# Quantum Chemistry of Atoms and Molecules

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## Lecture – 29
## 2s Orbital

I hope you are enjoying this picture drawing session we have shown you some beautiful pictures of 1s orbital already. Now in this module which is going to be a little short we are going to show you 3s as well but before that let us complete our discussion of 2s orbital. We have shown you what 2s orbital looks like already you get a node at r = 2a/Z and we have shown you how if we plot it in three dimensions, we can get a depiction like this. Please do not forget that this vertical axis is wave function.

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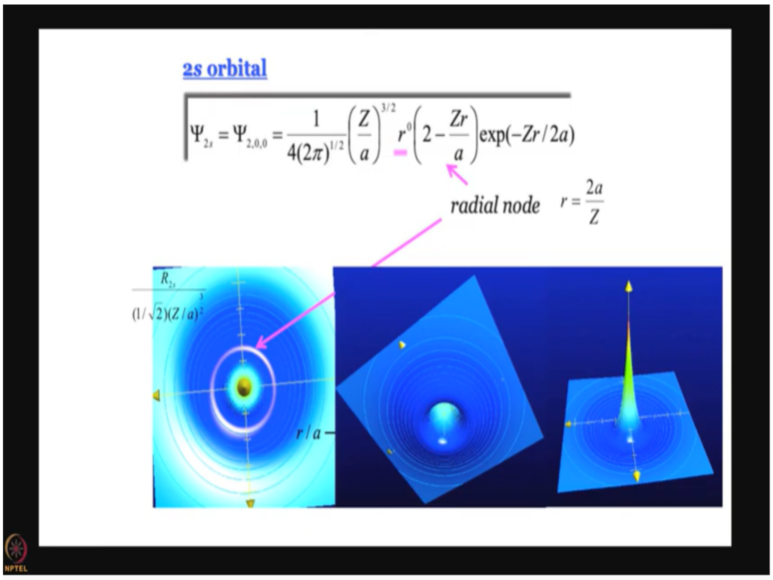


Nothing else wave function so from there you can generate this contour diagram and what you see in white here is really the radial node where r = 2a divided by Z and we also gave you this kind of a view if you look from the bottom you see these contours and you can see this big peak that is there inside. But there is only the orbital but I do not have on these slides but I have shown you in the previous module is that what happens when you consider size square.

And what happens well capital R square in this case one and the same and what happens when you multiply that capital R square by small r square and get the radial probability density. Okay now let us go back to this definition that we like to debunk so much that an orbital is a region of space where probability of finding the electron is maximum. Well the definition is there in so many places there must be something in it right so let me just modify it a little bit and say that an orbital can be used to determine the space the region of space where finding probability of finding the electron is maximum.

Let me say that once again an orbital can be used to define the region of space where probability of finding the electron with that wave function is maximum how do you do that? Well you have these curves right well you have psi psi star d tau if you integrate then what happens.

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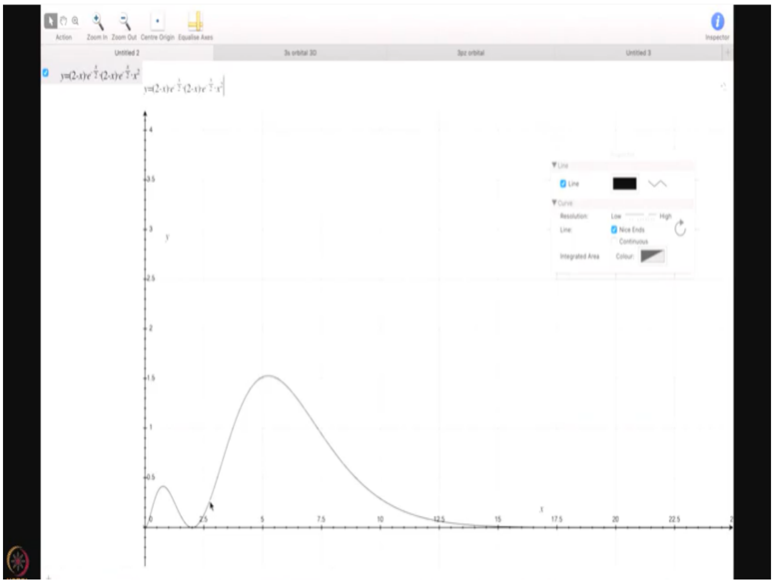

