

Lecture 3: Electrons in Atoms

Discovery of electron

In 1897, when the first experimental evidence for the internal structure of atoms was discovered when the British physicist J. J. Thomson was investigating “cathode rays,” the rays that are emitted when a high potential difference (a high voltage) is applied between two metal electrodes in an evacuated glass tube. Thomson showed that cathode rays are streams of negatively charged particles coming from inside the atoms that made up the negatively charged electrode, the cathode. Thomson found that the charged particles, which came to be called electrons, were the same regardless of the metal he used for the cathode. He concluded that they are part of the makeup of all atoms. Thomson was able to measure the value of e/m_e , the ratio of the magnitude of the electron’s charge e to its mass m . Mulliken later determined charge (oil drop experiment).

Rutherford experiment

Although electrons have a negative charge, an atom has zero charge. Therefore, an atom must contain enough positive charge to cancel the negative charge. But where was the positive charge? Thomson suggested a model of an atom as a blob of a positively charged, jellylike material, with the electrons suspended in it like raisins in pudding. However, this model was overthrown in 1908 by another experimental observation. Ernest Rutherford knew that some elements, including radon, emit streams of positively charged particles, which he called particles (alpha particles). He asked two of his students, Hans Geiger and Ernest Marsden, to shoot particles toward a piece of platinum foil only a few atoms thick. If atoms were indeed like blobs of positively charged jelly, then all the particles would easily pass through the diffuse positive charge of the foil, with only occasional slight deflections in their paths. Geiger and Marsden’s observations astonished everyone. Although almost all the particles did pass through and were deflected only very slightly, about 1 in 20 000 was deflected through more than 90°, and a few particles bounced straight back in the direction from which they had come. “It was almost as incredible,” said Rutherford, “as if you had fired a 15-inch shell at a piece of tissue paper and it had come back and hit you.”

Planetary model fails

It failed since accelerating electron in a curved orbit will continuously emit radiation- classical EM theory. Hence the electron would immediately collapse into the nucleus.

Photoelectric effect

Electrons emitted from a metal surface upon irradiation above a certain frequency. The kinetic energy increases with frequency above the threshold frequency. This is contrary to what is known in classical physics.

Classical physics predicted that kinetic energy would not change with the frequency of light. Nothing in classical physics connected frequency to energy. In addition, it predicted that KE should be dependent on the Intensity of light. The observation was the KE of electrons had nothing to do with the intensity of light. It was a real conundrum.

The KE vs frequency plot for different metals were same and found to be equal to Planks constant.

Just a few years earlier, Max Plank was interested in the origin of black body radiation.

Black Body Radiation

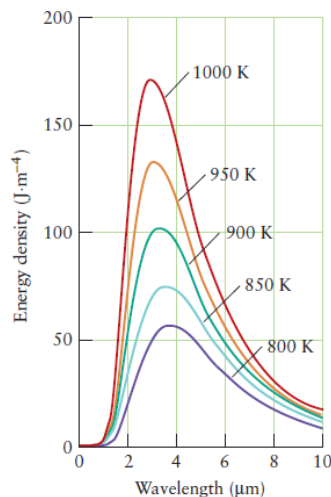


FIGURE 1.12 The intensity of radiation emitted by a heated black body as a function of wavelength. As the temperature increases, the total energy emitted (the area under the curve) increases sharply, and the maximum intensity of emission moves to shorter wavelengths.

For nineteenth-century scientists, the obvious way to account for the laws of black-body radiation was to use classical physics, the theory of motion devised by Newton two centuries previously, to derive its characteristics. However, much to their dismay, they found that the characteristics they deduced did not match their observations. Worst of all was the ultraviolet catastrophe: classical physics predicted that any hot body should emit intense ultraviolet radiation and even x-rays and γ-rays! According to classical physics, a hot object would devastate the countryside with high-frequency radiation. Even a human body at 37 °C would glow in the dark. There would, in fact, be no darkness.

