Algebraic solution to the 3d harmonic oscillator

Nathaniel Craig

Our next goal is the hydrogen atom, but as a warmup, I'd like to first consider the algebraic solution to the 3d harmonic oscillator in spherical coordinates. As you have already seen, the solution in Cartesian coordinates is relatively simple: separable solutions factorize, and we can use three copies of our one-dimensional algebraic approach to find the energy eigenstates. But this approach somewhat obscures the physical meaning of the solutions – the potential is spherically symmetric, so the most natural coordinate system for the solutions is the one that manifests this symmetry.

For harmonic oscillator in three dimensions, the potential in spherical coordinates is simply

$$V(r) = \frac{1}{2}m\omega^2 r^2$$

The angular dependence of the energy eigenstates in spherical coordinates is entirely encoded by the spherical harmonic Y_ℓ^m. Our task is now simply to solve the radial dependence to find the radial wavefunction $R_\ell(r)$. The effective radial Hamiltonian H_ℓ is simply

$$H_\ell = \frac{p_r^2}{2m} + \frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

This radial Hamiltonian has the form of the sum of squares. When we encountered such a Hamiltonian for the 1d harmonic oscillator, this suggested that we try to write it as the product of two operators. This turned out to lead us to a complete algebraic solution! So let's do the same thing here. Consider the operator

$$a_\ell \equiv \frac{1}{\sqrt{2m\hbar\omega}}\left[ip_r - \frac{(\ell+1)\hbar}{r} + m\omega r \right]$$

In analogy with the 1d harmonic oscillator, this will be our lowering operator. Its hermitian conjugate $a_\ell^\dagger$ is the raising or creation operator. As you can check, these operators satisfy the following commutation relation:

$$[a_\ell, a_\ell^\dagger] = \frac{(\ell+1)\hbar}{m\omega r^2} + 1$$

This is more complicated than the commutation relation satisfied by the raising/lowering operators of the 1d harmonic oscillator, but still relatively compact. Now notice that the product of $a_\ell^\dagger$ and a_ℓ is

$$a_\ell^\dagger a_\ell = \frac{1}{2m\hbar\omega}\left(-ip_r - \frac{(\ell+1)\hbar}{r} + m\omega r\right)\left(ip_r - \frac{(\ell+1)\hbar}{r} + m\omega r\right) \tag{1}$$

$$= \frac{1}{2m\hbar\omega}\left(p_r^2 + \frac{\ell(\ell+1)\hbar^2}{r^2} + m^2\omega^2 r^2 - (2\ell+3)\hbar m\omega\right) \tag{2}$$

so that we can write the radial Hamiltonian H_ℓ as

$$H_\ell = \hbar\omega\left(a_\ell^\dagger a_\ell + (\ell + 3/2)\right)$$

This looks a lot like the harmonic oscillator in 1d, albeit with the appearance of extra ℓ dependence. And notice that we have already picked up something that looks like the ground state energy, complete with the factor of $3/2$ you found in Cartesian coordinates.

Now notice something interesting: we can write the commutator of a_ℓ and $a_\ell^\dagger$ in terms of the radial Hamiltonian H_ℓ and the radial Hamiltonian corresponding to $\ell+1$:

$$[a_\ell, a_\ell^\dagger] = \frac{H_{\ell+1} - H_\ell}{\hbar\omega} + 1$$

This is because

$$H_{\ell+1} - H_\ell = \frac{\hbar^2}{2mr^2}\left[(\ell+1)(\ell+2) - \ell(\ell+1)\right] = \frac{\hbar^2(\ell+1)}{mr^2}$$

This observation allows us to easily work out the commutator of a_ℓ and H_ℓ, for example:

$$[a_\ell, H_\ell] = \hbar\omega[a_\ell, a_\ell^\dagger a_\ell] = \hbar\omega[a_\ell, a_\ell^\dagger]a_\ell = (H_{\ell+1} - H_\ell + \hbar\omega)a_\ell$$

Now imagine we knew a radial eigenstate R_ℓ with energy E_n,

$$H_\ell R_\ell = E_n R_\ell$$

Then acting on both sides with a_ℓ and commuting it past H_ℓ with our above commutator gives

$$E_n a_\ell R_\ell = a_\ell H_\ell R_\ell = (H_\ell a_\ell + [a_\ell, H_\ell]) R_\ell = (H_{\ell+1} + \hbar\omega) a_\ell R_\ell$$

Cleaning things up, we have

$$H_{\ell+1}(a_\ell R_\ell) = (E_n - \hbar\omega)(a_\ell R_\ell)$$

This means that acting on R_ℓ with the lowering operator a_ℓ gives us a new radial state $a_\ell R_\ell$, which is *not* an eigenstate of H_ℓ, but *is* an eigenstate of a radial Hamiltonian $H_{\ell+1}$ with a larger separation constant $\ell + 1$ and smaller energy eigenvalue $E_n - \hbar\omega$. As we'll see next, this is enough to obtain a complete algebraic solution to the 3D harmonic oscillator, and provides a blueprint for the algebraic solution to the hydrogen atom.