Let me take you back to that plot maybe we will work in one dimension well two dimensions say this one right this is a plural plot of r square capital R square for 2s against r okay we talked about radial probability distribution function. Suppose I want to know what is the total probability well I can say it without doing anything total probability is 1 but if I am to get total probability is equal to 1 then I have to integrate from 0 to infinity right.

That is not something that we want to do but one thing that comes out very nicely is if you just look at the numbers now remember x-axis is in terms of a0 for Z= 1 let us put Z =1 for now this is 2a0 actually it is 2a0/Z. So if you go up to infinity then probability of finding the electron is 1 suppose I do not go up to infinity maybe I will increase this a little bit right now it is up to 16 so let me make it up to 25 or something yeah.

So while it is true that this function goes on until infinity I hope that you will agree with me that it does not matter if I assume that if I work with the function up to a limit of say 15 angstrom because beyond 15 angstrom is very little so if I take area of this curve maybe 99.999% of it will be there until this 15 angstrom or so beyond that you have a very small amount of probability.

So even though the orbital goes up to infinity there is no need for us to work up to infinity it is enough if we go up to 15. Now let us think like this let us say I draw I take this radius of 15 angstroms this is going to 15 angstroms for hydrogen right well assuming Bohr radius to be 1 angstrom it is not exactly 1 angstrom so that factor will be there. So, let us say I go up to 15 angstroms somewhere here.

So, probability of finding the electron inside a sphere of that radius will be how much 99.999% if I draw that sphere then this surface of the sphere encompasses 99.999% probability of finding the electron that surface is called a constant probability surface. So, if I want to draw a 99.999% surface then perhaps, I have to take a radius of 15. Suppose I am okay with say 95% where will I have to truncate 95% will be somewhere here actually yeah maybe here.

So, let us say 11 angstroms if I draw a circle of 11 angstrom then that circle would contain 95% probability of occurrence of the electron right. So, this way we can draw surfaces and when we draw the surface we might as well draw another circle inside it because this circle of say radius 2 angstrom well 2a0 angstrom is going to be the nodal surface. The nodal surface here radial node is going to be a sphere right surface of a sphere.

So, you might as well draw that because there is no probability density of finding and the electron at that particular surface. So that is how we often designate probabilities and more often than not we mistake those plots to be orbitals they are not. Those are plots of probability of finding electrons in particular orbitals they are constructed using the orbitals okay. So, let us I hope that we will not have any further confusion in this matter anymore we have talked about constant probability surfaces.

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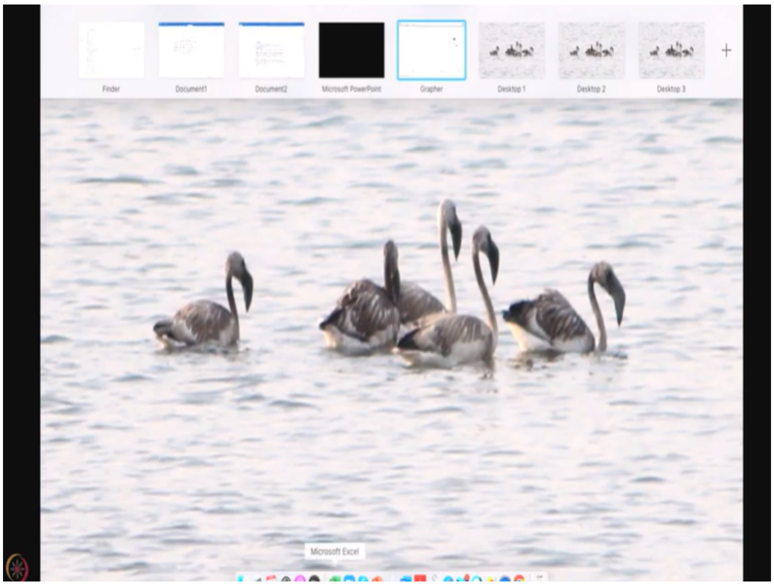

And let me show you some ways in which these probabilities can be determined. So, let us not think for a moment that probabilities are not important probabilities are all important. When we want to talk about things like bonding, we want to know what is the region where probability of finding the electron is more where what is the region where it is less right so we have to work it out.