Plank's hypothesis

Plank proposed that in these materials there must be oscillators which must be giving off radiation and this radiation was being emitted in quanta or chunks. Using this idea and some statistical mechanics he was able to calculate the shapes of these curves. He got the shape correct but to get the intensity correct he had to use scaling factors in front of the frequency of his oscillators and that is what we know as the Planck's constant.

Einstein's hypothesis of the PE effect

Einstein was amazed that the same number comes in the slope of graph of KE vs photoelectric effect. He then put this into the equation: $E = h\nu - h\nu_0$. Since ν is the energy of the incident radiation, $h\nu$ is the energy of the incident radiation. That is how $E = h\nu$ comes up- from photoelectric effect.

In classical EM there is no relation between Energy and frequency. You can have any frequency but the energy comes quantized because of the factor h . Later it was called the energy of photon.

For PE effect, you have to get a packet of energy or a quantum of energy i.e. sort of a particle. The first evidence of particle nature of light. Einstein went on to show a more convincing example for the particle like nature of radiation....he showed that a particle has momentum. Even though a photon doesn't have mass- rest mass as the physicists would say. Momentum $p = mv$. What Einstein showed from the relativistic equation of motions, that a photon having frequency γ has a momentum

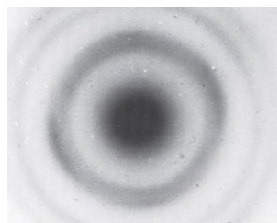
$p = h \nu / c$. Since $\lambda = c / \nu$, we can write: $p = h / \lambda$. That is the photon momentum. The Compton experiment demonstrated that photon had momentum.

How does the light behave during experimental conditions- as a wave or as a particle? There is no contradiction- it is the fundamental property of radiation.

Lecture 4: Matter as waves

Davison and Grammer experiment

The wavelike character of electrons was confirmed by showing that they could be diffracted. The experiment was first performed in 1925 by two American scientists, Clinton Davisson and Lester Germer, who directed a beam of fast electrons at a single crystal of nickel. The regular array of atoms in the crystal, with centers separated by 250 pm, acts as a grid that diffracts waves; and a diffraction pattern was observed. Since then, heavier particles, such as molecules, have also been shown to undergo diffraction, and there is no doubt that particles have a wavelike character. Indeed, electron diffraction is now an important technique for determining the structures of molecules and exploring the structures of solid surfaces.



What about your and mine wave-length. The wavelength of cricket ball – it is 10^{-34} m. The size of a nucleus- 10^{-14} m. Hence this will not have any consequence in our macroscopic world. Because to see any effects from this small wave-length, we need to have two nickel atoms or slits as small as these.

Uncertainty Principle

The discovery of wave–particle duality not only changed our understanding of electromagnetic radiation and matter, it also swept away the foundations of classical physics. In classical mechanics, a particle has a definite trajectory, or path on which location and linear momentum are specified at each instant. Think of the trajectory of a ball: in principle, we can state its location and momentum at every moment of its flight. However, we cannot specify the precise location of a particle if it behaves like a wave: think of a wave in a guitar string, which is spread out all along the string, not localized at a precise point. A particle with a precise linear momentum has a precise wavelength; but, because it is meaningless to speak of the location of a wave, it follows that we cannot specify the location of a particle that has a precise linear momentum. The wave–particle duality of matter means that the electron in a hydrogen atom cannot be described as orbiting the nucleus with a definite trajectory.

