Chemistry Atomic Structure and Chemical Bonding
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Lecture – 26
Hydrogen Atom: Radial and Angular Solutions and Animations Part II

Welcome back to the lectures on the Hydrogen Atom. The lecture today is on the animated view and visualization of the d and the f orbitals. As I said in the last part of the last lecture this is purely a visualization for some of the orbital or some of the angular parts of the orbital. D orbitals and f orbitals are quite interesting for the molecular systems particularly for the atoms in the I mean elements in the transition metal rate, and also the inner transition metals such as the lanthanides and actinides series.

Therefore, a visualization of some of these f orbitals helps you to imagine I mean in the case of say crystal field theory when you study the charge distribution of the ligands and the orbitals of the energies of the orbitals, you can see why the conclusions are important. So, let me start by recalling what the d orbital angular part of the function is.

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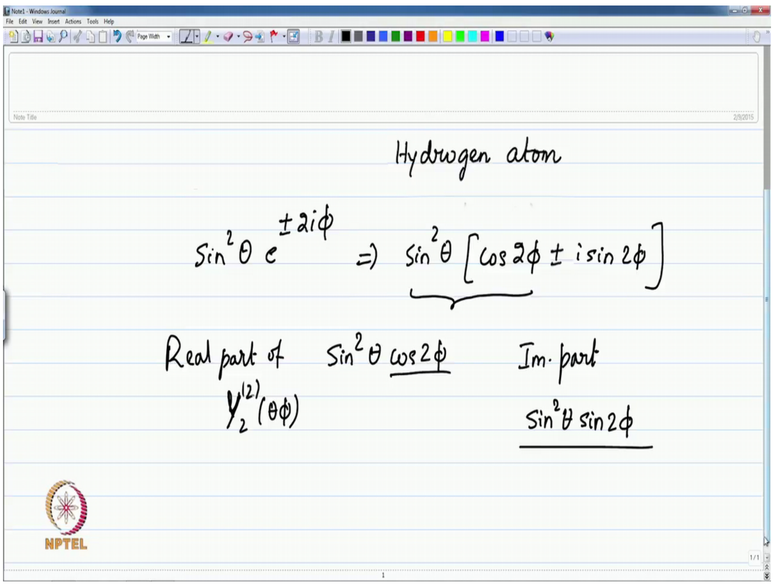

This is the part 4 of the 5th literature lecture on the d and f orbital views in quantum mechanics ok.

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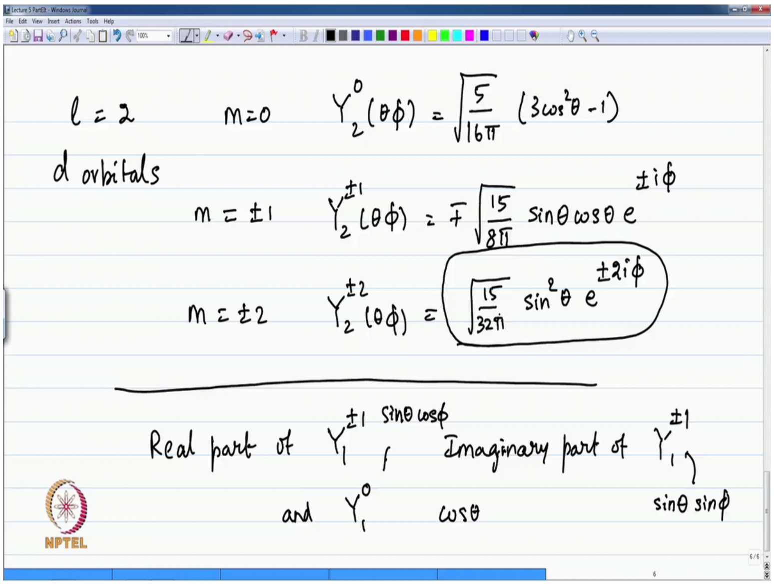

The d orbitals correspond to the quantum number l with a value 2 and there are 5 d orbitals with the quantum number m being 0 or plus minus 1 or plus minus 2. And the spherical harmonics second rank tensor with the spherical component 0. I am not introduced this terminology until now, but keep this in mind, the spherical harmonics l and m or also referred to by the tensorial rank. People have some other mathematics lectures to determine what tensors are and understand them, but please take it from me that these are second rank tensors representation in a spherical coordinate system with the component in the spherical coordinate system being 0 or plus minus 1 or plus minus 2, now that is the mathematics.