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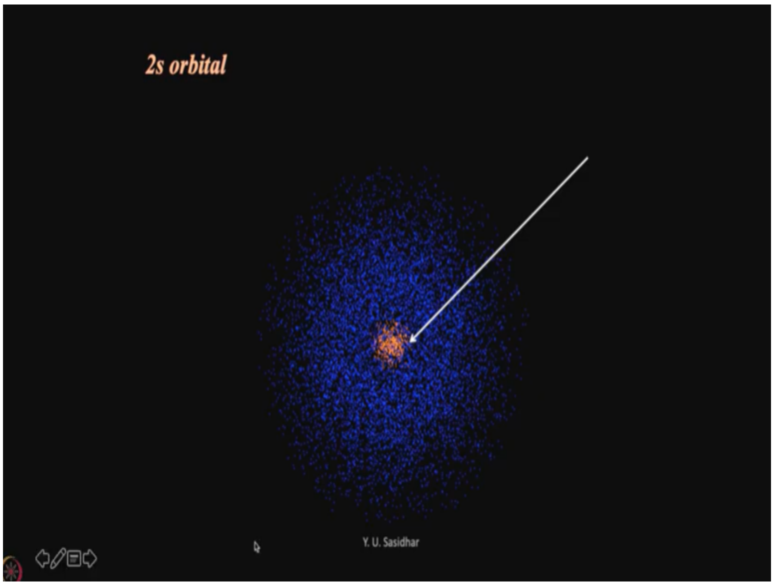


So how do you designate it well this fear this is how one can designate it. We use different colours okay you put dots more dots where probability is maximum. So as you see if you go out along a radius density of dots here is more as you go further out density of dots decreases and finally you there is hardly anything right so it is sort of like a galaxy lot of stars and then towards the fringe of a galaxy it fades out and then there is nothing okay something like that it does not mean that it is actually 0.

It is just that the density of dots is so few that you do not see it okay and inside you use dots of different colour to designate the sign is different sign of the wave function probability or probability density is always positive. So, sign of the wave function can also be conveniently shown in figures like this using coloured dots.

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Well another way in which you can show it is this kind of 3d dimensional Pac-man kind of figures where you show a section draw a solid figure with one particular colour inside whenever the sign changes draw another solid figure I like the this one is prettier but the previous one actually contains more information because it sort of tells you at what kind of radius you have the maximum probability of occurrence.

Okay this is a more qualitative definitely better looking depiction but please do not forget these are not orbitals these are using orbitals depictions of regions of space where probability of well it is a depiction of probability distribution of these 2s electrons okay they are not orbitals, orbitals have been used here and once again let me thank professor Sasidhar for having created these beautiful images almost 20 years ago.

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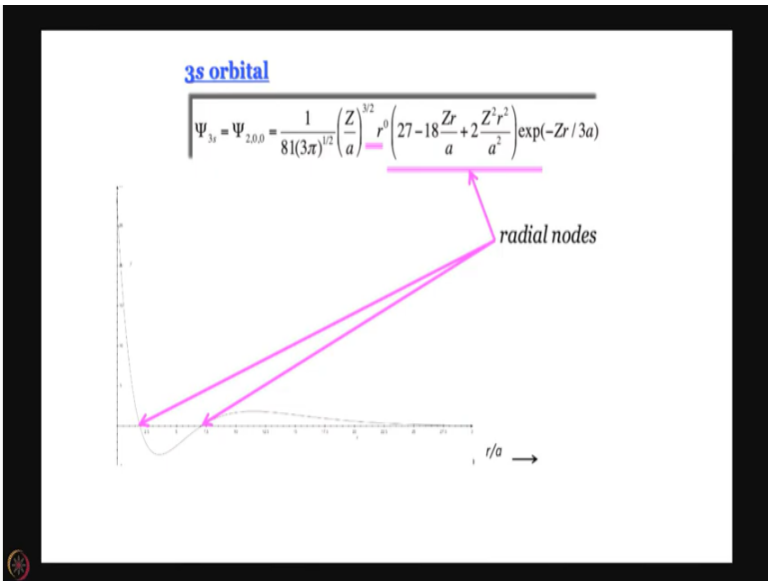