The popular picture of an electron in orbit around the nucleus is just plain wrong! The difficulty will not go away. Wave–particle duality denies the possibility of specifying the location if the linear momentum is known, and so we cannot specify the trajectory of any particles exactly. The uncertainty is negligible for heavy particles, but for subatomic particles it can be huge. Thus, if we know that a subatomic particle is *here* at one instant, we can say nothing about where it will be an instant later! The impossibility of knowing the precise position if the linear momentum is known precisely is an aspect of the complementarity of location and momentum— if one property is known the other cannot be known simultaneously. The Heisenberg uncertainty principle, which was formulated by the German scientist Werner Heisenberg in 1927, expresses this complementarity quantitatively. It states that, if the location of a particle is known to within an uncertainty x , then the linear momentum, p , parallel to the x -axis can be known simultaneously only to within an uncertainty p , where

$$\begin{array}{c} \text{Uncertainty in} \\ \text{momentum} \end{array} \quad \overline{\Delta p} \quad \times \quad \begin{array}{c} \text{uncertainty in} \\ \text{position} \end{array} \quad \overline{\Delta x} \quad \geq \frac{1}{2} \hbar \quad (8)^*$$

The symbol \hbar , which is read “h bar,” means $h/2\pi$, a useful combination that is found widely in quantum mechanics.

The uncertainty principle has negligible practical consequences for macroscopic objects, but it is of profound importance for very precise measurements dealing with subatomic particles, such as the locations and momenta of electrons in atoms, and the interpretation of their properties.

Lecture 5

Schrodinger Equation

This led to realizations that we need to treat electrons as waves. Electron in an atom cannot be treated as a particle- maybe we have to treat its wave-like properties. That led Schrodinger to write down an equation of motion of waves...

If a particle has a wavelength in the size of its environment, maybe the wavelength has an effect.

An equation of motion for matter waves: $H\psi = E\psi$

Schrodinger Equation

Schrodinger assumed that maybe he needed to treat the electron was a wavemaybe the electron in the H-atom can not be treated as a particle but as wave.....electron has a de Broglie wavelength in the order of size of its environment and maybe in these cases the electron needs to be treated as a wave...not a particle using classical mechanics

The reason we do not pay order to our wavelengths is that it is in the order of 10^{-30}m , which is much larger than the size of the environment

He wrote an equation of motion for waves: $H\psi=E\psi$, ψ is a wave...it is going to be called a wave function, the electron is going to be treated as a wave function.....The energy E here is the binding energy of the electron in the atom. The "H" is called the Hamiltonian operator....that operator is specific to a particular problem....we will look at the Hamiltonian operator for a H-atom.....this operator is operating on ψ and giving back the same function times the binding energy. How did he derive this equation?

What he did was to just guess at a wave function....he would say let us guess this wave function:

$$\psi(x) = 2^{-a} \cos\left(\frac{2\pi x}{\lambda}\right)$$

He needs to know how ψ changes with x , in an equation of motion if we want to know how ψ changes with x , would just take the derivative:

Rate of change of ψ with x :

$$\frac{d\psi(x)}{dx} = -2a \left(\frac{2\pi}{\lambda}\right) \sin\left(\frac{2\pi x}{\lambda}\right)$$
$$\frac{d^2\psi(x)}{dx^2} = -2a \left(\frac{4\pi^2}{\lambda^2}\right) \underbrace{\cos\left(\frac{2\pi x}{\lambda}\right)}_{\psi(x)}$$
$$\frac{d^2\psi(x)}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x) \Rightarrow \text{derive. Schrodinger equation}$$

This is a classical wave equation....have just taken derivative....there is nothing quantum mechanical about it. Here comes the big leap Schrodinger made:

He substituted for λ , the momentum p for the particle....since it is a matter wave....he could do it since de Broglie taught him how to do that. De Broglie said:

$$\lambda = \frac{h}{p}$$

$$\text{Then } \Rightarrow \frac{d^2 \psi(x)}{dx^2} = -\frac{p^2}{\hbar^2} \psi(x) \quad \hbar = \frac{h}{2\pi}$$

We have an equation of motion of a matter wave....we have an equation which tells how the $\psi(x)$ changes with x and I have the momentum of the particle buried in here.....

$$E = K + U = \frac{p^2}{2m} + U(x)$$

$$p^2 = 2m[E - U(x)]$$

$$\frac{d^2 \psi(x)}{dx^2} = -\frac{2m}{\hbar^2} [E - U(x)] \psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x) \psi(x) = E \psi(x)$$

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \psi(x) = E \psi(x)$$

H

$$\hat{H} \psi(x) = E \psi(x)$$

The Hamiltonian is a combination of kinetic energy operator and a potential energy operator....the key is the substitution of a de Broglie equation into an ordinary wave equation...

