HARMONIC OSCILLATOR GROUND STATE - NUMERICAL SOLUTION

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Although the examples of the Schrödinger equation that we've looked at have all had exact analytic solutions, in practice this is quite rare. Usually we need to resort to a numerical solution on a computer. We can illustrate the technique using a familiar potential such as the harmonic oscillator. In the analytic solution, we arrived at the following differential equation

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

where we've used dimensionless parameters

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

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

What we really want from a solution of this equation are the acceptable values of the energy, that is, values for which the wave function is normalizable, which means it goes to zero at infinity. We can therefore try various values for ϵ and try to home in on values that satisfy this condition. This technique is sometimes called 'wagging the dog', because we are holding onto the tail (the end result) and then seeing what sort of a solution produces this result.

Numerical solution of differential equations is quite easy in Maple. For the above equation, we set up the problem with the Maple statement

*sol := dsolve({diff(p(y),y$2)=(y^2-eps)*p(y), p(0)=1,D(p)(0)=0}, p(y), type=numeric,parameters=[eps])*

The term *diff(p(y),y$2)* is Maple notation for d^2p/dy^2. As this is a second order equation we need to specify two initial conditions, so we've given $\psi(0) = 1$ and $\psi'(0) = 0$ as an example here. (The Maple phrase *D(p)(0)* means the first derivative of *p* evaluated at $y = 0$.)

Then we specify that the solution we want is *p(y)*, that it should use a numeric solution method, and that there is one parameter called *eps*. When we

enter this command into Maple it responds by defining a procedure which it will use to calculate the solution. The procedure is named *proc(x_rkf45)*. The actual name isn't important here, but the 'rk' bit means it's using a Runge-Kutta method for the solution (if you're interested).

To generate a solution, we need to provide values for all the parameters, so we give the command

sol(parameters=[0.9])

This sets $\epsilon = 0.9$. We can then determine the solution at a particular point if we want, by calling *sol(y)*, where *y* is a particular value. Maple will produce the values of *p(y)* and *p'(y)* at that point.

For our purposes, however, we would like a plot of the solution over a given range so that we can see whether the wave function tends to zero for large y. Maple provides the *odeplot* command for this. To use it, we need to include the *plots* library, so the command is

plots[odeplot](sol, [y,p(y)], -5..5)

This tells Maple to draw a plot of *p(y)* in the range $y \in [-5, 5]$.

Assuming we don't know the correct values for ϵ, we need to make an initial guess and then try to narrow it down. We also need to specify the initial conditions for ψ and ψ'. For even functions, we know that $\psi'(0) = 0$ (assuming the first derivative is continuous, which is true for the harmonic oscillator). The precise value of $\psi(0)$ itself doesn't really matter, as long as it's non-zero, since any multiple of a solution is also a solution.

For odd functions, we know $\psi(0) = 0$. Here, the actual value of $\psi'(0)$ doesn't matter, as long as it's non-zero.

Since the potential is even, we know that the solutions will be even or odd. If we're being honest and assuming that we haven't worked out the analytic solution, we really don't know which energy states are even and which are odd. For the ground state, the solution actually is even, so we can demonstrate the technique by assuming this to start with. We'll take $\psi(0) = 1$ and $\psi'(0) = 0$, and try an initial value of $\epsilon = 0.9$. We get Fig. 1.

As you can see, the wave function heads off to $+\infty$ on both sides, so $\epsilon = 0.9$ isn't a valid value. If we try $\epsilon = 1.1$, we get Fig. 2.

This time, the wave function goes to $-\infty$, so we can guess that somewhere in the middle it does tend to zero.

We can try values of ϵ successively closer to 1.0 on both sides and watch what happens. For $\epsilon = 0.999$ we get Fig. 3.

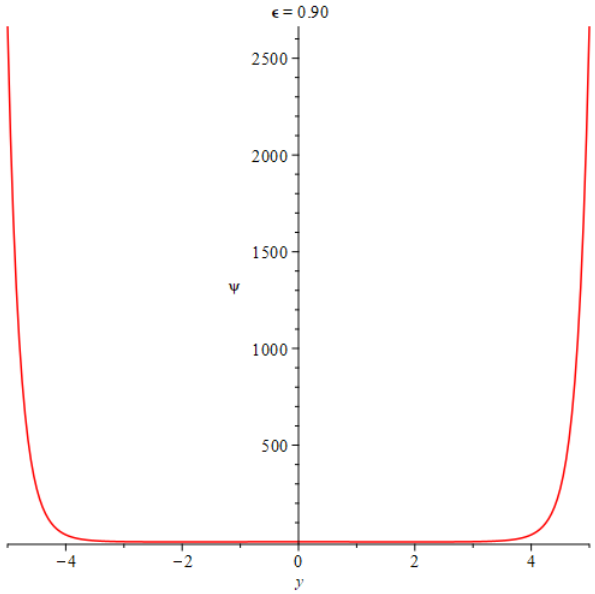

FIGURE 1.