Okay now let us go to 3s orbital, 3s orbital as we know has a polynomial of second order. So yeah 3s orbital remember has in its expression a polynomial of second-order the three terms. So polynomial of second-order equated to 0 gives you two roots and you can work out what these roots are I think they are 1.9 and 9 if you just take Z to be 1 and a to be 1. So, it they occur in two different places in fact you see what the values are here okay if you have 2 radial nodes.

So when you start at r = 0 at the nucleus you can start with a positive value of the wave function it falls off to 0 that is a node changes sign then it has to rise again so there is a minimum point then there is another node rises again and falls off to 0 at well again asymptotically okay this is 3s orbital once again we see that the innermost part is most if I can say intense followed by the second part the third part seems to have the least height okay. Once again when you multiply by r square will take square of this multiplied by r square even though it is repetitive, I will just do it for you.

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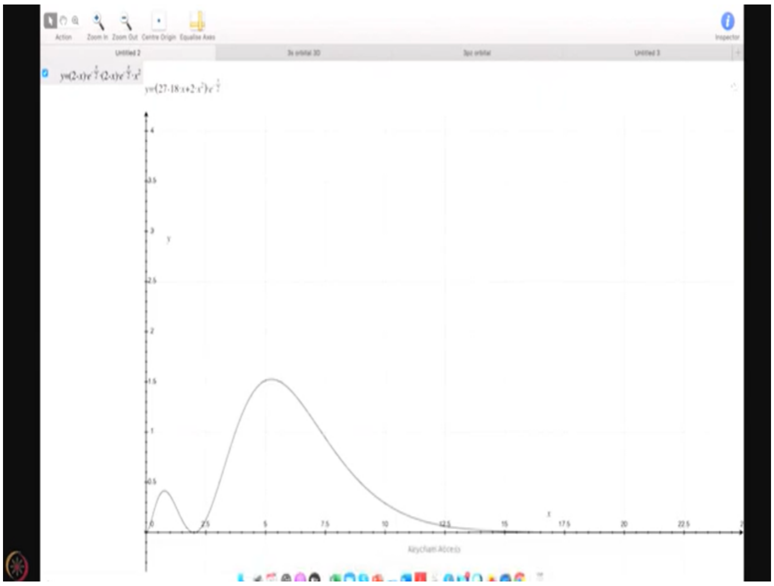

What was the expression 27 - 2x 18 + 2x I think please do not try to remember these expressions as you can see, I do not remember them myself there is no need yeah 27 - 18 x + 2x square that kind of an expression? So I can write 27 - 18 star 18 into x + 2x square okay that will get rid of everything else and while doing all this let us not forget that this factor is multiplied by an exponential term and I will take you back in case you have not noticed what the exponential term is the exponential term is e to the power – Zr/3a for our purpose will set Z to 1 a to 1 it will be Z divided by 3. Let us see.