Schrodinger's equation is to quantum mechanics what Newton's equation is to classical mechanics.....Newton's equation will not work on something whose wavelength is the size of its environment....Classical mechanics is a subset of quantum mechanics...it is embedded in it...

For H-atom, we have to think of wave function in 3-D....typically we would use x, y, zbut this problem is much more solvable if we use spherical co-ordinates....instead of x, y , and zwe will

replace with R , θ and ϕ . Set up H for H-atom using spherical coordinates.... in 3-D we would have a partial differential equation which has a double derivative with respect to x , y and zmakes the problem unsolvable. But when we move it to the spherical coordinates...this can be solved

Spherical coordinates: Like latitude and longitude. θ ranges from 0 to π while ϕ ranges from 0 to 2π .

Solving the Schrodinger equation means calculate these E 's, i.e. the binding constants of the electron to the nucleus, called the Eigen Value ...the other thing we are going to solve for is ψ , that is the actual form of the wave function...that we can get out of solving the diff eq. The functional form will be complicated.....but we will look at them later. Those wave functions are what you have studied in school- they are the orbitals: s, p, d and f. They come from solving the Schrodinger equation. They are what is known as the spatial part of the wave function....there is also what is known as the spin part of the wave function....we are going to use orbitals and wave function sort of interchangeably.

The Schrodinger equation solution is going to show that the H-atom is stable....this is in contrast to classical ideas.

$$E = -\frac{1}{n^2} \left[\frac{me^4}{8\epsilon_0^2 h^2} \right] \Rightarrow R_H \text{ Rydberg constant}$$

$$R_H = 2.17987 \times 10^{-18} \text{ J}$$

$$E = -\frac{R_H}{n^2}$$

n = principal quantum no.
 allowed values $\Rightarrow n = 1, 2, 3, \dots \infty$

Allowed energies in H atom are quantized written in terms of quantum numbers

These values tell us the energies the electron is supposed to have when it is bound to the hydrogen nucleus. When $n=1$, binding energy is $-R_H$. When $n=2$, binding energy is $1/4^{\text{th}}$ of $-R_H$binding energy decreases as n increases. When $n=\text{infinity}$, the electron and nucleus are not bound to each other. The energies are discrete....they are quantized. This means only certain specific values are allowed...for example, values between $-E$ and $-E/4$ are not allowed. How did this quantization come from- by solving the Schrodinger equation. When you solve diff eq to solve a physical problem, in order to make it specific for the physical problem you include boundary conditions, here the allowed values of θ and ϕ .

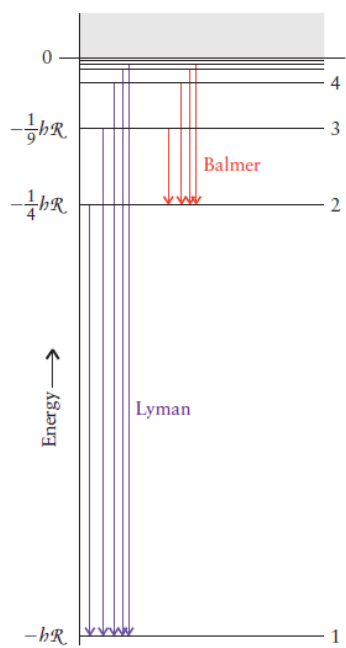
Significance of binding energies: When electron is bound to the nucleus with energy $-R_H$, we say that the Hydrogen atom is in the $n=1$ state, the ground state. It is the lowest energy state- the electron is most strongly bound. The physical significance is that the binding energy is (-) ionization energy. The $n=1$ is the first excited state, consequently the ionization energy from the less excited state is less.

