HARMONIC OSCILLATOR - ASYMPTOTIC SOLUTION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.3.

In the summary of the quantum harmonic oscillator, we saw that we need to solve the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}kx^2\psi = E\psi \tag{1}$$

There are two popular ways of approaching this problem. Here we will examine the more direct of the two, in which we use some methods typical in the solution of differential equations. The other method is based on algebra more than calculus and we'll leave that for another post.

First, a quick review of the potential in this equation. The constant k determines the strength of potential, and is related to the mass m of the oscillator and the frequency of oscillation ω by

$$\omega=\sqrt{\frac{k}{m}} \tag{2}$$

Using this relation, we can rewrite the Schrödinger equation as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \tag{3}$$

The standard method of solving this equation involves two stages. First we find what the solution looks like for very large values of x (the *asymptotic* behaviour). We then factor this asymptotic behaviour out of the overall solution ψ and try to solve a new differential equation for what is left over. This second equation is solved by expressing the solution as a power series in x, and using the physics to constrain the coefficients in the series.

In principle, we could skip the first step and attempt to find a series solution starting from the Schrödinger equation, but it turns out that the two stage process is a bit less messy (although things still do get fairly complicated, as you'll see).

First, things get a bit clearer if we introduce a couple of new symbols. We define a new spatial variable:

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{4}$$

and, for the energy:

$$\varepsilon \equiv \frac{2E}{\hbar\omega} \tag{5}$$

To transform the spatial variable, we also need to transform the second derivative, which we can do if we note that

$$dy = \sqrt{\frac{m\omega}{\hbar}}dx \tag{6}$$

$$\frac{d\psi}{dy} = \sqrt{\frac{\hbar}{m\omega}}\frac{d\psi}{dx} \tag{7}$$

$$\frac{d^2\psi}{dy^2} = \frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2} \tag{8}$$

Therefore, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2}+\frac{1}{2}m\omega^2\frac{\hbar}{m\omega}y^2\psi = E\psi \tag{9}$$

$$-\frac{\hbar\omega}{2}\frac{d^2\psi}{dy^2}+\frac{\hbar\omega}{2}y^2\psi = E\psi \tag{10}$$

$$\frac{d^2\psi}{dy^2} = (y^2-\varepsilon)\psi \tag{11}$$

Now that we have transformed the equation to a cleaner form, we can try to solve it. The problem is to solve this differential equation:

$$\frac{d^2\psi}{dy^2} = (y^2-\varepsilon)\psi \tag{12}$$

First, we try to find the solution of this equation for very large y. In this limit, the equation is, approximately:

$$\frac{d^2\psi_a}{dy^2} \approx y^2\psi_a \tag{13}$$

The idea is that if we can find a solution $\psi_a(y)$ of this approximate equation, then we can write the *actual* solution as a product of the approximate solution and some other function $f(y)$:

$$\psi(y) = \psi_a(y) f(y) \tag{14}$$

where $f(y)$ can be solved as a power series in y.

So can we find the asymptotic solution ψ_a? The *exact* solution of the approximate equation 13 involves Bessel functions, but since the equation is only an approximate equation, and we are interested only in its behaviour for large y, we don't need an exact solution. If we try

$$\psi_a(y) = Ae^{-y^2/2} + Be^{y^2/2} \tag{15}$$

we find

$$\psi_a'(y) = -Aye^{-y^2/2} + Bye^{y^2/2} \tag{16}$$

$$\psi_a''(y) = A(y^2-1)e^{-y^2/2} + B(y^2+1)e^{y^2/2} \tag{17}$$

For large values of y, the second derivative is approximately:

$$\psi_a''(y) \approx Ay^2e^{-y^2/2} + By^2e^{y^2/2} \tag{18}$$

$$= y^2\psi_a \tag{19}$$

So as an approximation for the asymptotic behaviour, ψ_a seems to fit the bill. Also, since the final wave function has to be normalizable, we can't have the asymptotic function blowing up to infinity, so we must take $B = 0$. If we leave the overall normalization until the end, we can also absorb A into whatever normalization we do at the end, so we can take

$$\psi_a(y) = e^{-y^2/2} \tag{20}$$

This means we are taking for the overall wave function:

$$\psi(y) = e^{-y^2/2} f(y) \tag{21}$$

At this point you might be feeling a bit soiled, since it seems that we've used a lot of approximating and hand-waving to get to this point. However, all this hand-waving has merely given us a possible form for the final solution; we still need to find $f(y)$, and we do that by substituting equation 21 back into the original equation 12 and finding the solution for $f(y)$. It doesn't really matter how we arrived at equation 21; the acid test is when we substitute it back into equation 12 and try to find $f(y)$. If we can do that, then this is an *exact* solution to the original Schrödinger equation.

Anyway, enough hand-waving. Has finding the asymptotic form helped at all? When we do the substitution, we need to calculate the second derivative of $\psi(y)$:

$$\frac{d\psi}{dy} = \left(\frac{df}{dy} - yf\right)e^{-y^2/2} \tag{22}$$

$$\frac{d^2\psi}{dy^2} = \left(\frac{d^2f}{dy^2} - 2y\frac{df}{dy} + (y^2-1)f\right)e^{-y^2/2} \tag{23}$$

Substituting this back into equation 12 gives us

$$\frac{d^2f}{dy^2} - 2y\frac{df}{dy} + (\varepsilon - 1)f = 0 \tag{24}$$

It is this equation that we wish to solve by taking $f(y)$ to be a power series in y. But that's probably enough for one post, so we'll leave that bit to the next post.

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