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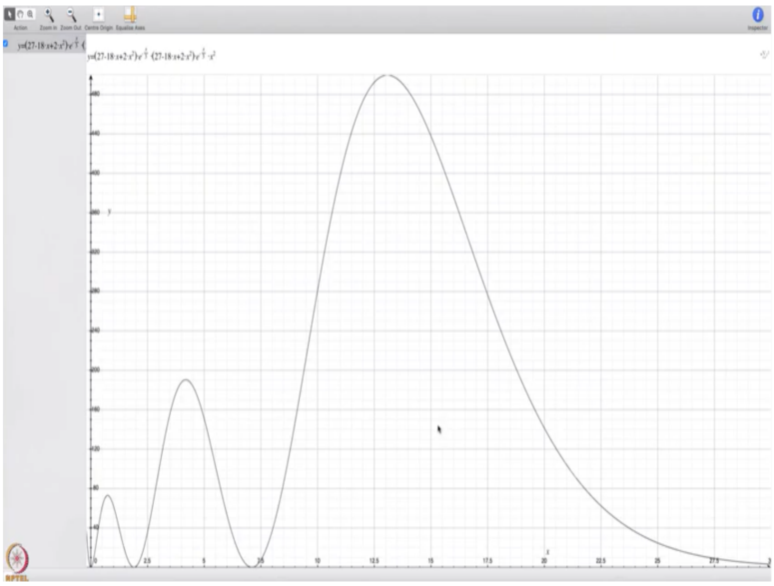

So we have seen the functional form for the 3s orbital so let me just put that in 27 - 18 into x remember x here is actually r what we have studied there and I am not using Z I have set Z to be 1 I am writing this in terms of a0 so a0 is also said to be 1 so all that is fine. So simply I get 27 – 18x + 2x square multiplied by e to the power – x/3 remember the exponential term earlier it was e to the power minus x/2 this time it is x/3.

And here it is this is your 3s orbital that seen some depiction already but here you have seen how it shows up when I key in the expression this is what I get so not very difficult to understand you have an exponential decay that is why at x= 0 we have a maximum and then you have a decay but then this decay is modulated by this factor by which it is multiplied which is a polynomial and since the polynomial is of second order it becomes equal to 0 for two values of x.

So here it is 0 here it is 0 and then x it becomes 0 asymptotically at r = infinity okay so this here is your 2d depiction of 3s orbital will show you the 3d depiction also before that let me do something. Let me take this whole thing multiplied by itself and multiply it by r square here x is r what am I doing here I am trying to plot the radial probability distribution function am I not so capital R square multiplied by small r square that is what we are doing.

So this is what we get e of course you have to zoom out and then we will fix it okay this is more like it well because you do not see anything here but we will just take care of that in a moment we started from - 0.2 went up to 30 so that is what will keep now y-axis we will have to see here actually we do not need anything in minus maybe I will keep - 1 or something and we have gone up to 500 here.

So let us make that 510 here you are see what happened remember what the original wave function was it had 3 portions that is right but at the centre nearest to the nucleus it had the maximum value of psi and then it decayed went to 0 cross 0 so that was an node then turned again cross once again and then went through another maximum did that once again finally went to 0.

So then these 3 parts that you had this part was a maximum most intense you can say followed by this followed by this I am going to show the wave function once again but the moment I multiplied by r square after squaring the wave function itself this outer lobe has become the major lobe. So, if you just look at the wave function this is this looks like the smallest part but the moment you take care of the volume element which is simply small r square in this case it blows up okay.

So, let me just show you once again I will take all this out now it is very simple we just have to change frame limits once or twice maybe go back to the original figure. That make that look a little better yeah see what I was saying the outer lobe is actually quite small if you just look at the wave function but we will let us see what happens when we take square of that. So even though the square of it this part has blown up followed by this and this is what it is even if we take high psi stars high psi well i square in this case or capital R square in this case what is it probability density.

So probability density is maximum near the nucleus and then it has like smaller regions as you go higher further out but the moment you multiply it by the volume element component of volume element small r square in this case the outer lobe which had least probability density at least in the maximal position that becomes the biggest one I wish I had better memory so that I would remember what the value was earlier maybe the same value after all.

Yeah see now this actually has greater probability so this is something that demonstrated very nicely the difference between probability density and probability even though probability density is minimum in this region because of the volume element probability is actually maximum okay this is the point that I perhaps have said earlier or perhaps I will say once again it is a very important point it is important to understand it is not just the density probability is also governed by the volume element that you are considering. Okay so this was in two dimensions let us now go over and show you the three-dimensional plot.