The Schrodinger equation solution also predicts energy levels of all 1 electron atoms such as He^+ .

The energy is predicted by:

$$E = -\frac{Z^2 R_H}{n^2} \Rightarrow Z e = \text{charge of nucleus}$$

$Z e \times e \Rightarrow \text{Coulomb interaction}$



$$\Delta E = -R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Lecture 6

N principal quantum number: 1,2,3 up to ∞

Ψ in general is a function of r, θ, ϕ and t denoted as $\Psi(r, \theta, \phi, t)$. We will look at wave functions which are called stationary waves, i.e. Ψ which are not dependent on t . This means we will not look at a wave function when a chemical reaction is happening, it will be before and after. In those cases we are looking at Ψ when the atom is stable and sitting idle. The Ψ we will look at will be $\Psi(r, \theta, \phi)$ also known as time-independent QM. When we go and solve Schrodinger equation for $\Psi(r, \theta, \phi)$, two more quantum numbers drop out in the differential equation.

We get a new quantum number l , called the angular momentum quantum number because it dictates how much angular momentum the electron has. It also has allowed values. They are 0, 1, 2, ..., $(n-1)$. Why should it be smaller than n . Classically thinking l would denote the angular momentum.

The third quantum number which drops out is m , called the magnetic quantum number, since it dictates how an atom moves in a magnetic field. But more precisely what m is the z -component of the angular momentum l . The allowed values of m are $m=0, +1, +2, \dots, +l$. The largest value is l . Since it is a z component it also has direction, so m can be $-1, -2, \dots, -l$.

For $n=1, l=0, m=0$called 100 state and if we have an electron in the 100 state we are going to describe the electron by a wave function ψ_{100} .

For $n=2, l=0, m=0$: the wave function is ψ_{200} . The other wave functions possible for $n=2$ are ψ_{210}, ψ_{211} and ψ_{21-1} . All these four states have the same energy i.e. $-R_H/4$. They are what we call degenerate.

The other way of representing the wave function is an orbital...the orbital is actually the wave-function. If $l=0$, we call it s . For $l=1$, we call it p . If $l=2$, we call it d . So all ψ_{210}, ψ_{211} and ψ_{21-1} would be called $2p$.

When $l=1, m=0$, we call it p_z . When $m=1$, it is p_x and when $m=-1$ it is p_y . This is not fully correct because the Schrodinger equation solution of ψ_{211} and ψ_{21-1} are complex wave functions. For us to think about p_x and p_y wave functions, we take a linear combination. p_x is $\psi_{211} + \psi_{21-1}$ while p_y is $\psi_{211} - \psi_{21-1}$ - this gives you real functions.

For $n=1$, only one state. In $n=2$, four degenerate states. For $n=3$, 9 states.

For $l=2, m=-2$ is $3d_{xy}$, $m=-1$ is d_{yz} , $m=0$ is d_{z^2} , $m=1$ is d_{xz} , $m=2$ is $d_{x^2-y^2}$.

For $m=-2, -1, +1$ and $+2$, those wave functions when we solve Schrodinger's equation are complex wave functions. Again we take linear combination to make them real. For $m=0$ the d_{z^2} is a real function.

Lecture 7

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For $m= -2, -1, +1$ and $+2$, those wave functions when we solve Schrodinger's equation are complex wave functions. Again we take linear combination make them real. For $m=0$ the d_{z^2} is a real function.

