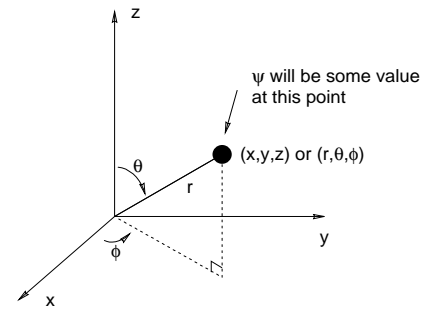The solution to the Schroedinger equation for the hydrogen atom (or other single-electron species with nuclear charge Z greater than 1) consists of two parts, a total energy, E_n, and a function Ψ_{nlm} (psi, pronounced "SIGH"):

ψ will be some value at this point
(x,y,z) or (r,θ,φ)

$$E_n = \left(\frac{-Z^2}{n^2}\right)\frac{(e_+^2)}{2a_o}$$

where

$$a_o = \frac{h^2}{4\pi^2 m_e(e_+^2)} = \text{the "Bohr" radius, } 0.53\times10^{-10}\ m$$

and

$$m_e = \text{the mass of the electron, } 0.00091\times10^{-27}\ kg$$
$$e_+ = \text{the basic unit of charge, } 1.6\times10^{-19}\ Coulombs$$

$$\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r) \times \Theta_{lm}(\theta) \times \Phi_m(\varphi) \qquad r\ \text{radial or "altitude", } \theta(theta)\ \text{latitude, and } \varphi(phi)\ \text{longitude}$$

$$R_{nl}(r) = (2Z/na_o)^{3/2}\left(\frac{(n-l-1)!(n+l)!}{2n}\right)^{1/2}(2Zr/na_o)^l e^{-Zr/na_o}\sum_{j=0}^{n-l-1}\frac{(-2Zr/na_o)^j}{j!(n-l-j-1)!(2l+j+1)!}$$

$$\Theta_{lm}(\theta) = 2^{-l-1/2}l![(2l+1)(l-|m|)!(l+|m|)!]^{1/2}|\sin^{|m|}\theta|\sum_{j=|m|}^{l}(-1)^{l-j}\frac{(1+\cos\theta)^{j-|m|}(1-\cos\theta)^{l-j}}{j!(l+|m|-j)!(l-j)!(j-|m|)!}$$

$$\Phi_m(\varphi) = (2\pi)^{-1/2}(\cos m\varphi + i\sin m\varphi)$$

Note that there is actually a whole set of "correct" solutions to the Schroedinger equation. To get any solution, replace n, l, and m with "reasonable" integers and Z with the nuclear charge. For example, setting the parameters $n = 1$, $l = 0$, and $m = 0$, we get for the hydrogen atom ($Z=1$):

"altitude" part	latitude part	longitude part

$$R_{10}(r) = \frac{2}{a_o^{3/2}}e^{-r/a_o} \qquad \Theta_{00}(\theta) = \frac{1}{\sqrt{2}} \qquad \Phi_0(\varphi) = \frac{1}{\sqrt{2\pi}}$$

and

$$\Psi_{100} = \left(\frac{1}{\pi a_o^3}\right)^{1/2}e^{-r/a_o} \qquad E_1 = \frac{-(e_+)^2}{2a_o} = -2.17\times10^{-18}\ Joules$$

Origin of the rules for *n*, *l*, and *m*. If you look carefully, the "rules" we learn for *n*, *l*, and *m* are present in the solution. Look for places, for example, where *n* is in the denominator, as $1/n$. How does that restrict the possible values for *n*? Similarly, there are several factorials in this equation, such as $(n + l)!$. That means the product of all the integers from 1 to $n+l$. For example, $5! = 120$.

$$5! = 1 \times 2 \times 3 \times 4 \times 5 = 120$$

Factorials can only be taken of nonnegative integers. (0! is defined to be 1, but "–1!" is meaningless.) The presence of certain factorial terms in the solution of the Schroedinger equation places strict restraints on the values of *n*, *l*, and *m*. (Can you find those terms?)

Degenerate states and hybridized orbitals. In addition, notice that the only quantum number that appears in the energy formula is *n*. That means that states with the same *n* but different *l* and/or *m* all have the same energy. They are *degenerate*. In fact, for any value of *n* there are n^2 degenerate states. For example, when $n = 2$ there are 4 states, commonly referred to as 2*s*, 2*px*, 2*py*, and 2*pz*. (For $n = 3$ what are the common names for the orbitals?) Any linear combination of degenerate states is still a solution of the equation. For example, $2s + 2px$ or $2s − 2px$ are perfectly fine solutions to the equation. They are sometimes referred to as *hybrid states* or *hybridized orbitals*.

Orbital size and *Z/n*. Whenever *r* appears in the radial part of the wave equation, it appears in the form "*Zr/n*." Thus, "*Z/n*" is a *scaling* term that changes the size of the orbital. When Z is large, that is, when there is a strong nuclear charge, the orbital is "shrunk" by a factor of Z. For example, for Li^{+2}, where $Z = 3$, the 1*s* orbital is exactly the same as the 1*s* orbital for hydrogen, but 1/3 the size. In contrast, when *n* increases, the orbital becomes larger. Thus, a 2*s* orbital is about twice the size of a 1*s* orbital. (In as much as one can refer to the "size" of an orbital, seeing as orbitals extend an infinite distance from the nucleus.)

Orbital type and the quantum number *l*. To a large extent, it is the quantum number *l* that determines the type, or overall shape, of an orbital. This is because the theta part of the wave function involves factors involving cosine theta taken to powers of *l*. For example, when $l = 0$, we have a spherically symmetric orbital (*s*). When $l = 1$, we have a *p* orbital. (So what do we have when *l* equals 2 or *l* equals 3?)

