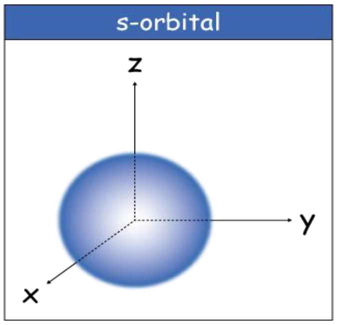
THE SHAPES OF THE ORBITALS

The lowest energy orbital, with L=0, is called an **s-orbital**. Its shape is always a sphere, as shown on the right.

In the spherical harmonic functions that describe the spaces that electrons occupy, when the quantum number L is zero, the quantum number m_L must also be zero, and the only possible 3-D shape that can arise is the sphere. There are no sub-orbitals of an s-orbital

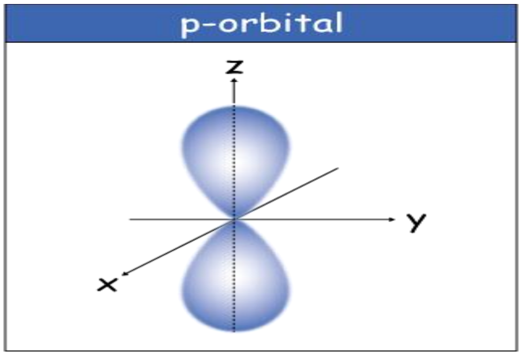
We interpret this sphere as the region within which it's most likely to find an electron if we *could* find it. Remember that an electron bound to an atom is acting much more like a wave than a tiny particle.

Every shell (labeled by n) has one s-orbital, each larger than the one below it.



Each s-orbital can hold, at most, two electrons, and those must have paired spins, one a +1/2, the other a -1/2.

It's another quirk of quantum behavior that we just have to get used to: No two electrons bound to an atom can have exactly the same set of quantum numbers, n, L, m_L and m_S.



P-orbitals are where things start getting interesting. How on Earth does this strange dumbbell shape arise?

We have to remember where we began. Electrons must be understood on their own terms. These orbital shapes arise from the solutions to the Schrödinger equation which exactly reproduce all that is known about the H-atom. They are what they are.

P-orbitals actually resemble some of the kinds of patterns you might observe if you could see electromagnetic waves coming off of an antenna.

The p-orbitals look like this because electrons act more like waves than particles when they're bound to atoms.

One of the ways waves interact is to **interfere** with one another, and that interference can lead to "**nodes**" like the pinched-off area in the middle of this p-orbital.

There are three p sub-orbitals, only one of which, the p_z orbital, is drawn above. There are also p-orbitals that lie along the x- and y-axes, p_x and p_y. The point is not really that they lie along these axes specifically, but that they exist at 90˚ angles to one another in 3 dimensions (another way to say this is that they're **orthogonal**). This has been verified in many experiments.

In an atom, each p sub-orbital can hold two electrons, as long as their spins are different.

For example, two electrons in the p_y orbital of the first energy level of an atom would have the quantum numbers n, L, m_L, m_s = 1, 1, 1, ±1/2 - unique sets of quantum numbers. Each p-orbital (including all three sub-orbitals) can hold six electrons. For each value of the quantum number n, there is a p-orbital (which consists of three sub-orbitals), which can hold six electrons.

It's getting weird: d-orbitals

D-orbitals (L = 2) are composed of five different types of sub-orbitals, labeled by m_L = -2, -1, 0 1, 2.

While the shapes of many of the d sub-orbitals are reminiscent of the p-orbitals, they are different. One, the d_z2 orbital is bizarre indeed, containing one **toroidal** (donut-shaped) region. Nevertheless, these orbitals represent the regions in which an electron with the energy of a d-orbital are most likely to be found.