Shapes of the wave functions

What do these wave functions actually look like:

$$\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi)$$

TABLE 2.1 Hydrogenlike Wavefunctions* (Atomic Orbitals), $\psi = RY$

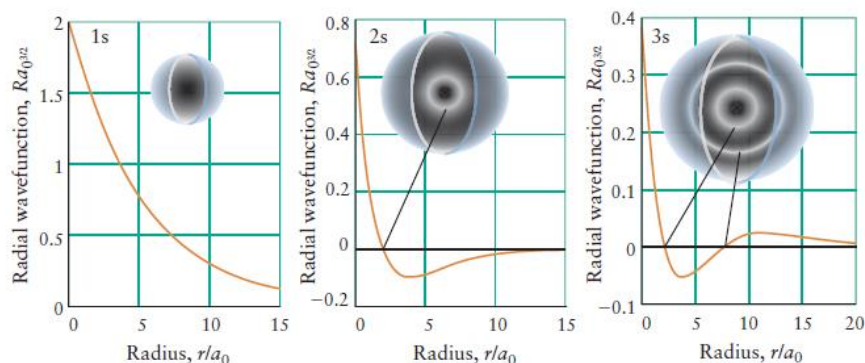
(a) Radial wavefunctions			(b) Angular wavefunctions		
n	l	$R_{nl}(r)$	l	" m_l " [†]	$Y_{lm_l}(\theta, \phi)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$	0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$	1	x	$\left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \cos \phi$
2	1	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$	1	y	$\left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \sin \phi$
3	0	$\frac{2}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2} \left(3 - \frac{2Zr}{a_0} + \frac{2Z^2r^2}{9a_0^2}\right) e^{-Zr/3a_0}$	1	z	$\left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$
3	1	$\frac{2}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/3a_0}$	2	xy	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \sin 2\phi$
3	2	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$	2	yz	$\left(\frac{15}{4\pi}\right)^{1/2} \cos \theta \sin \theta \sin \phi$
			2	zx	$\left(\frac{15}{4\pi}\right)^{1/2} \cos \theta \sin \theta \cos \phi$
			2	$x^2 - y^2$	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \cos 2\phi$
			2	z^2	$\left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$

*Note: In each case, $a_0 = e_0 h^2 / \pi m_e e^2$, or close to 52.9 pm; for hydrogen itself, $Z = 1$.

[†]In all cases except $m_l = 0$, the orbitals are sums and differences of orbitals with specific values of m_l .

The angular part of s wave function is not angle dependent.

Let us look at the radial part.....first let us observe the s orbital:

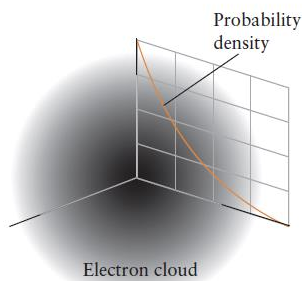


For 1s, the exponential drop is the result of the function having e^{-r/a_0} . The wave function at all values of r has a positive value. What about 2s wave function: the plot is shown above. We start at a large positive value and we get to a value of r where ψ becomes 0, that is a radial node. This radial node occurs at $r=2a_0$. The wavefunction gets more and more negative, starts increasing again and then approaches 0. At the radial node the wave function changes sign, the amplitude of the wave function becomes positive to negative. Sign of amplitude important because in a chemical reaction when two atoms come together and two electrons that are represented by are overlapping....if we bring them together.....they need to have the same sign of the amplitude for constructive interference- chemical bonding. Ψ_{300} has two nodes: at $1.9 a_0$ and $7.1 a_0$.

What does the wave function actually mean and how does it actually represent the electron....this was a very puzzling question....how does this represent where the particles are....the answer to this question is that there is no answer to this question. Wave function is just a mathematical function...a wave function is a wave function- you can not draw a correct analogy to the classical world. However, Max Born said that if I take the wave function and I square it, if I interpret that as a probability density then I can interpret all the predictions made in the Schrodinger equation within that framework.

$$[\Psi_{n\ell m}(r, \theta, \phi)]^2 = \text{probability density i.e. probability/unit volume}$$

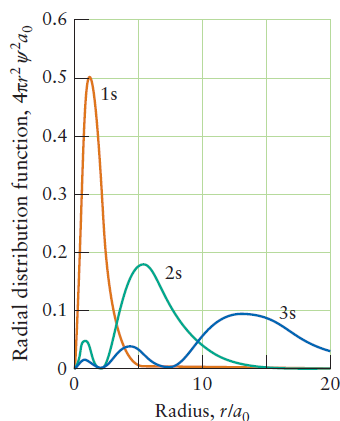
That really works. The interpretation agrees with our observations and hence we believe it to be correct. But it is just an assumption. It is just an interpretation....there is no derivation for it....it just works.