Imaginary solutions. The quantum number *m* only appears in the "longitude" term, where it can be thought of as setting the direction or orientation of the orbital. Notice that in that term there is the imaginary number *i*, the square root of minus one. This part of the solution poses a distinct problem. When $m = 0$ this term disappears, but when *m* is nonzero, in order to show "real" solutions, pairs of imaginary solutions have to be combined together. For example, what are commonly called the *px* and *py* orbitals are actually linear combinations of $m = 1$ and $m = -1$ when $l = 1$.

$$\Phi_1(\varphi) = (2\pi)^{-1/2}(\cos\varphi + i\sin\varphi)$$

$$\Phi_{-1}(\varphi) = (2\pi)^{-1/2}[\cos(-\varphi) + i\sin(-\varphi)]$$
$$= (2\pi)^{-1/2}(\cos\varphi - i\sin\varphi)$$

$$\Phi_{p_x}(\varphi) = \frac{1}{2}[\Phi_1(\varphi) + \Phi_{-1}(\varphi)] = (2\pi)^{-1/2}\cos\varphi$$

$$\Phi_{p_y}(\varphi) = \frac{1}{2}[\Phi_1(\varphi) - \Phi_{-1}(\varphi)] = (2\pi)^{-1/2}\sin\varphi$$

This is acceptable, because any two degenerate states can be combined to give a perfectly reasonable solution to the overall equation. (What do you suppose the combinations for $m = 2$ and $m = -2$ look like? What do we commonly call those orbitals?)

Radial and angular nodes. If you look closely at three-dimensional depictions of orbitals, you will find that there are two-dimensional surfaces—specifically spheres, planes, and cones—where there is absolutely no probability of finding the electron. These surfaces are called *nodes*. The radial part of the wave function ends up being an equation involving sums and differences of r taken to various powers. Equations of this type have *roots*—values for r for which the value is zero. These roots result in spherical nodes.
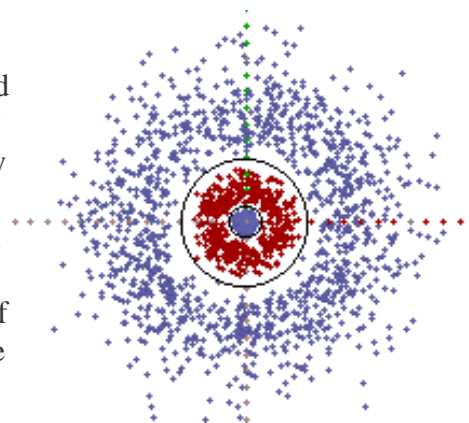

two spherical nodes ($n=3, l=2, m=0$)

The two angular parts of the wave equation (involving θ and φ) also produce nodes. Here the nodes appear due to the presence of sines and cosines in the equation. These functions go to zero at regular intervals, such as every 180° for $\sin(x)$ and $\cos(x)$, or every 90° for $\sin(2x)$ and $\cos(2x)$. These nodes can take the shape of cones or planes, depending upon the values of m and l.
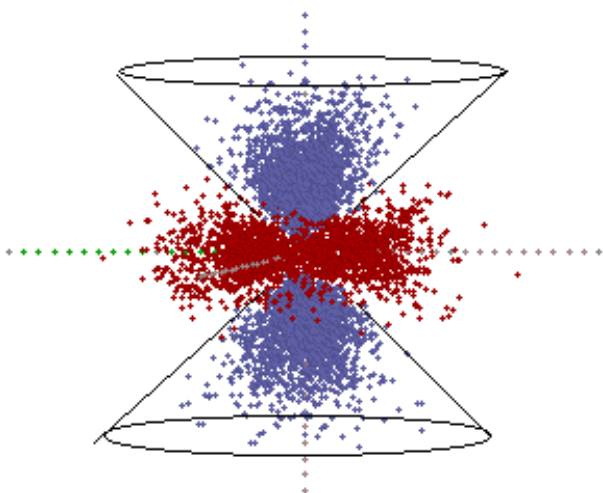
two conical nodes ($n=3, l=2, m=0$)
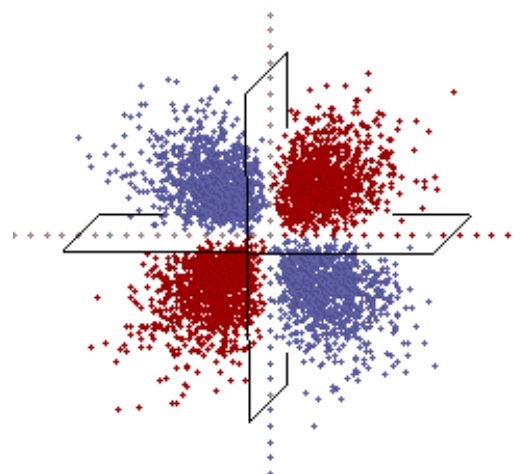
two planar nodes ($n=3, l=2, m=\pm1$)

The exact number of radial nodes and angular nodes for an orbital can be determined just from knowing the values of n and l. (The exact relationships are left as an exercise for the reader. See if you can figure it out based on what you know about the orbitals with n equal to 1, 2, and 3. How many radial nodes and how many angular nodes should there be for an orbital with quantum numbers $n = 5$ and $l = 3$—that is, a 5f orbital?)

It might seem odd at first that there be a surface where there is no possibility of finding the electron. However, it is also true that there is no possibility of finding the electron on *any* surface, node or otherwise. This is because the probability of an electron being "found" can only be determined for *volumes*, not surfaces. (Integration over all three dimensions is required to obtain a value for probability.) Thus, the fact that Ψ is zero on a surface need not be a concern. In any real volume the electron always has *some* probability of being found.