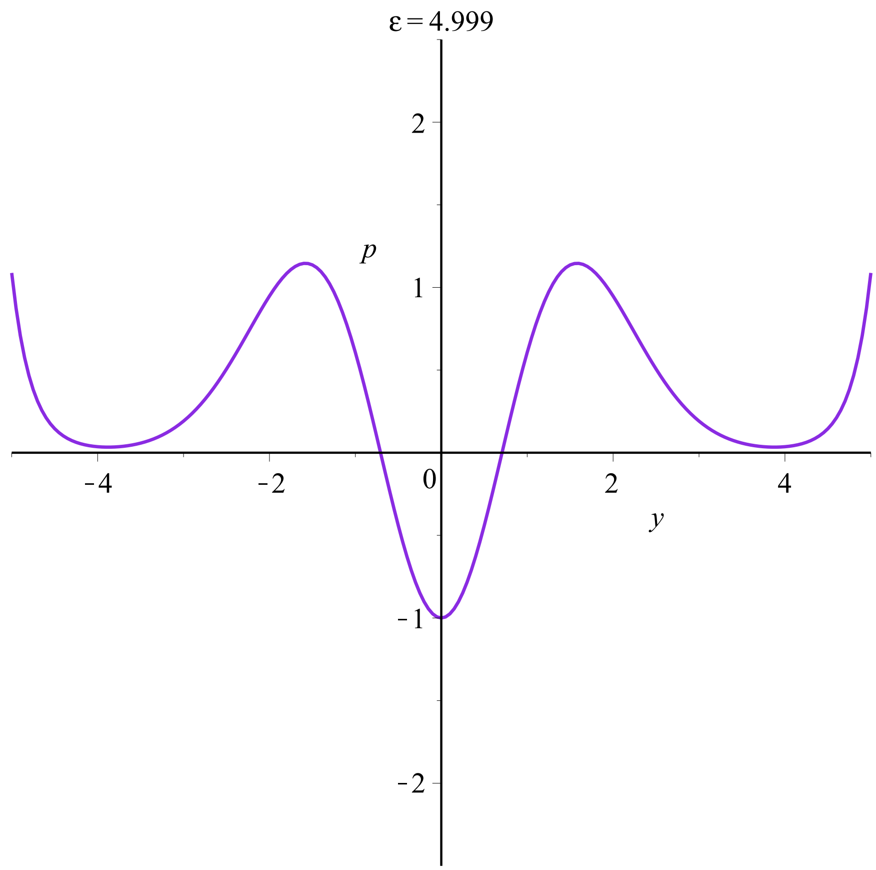
For $\varepsilon = 3.001$ we get



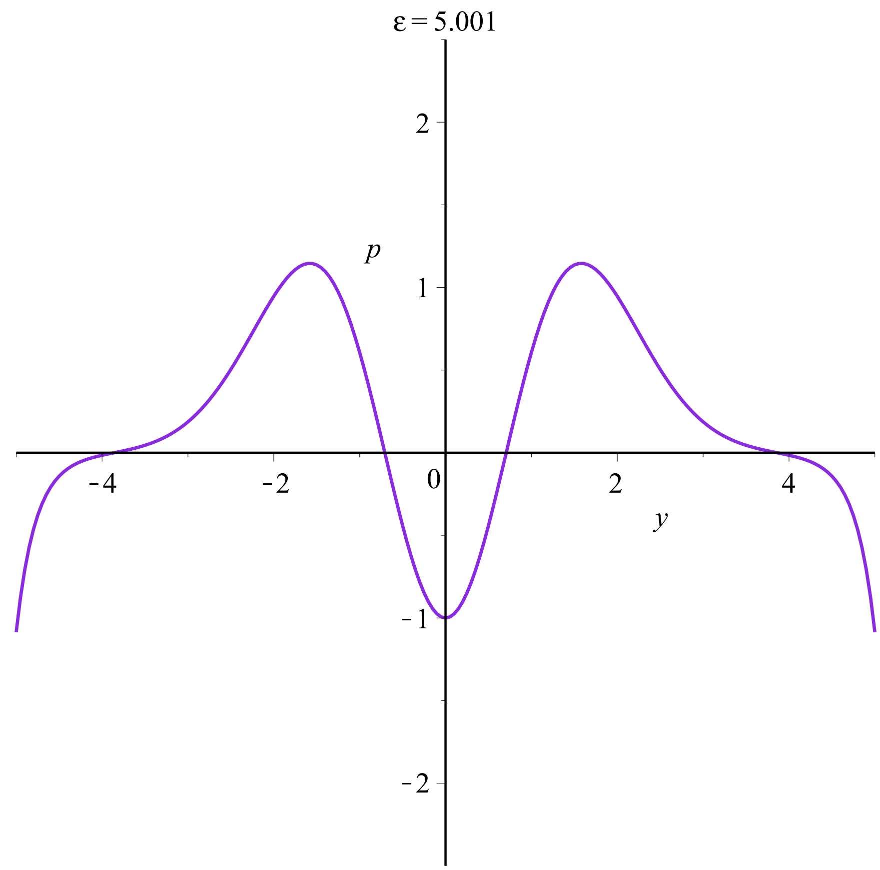
The two tails of the function have flipped, but the central region remains the same since it is constrained by the initial conditions. Finally, with $\varepsilon = 3.000$ we get the correct solution:



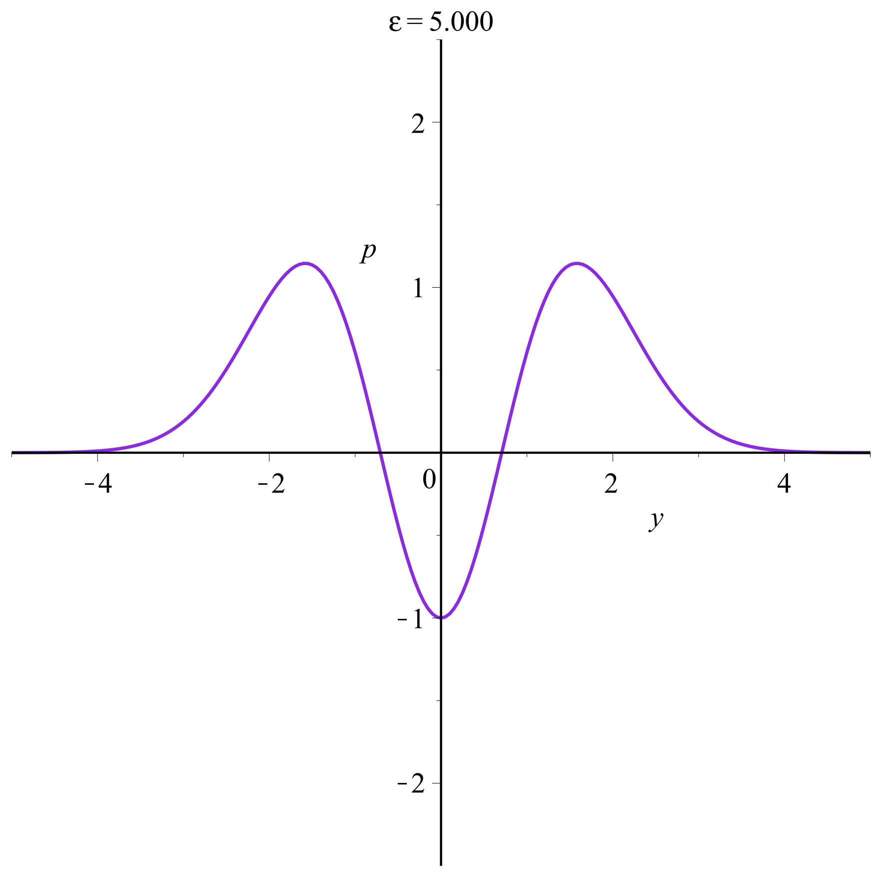
For the second excited state, the solution is even so we take $\psi(0) = -1$ (again, just for variety - the actual numerical value doesn't matter since any multiple of a solution is also a solution, and the *actual* value of $\psi(0)$ would be determined by normalization anyway) and $\psi'(0) = 0$. We try $\varepsilon = 4.999$ and get