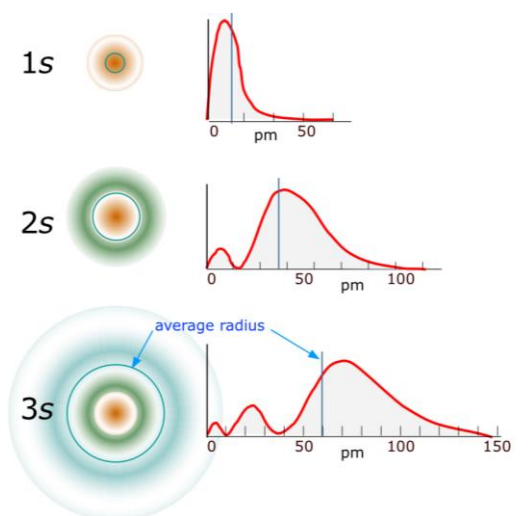


For 1s, probability of finding an electron per unit volume at some at some value of r , θ and ψ . It doesn't matter what θ and ψ is in this case as it is spherically symmetric. The 2s probability density is a maximum at the nucleus. It decays uniformly in all directions and it decays so much that at some point you have no probability density. It then increases again since it has changed sign.

We have talked about probability density but not probability yet. To determine probability, we are going to look at the radial probability distribution function. RPD is probability of finding an electron in a spherical shell. The spherical shell will be some distance away from the nucleus. The spherical radius r and a thickness dr . Then the RPD is the probability of an electron at a distance r with a thickness dr i.e. from a distance r to $r+dr$.

If we have to calculate probability (RPD), then we take the probability density (ψ^2) and then we can multiply by the unit volume that is $4\pi r^2 dr$. The result will be a probability.



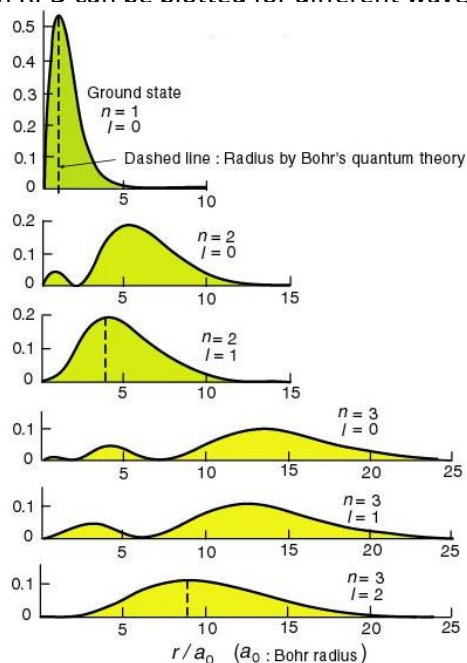


Radial probability distribution function $[4\pi r^2 R_{nl}^2(r)]$: For 1s, 2s and 3s, as r goes larger and larger, the value of the exponential function shoots up and the max value differs. For 2s, the second peak maxima has much more intensity. For 3s the third maxima has highest probability. As you from 1s to 2s to 3s the probability of finding the electron increases as you go slightly further away from the nucleus. For 1s the probability is much closer to the nucleus. The number of radial nodes increases as to go to higher quantum numbers. They are correlated by the equation:

$$\text{No of radial nodes} = n - l - 1$$

The closer it is to the nucleus the more tightly bound it is. So, the 1s is more tightly bound than 2s.