To recap, we found that the operator equation satisfied by radial eigenstates of the 3d harmonic oscillator in spherical coordinates,

$$H_\ell R_\ell = E_n R_\ell$$

could be solved by introducing a lowering operator

$$a_\ell \equiv \frac{1}{\sqrt{2m\hbar\omega}} \left[i p_r - \frac{(\ell+1)\hbar}{r} + m\omega r \right]$$

and the corresponding creation operator, $a_\ell^\dagger$, with commutator

$$[a_\ell, a_\ell^\dagger] = \frac{(\ell+1)\hbar}{m\omega r^2} + 1$$

The radial Hamiltonian H_ℓ could be written in terms of these as

$$H_\ell = \hbar\omega \left(a_\ell^\dagger a_\ell + (\ell + 3/2) \right)$$

We then noted that, given a solution R_ℓ with energy E_ℓ, then $a_\ell R_\ell$ was itself an eigenstate of $H_{\ell+1}$ with energy $E_n - \hbar\omega$ – the angular momentum was higher, and the total energy lower:

3

$$H_{\ell+1}(a_\ell R_\ell) = (E_n - \hbar\omega)(a_\ell R_\ell)$$

If we repeat this process over and over – that is to say, acting on $a_\ell R_\ell$ with $a_{\ell+1}$, etc. – we will eventually get to a state $R_\mathcal{L}$ that is an eigenstate of some radial Hamiltonian $H_\mathcal{L}$ where all of the radial kinetic energy has been exhausted. The specific value of $\mathcal{L}$ will be determined by the E_n you started with, but we only care that it exists. With little radial kinetic energy, this is the quantum mechanical equivalent of a circular orbit (as we will see, they still have a little bit of radial kinetic energy – this is the zero point energy in the radial direction). And although we have not rigorously established the connection to angular momentum yet, the fact that ℓ increases as the radial energy decreases means we are trading radial kinetic energy for angular momentum.

If we then acted on this state with $a_\mathcal{L}$, the radial kinetic energy would go negative. This is unphysical, so avoiding an unphysical conclusion implies that the state $R_\mathcal{L}$ should be annihilated by $a_\mathcal{L}$,

$$a_\mathcal{L} R_\mathcal{L} = 0$$

Knowing this, if we act on this state with $H_\mathcal{L}$, we have

$$H_\mathcal{L} R_\mathcal{L} = \hbar\omega \left(a_\mathcal{L}^\dagger a_\mathcal{L} + (\mathcal{L} + 3/2) \right) R_\mathcal{L} = (\mathcal{L} + 3/2)\hbar\omega R_\mathcal{L}$$

Now $\mathcal{L}$ is subject to the same constraints as general ℓ – it must be a non-negative integer. So it follows that the lowest-energy state of all corresponds to $\mathcal{L} = 0$, with energy $E = \frac{3}{2}\hbar\omega$, just as you found in Cartesian coordinates. Higher integer values of $\mathcal{L}$ correspond to higher-energy circular orbits. (Remember, the value of $\mathcal{L}$ depends on the energy E_n you started with).

There is one circular orbit corresponding to every non-negative integer. We can find the explicit functional form of each one of them because $a_\mathcal{L} R_\mathcal{L} = 0$ is actually a pretty simple first-order linear differential equation,

$$\left(\frac{\partial}{\partial r} + \frac{1}{r} - \frac{\mathcal{L} + 1}{r} + \frac{m\omega}{\hbar}r \right) R_\mathcal{L}(r) = 0$$

The solutions are

$$R_\mathcal{L}(r) = Cr^\mathcal{L} \exp\left[-r^2/4r_0^2\right]$$

where $r_0 = \sqrt{\hbar/2m\omega}$ is the natural scale of the exponential envelope and C is a normalization constant. Thus we have found a whole class of radial wavefunctions – the "circular" ones – explicitly. We can then find all of the other eigenstates by starting with a given circular wavefunction and acting with the raising operator $a_\mathcal{L}^\dagger$ to create a less "circular" state. Because the raising operator both differentiates and multiplies by powers of r, acting with it creates more nodes in the radial wavefunction. This makes sense: nodes mean larger kinetic energy.

The relation between different radial eigenstates, their total energy, and their angular momentum (encoded in ℓ) is best illustrated by the following picture:
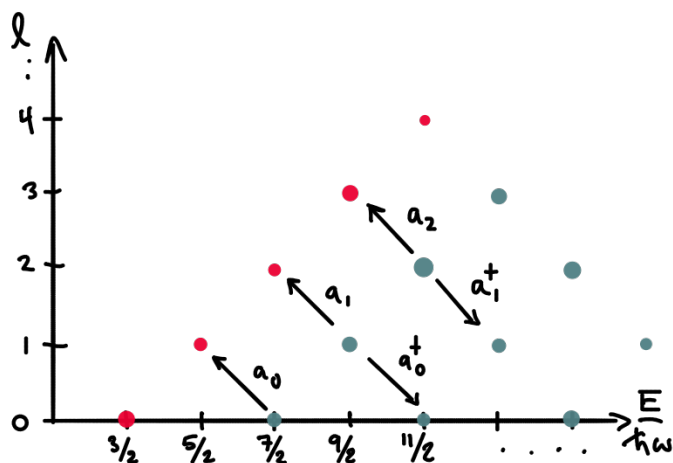
For the 1d harmonic oscillator, we used the raising and lowering operators to find one "ladder" of energy eigenstates. For the 3d harmonic oscillator, the appearance of ℓ means there is now a whole tower of ladders indexed by ℓ, with towers of raising and lowering operators also indexed by ℓ.

This is a beautiful and elegant way of solving the 3d harmonic oscillator, one that brings to bear all of the tools we have developed thus far in quantum mechanics. As we will now see, an analogous approach is perfect for the hydrogen atom as well.