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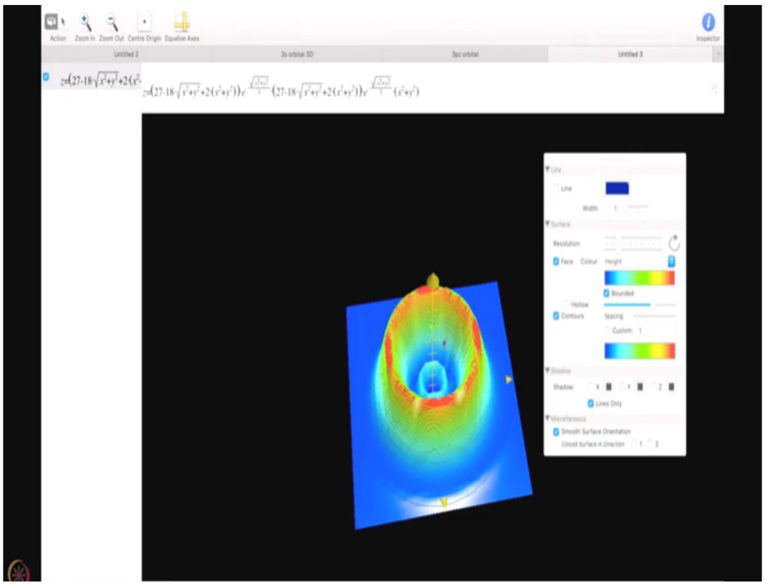

We will show you the three-dimensional picture okay this is your 3x for you and draw the frame limits it right from 30 same here this would be something like - 3 to 30 or so okay this is 3s orbital first look it might look exactly the same as 2s orbital but actually it is not you see we have this sharp part for small values of r then it goes through this first node and becomes negative and then goes to the second node and becomes positive.

Do you see this this is the second node becomes positive so this is your contour diagram this is the function so let us see that this orientation if you can see in three dimensions you can see this sharp and tall innermost portion followed by the negative basin followed by the positive small peak. So, let us see what happens when I take square of this and multiply it by your the volume element r square, square of this multiplied by r square would simply be x square + y square.

Yeah this is what it looks like so once again you can see the outermost lobe is the major lobe followed by a smaller one and you can hardly see the innermost one why is it that the trend has completely reversed because we multiplied by r square for some reason the 2d plot seems to be a problem but I think we have in any case showing you the result so we will come back to this one later.

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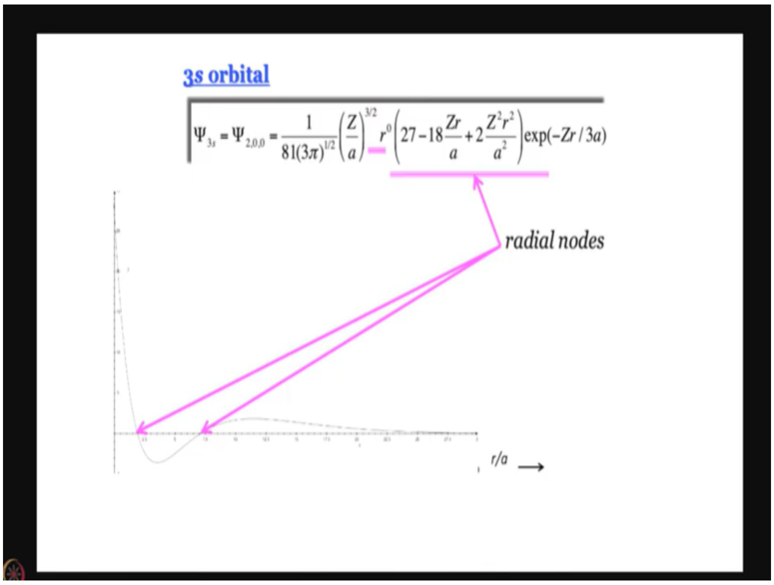


Okay so this is the plot that somehow, we could not plot in real time unfortunately something is wrong but you are familiar with this anyway and you have seen what it looks like in three dimensions.