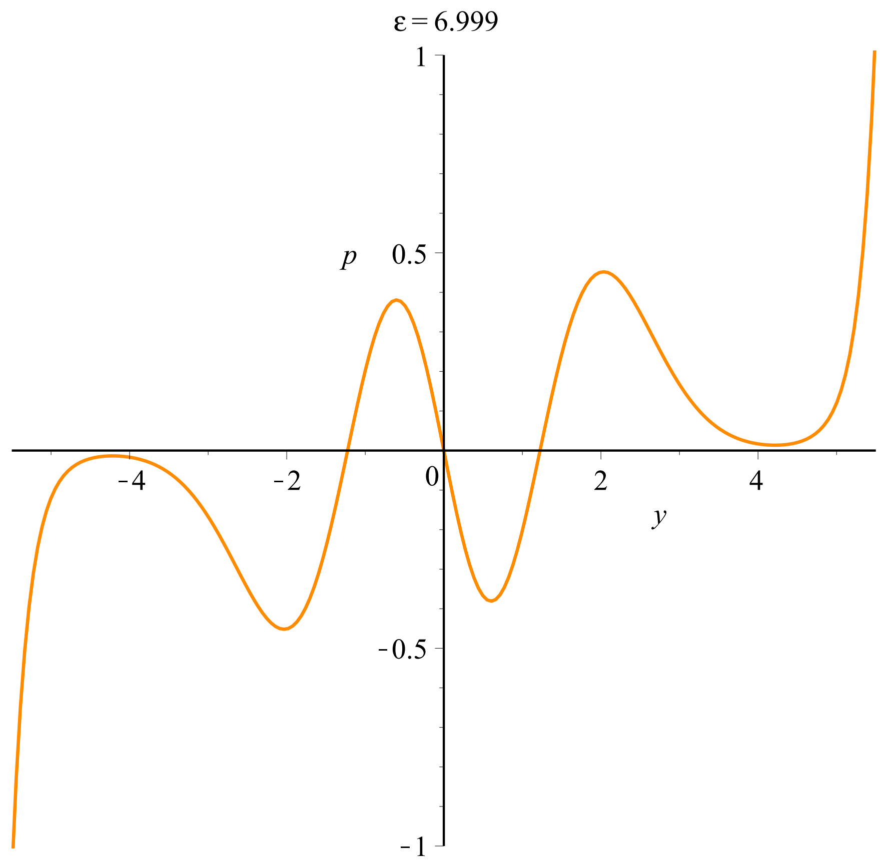
For $\epsilon = 5.001$ we have:



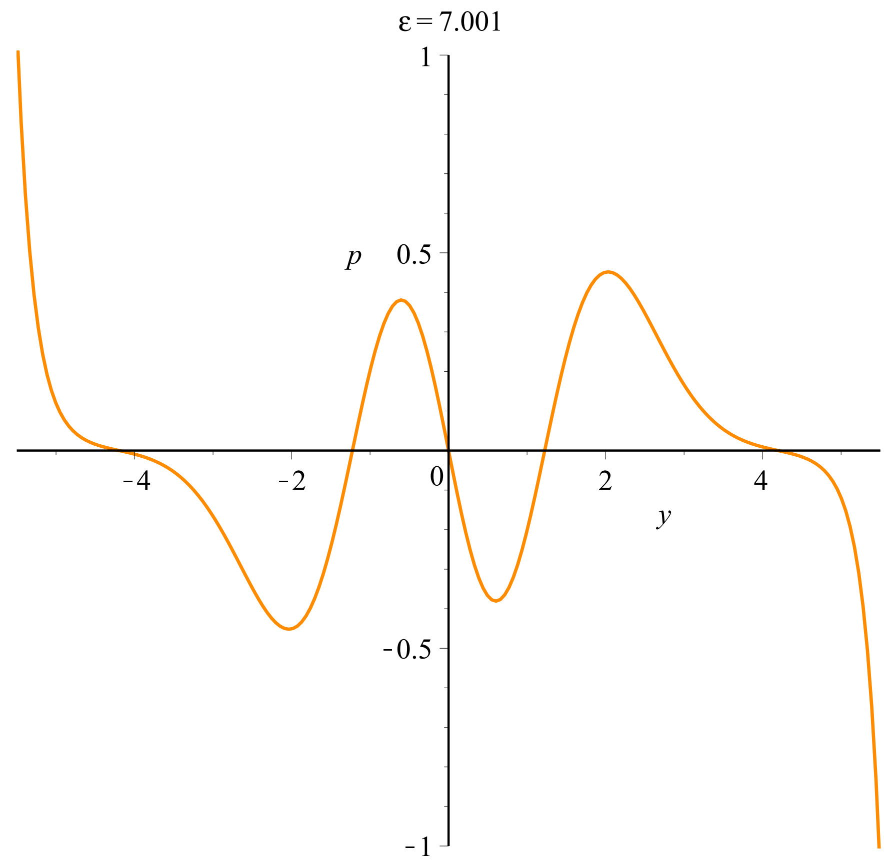
And finally for $\varepsilon = 5.000$ we get the correct solution:



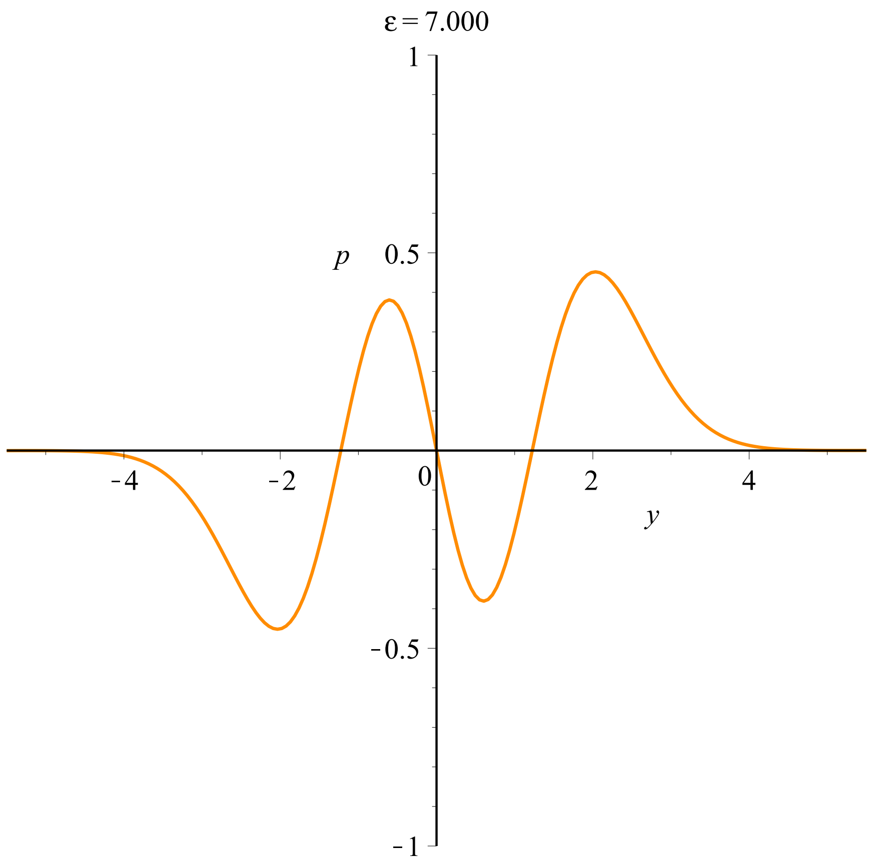
For the third excited state, the solution is again odd, so we revert to $\psi(0) = 0$ and $\psi'(0) = -1$. With $\varepsilon = 6.999$ we have:



For $\varepsilon = 7.001$ we have:



And finally for $\varepsilon = 7.000$ we get the correct solution:



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