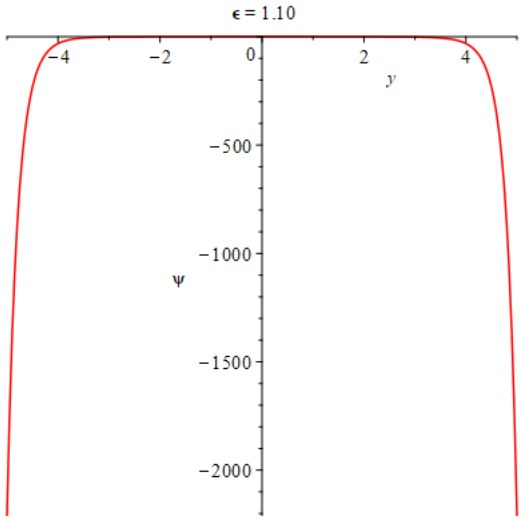

FIGURE 2.

Note the scale on the vertical axis is a lot smaller, and there is now a noticeable bump near $y = 0$. For $\epsilon = 1.001$, we have Fig. 4.

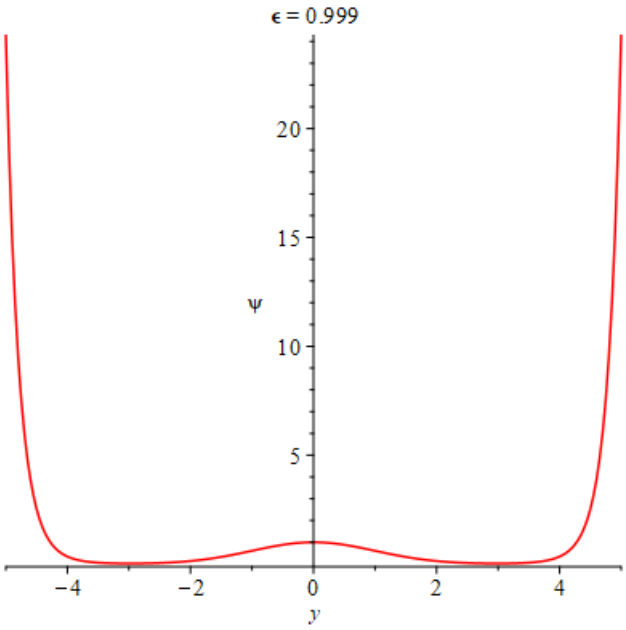

FIGURE 3.

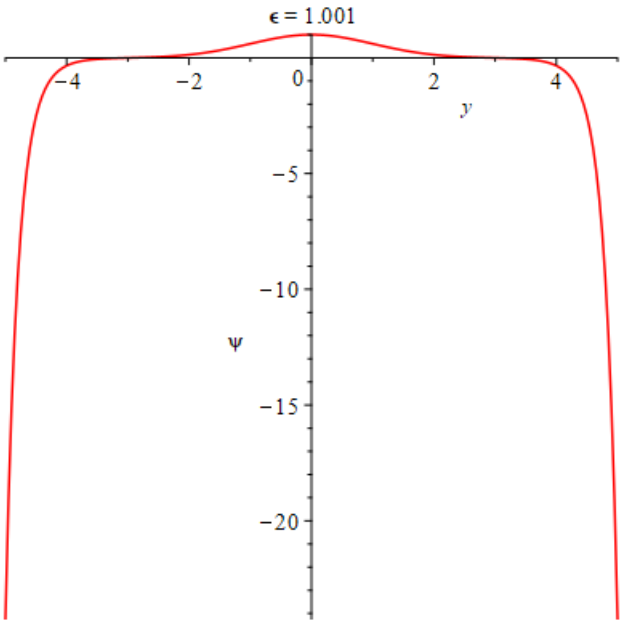

FIGURE 4.

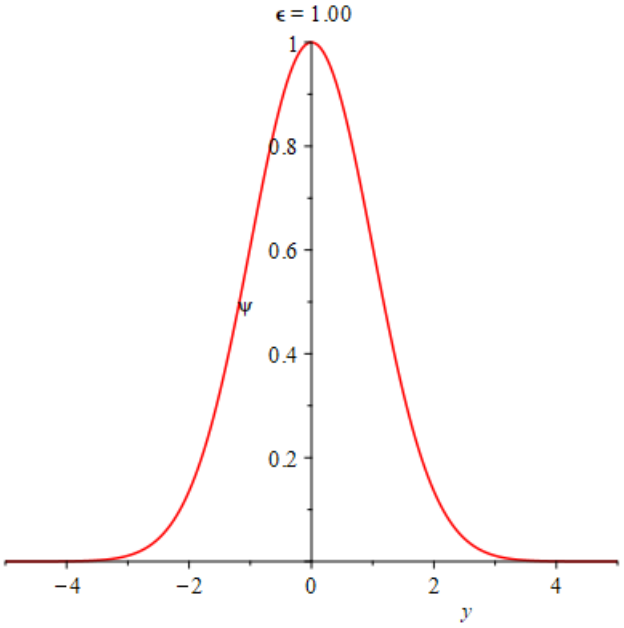

FIGURE 5.

It still goes to $-\infty$ but the bump around $y = 0$ is still there. Finally, just to confirm the numerical method does actually work for the correct value, we try $\epsilon = 1.0$ and get Fig. 5.

That looks right, so the method seems to be working.

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