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And from there one can construct this 3-dimensional probability plot of 3s orbital. Remember the colour denotes the sine of the wave function and the density of dots denotes the value of not the wave functions psi not its psi square but psi psi square multiplied by r square okay so this is how we often designate the orbitals but please remember these are not orbitals these are using orbitals we have worked out the regions the well the radial distribution of probability of 3s electrons.

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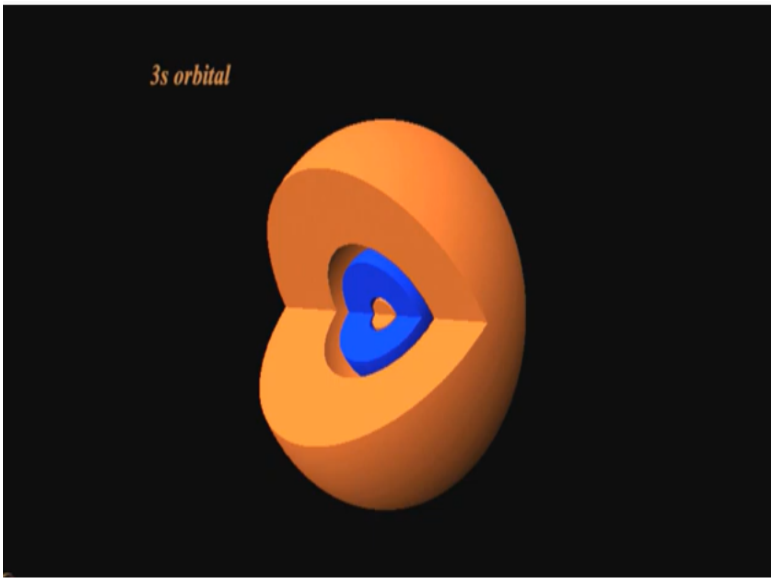


As usual you can draw it like this like professor Sasidhar had done.

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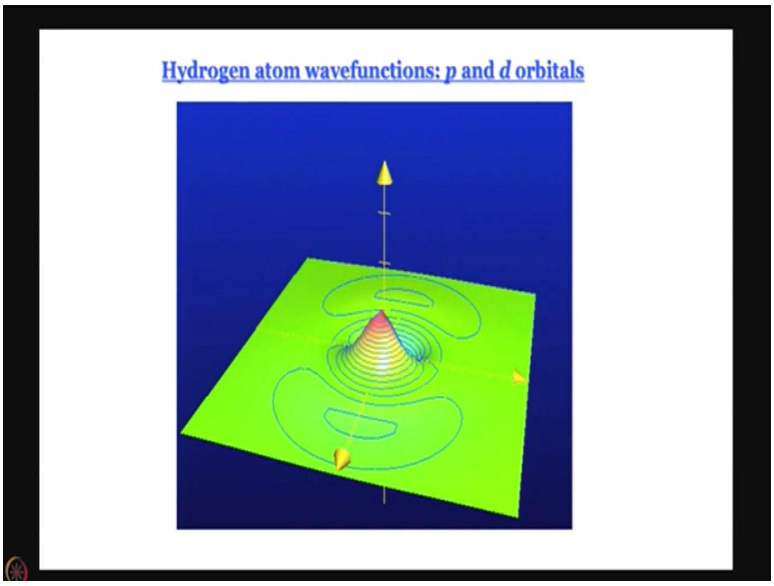


So, we have talked about 1s, 2s. 3s wave functions we have learned how to draw them in two dimensions and three dimensions remembering that one of the dimensions is always orbital we have also been able to plot for ourselves capital R square multiplied by r square the radial probability distribution function. But one thing that is common in all these orbitals is that all of these are dependent only on r there is no angular part the plot thickens the situation becomes more interesting when we go to p orbitals where it is not only about r.

But it is also about theta and Phi in the next module we are going to discuss the p orbitals and d orbitals and there we are going to learn where these px, py, pz and more interestingly dx square - y square dz square and so on and so forth where these orbitals get their subscripts from.