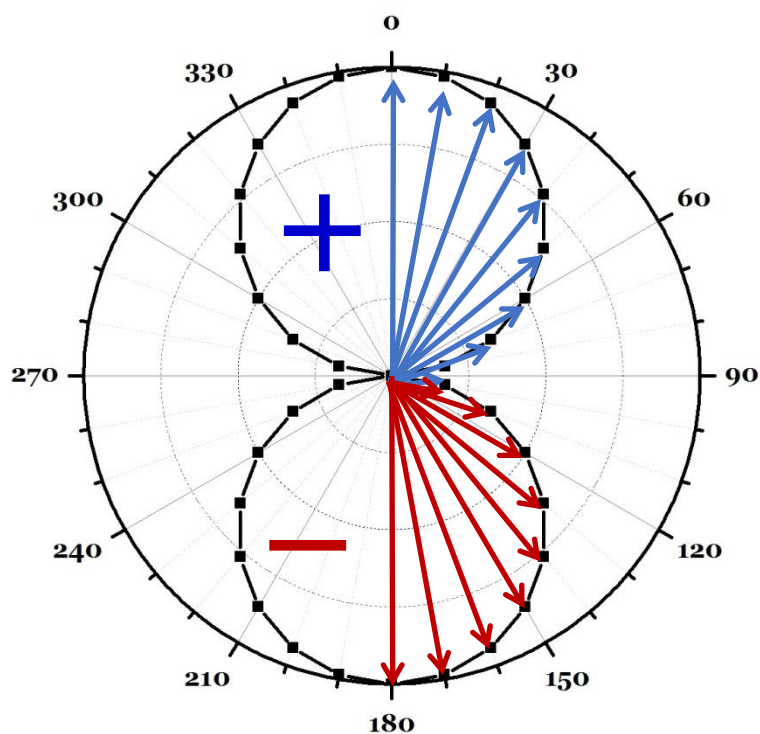
Such RPD can be plotted for different wave functions such as for 1s, 2s, 2p, 3s, 3p and 3d etc.



The most probable value of finding the electron will always be at the maxima of the RPD. For average radius, we need to integrate.

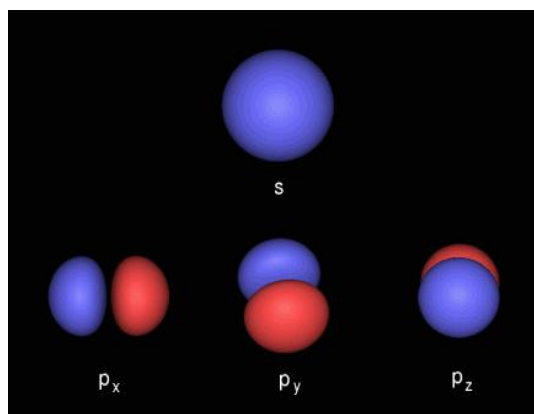
Now compare 2s and 2p. The most probable value of finding the electron for 2s is further away from the nucleus than 2p. However, for 2s there is a significant probability of finding the electron near the nucleus than 2p. In general average value of r gets smaller as l gets larger. These two facts which look contradictory are important, they dictate the behaviour of atoms.

For 2p_z, the wave function will change with r and θ , but not with ϕ . First let us look at the variation of $\cos \theta$ with θ . What we see here is a polar plot of the variation of $\cos \theta$ with θ .



The wave function changes direction (from +ve to -ve) as we go from 0 to π . The point where the wave function becomes 0 is called the node. This is called an angular node (different from radial node).

Then what really is an orbital?



We very familiar with the pictures depicted above. These are pictures we draw for our convenience. Orbitals have nothing to do with probability. Angular plots of $\psi(\theta, \phi)$ has no physical meaning – just mathematical functions - may be used to obtain information about probable electron distribution. But

can not be, in any way, regarded as the “picture” of an orbital. It is unfortunate that fuzzy drawings like these are often incorrectly represented as “orbitals”

However, ψ^2 might provide a better intuitive picture. However, you need to consider both the radial and angular part of the wave-function together and square of that wave function will give you sort of the most probable electron density.