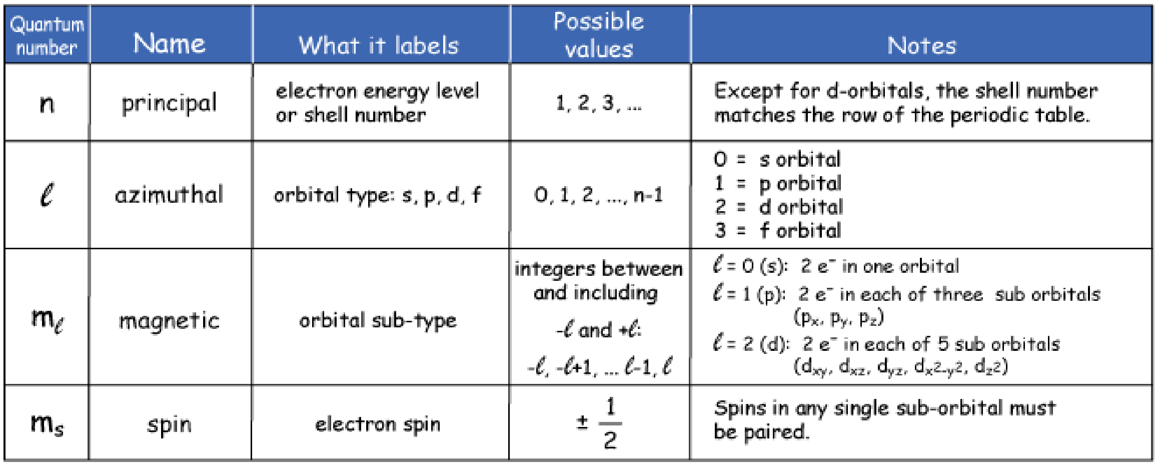
Because L = 0, 1, ... n-1, the lowest shell (quantum number n) to even have d orbitals is n = 3. The n= 3 shell contains s, p and d orbitals.

D-orbitals are what give metals their character. We'll get to that another time.

The d sub-orbitals are given names, analogous to p_x, p_y and p_z, of d_{xy}, d_{xz}, d_{yz}, d_{x2-y2}, and d_z^2.

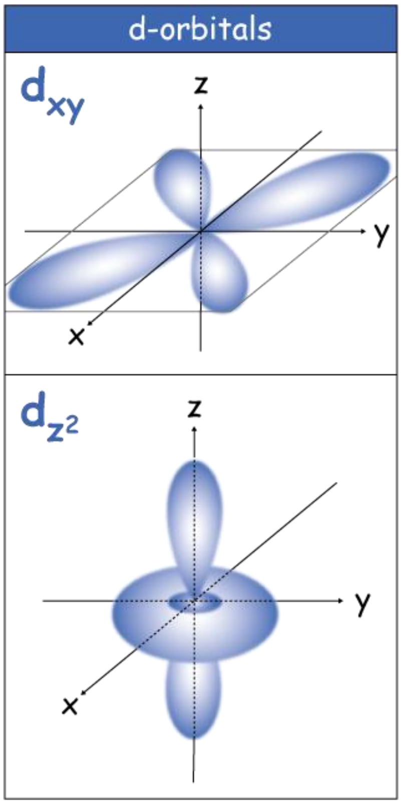
Each sub-orbital of a d-orbital can hold two spin-paired electrons, for a total of ten electrons in any d-orbital.

The table below summarizes the possible values of each of the quantum numbers.



Quantum number	Name	What it labels	Possible values	Notes
n	principal	electron energy level or shell number	1, 2, 3, ...	Except for d-orbitals, the shell number matches the row of the periodic table.
ℓ	azimuthal	orbital type: s, p, d, f	0, 1, 2, ..., n-1	0 = s orbital 1 = p orbital 2 = d orbital 3 = f orbital
m_ℓ	magnetic	orbital sub-type	integers between and including $-\ell$ and $+\ell$: $-\ell, -\ell+1, \ldots \ell-1, \ell$	$\ell = 0$ (s): 2 e^- in one orbital $\ell = 1$ (p): 2 e^- in each of three sub orbitals (p_x, p_y, p_z) $\ell = 2$ (d): 2 e^- in each of 5 sub orbitals (d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$, d_{z^2})
m_s	spin	electron spin	$\pm \frac{1}{2}$	Spins in any single sub-orbital must be paired.

Source: http://www.drcruzan.com/Chemistry_Electrons.html



What we've learned so far is that the mere presence of electrons in an atom (bound by attraction to the nucleus) creates a situation in which electrons behave like three-dimensional waves.

They interfere with one another in the way that waves do, and they occupy strangely-shaped regions of space modeled by functions called spherical harmonics. Which of these shapes (orbitals) the electron in an H-atom occupies depends on its total energy.

Source: http://www.drcruzan.com/Chemistry_Electrons.html