Now, the circle harmonics Y 2 0 has the functional form 3 cos square theta minus 1. And being m being 0, it does not have a 5 dependent part. The exponential i m phi gives you 1, because m is 0. The Y 2 plus minus 1 theta phi is quadratic in the trigonometric functions sine theta cos theta. And if you think of 3 cos square theta minus 1, 1 is nothing but sin square theta plus cos square theta. Therefore, this function is actually 2 cos square theta minus sin square theta. So, it is a homogeneous function trigonometric function of order 2.

And this is order 2 sin theta cos theta, but plus minus 1 means exponential i phi is plus minus i phi. And likewise plus minus 2 for the Y 2 2 tells you that the angular part has a trigonometric function, which is sin square theta and a phi dependent function which is exponential plus minus 2 i phi ok. We shall plot 1 or 2 of these. And let us start with the picture for Y 2 0.

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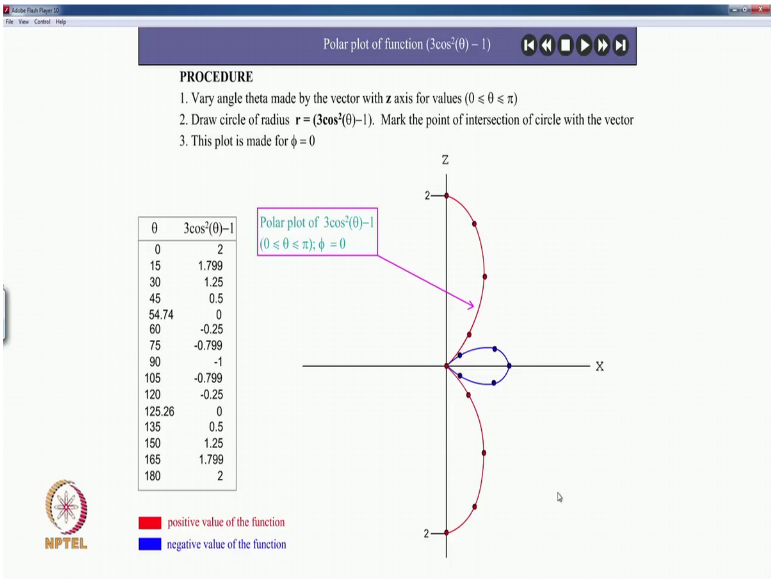

So, this is 3 cos square theta minus 1. I mean I am leaving out what is called the pre factor the normalization factor and all those things I mean they will only change the extension, but the shapes will remain the same. Therefore, we will keep 3 cos square theta minus 1, and we want to plot this in the polar system with the theta axis going from 0 to 90 to pi to 180 degrees. The values of 3 cos square theta minus 1 for various values of theta are given here in this table. And you can see that 3 cos square theta minus 1 goes to 0 at cos theta is equal to plus or minus 1by root 3.

Therefore, you see the plus 1 by root 3 corresponds to theta is equal to 54.74. And the minus 1 by root 3 corresponds to pi minus theta and that is 180 minus 54.74, which is 125.26. In between 54 and 0.74 and 125.26 3 cos square theta minus 1 is negative, because cos square theta is less than one-third. And at 90 degrees this is 0 therefore, this whole function is minus 1 maximally negative. So, from the magnitudes given here the variation is between 2, 0, minus 1, 0, plus 2.

Let us see the function plot. Remind yourself that we are plotting the value of 3 cos square theta minus 1 on the radius that makes an angle theta with the z axis that is a plot please recall that. So, at 54.74 it goes to 0. And then the function is negative, so I have a different color for the points with the blue dots and that is minus 1 exactly half of the height. Again the function goes back to 0 and starts increasing to larger values and reach 2. So, the graph is drawn by following the theta values, namely theta is equal to 0 up to 54.74. And then between 54.74 up to 125.26 and then for the increased value of theta you have. So, this is a continuous plot, now this is phi independent.

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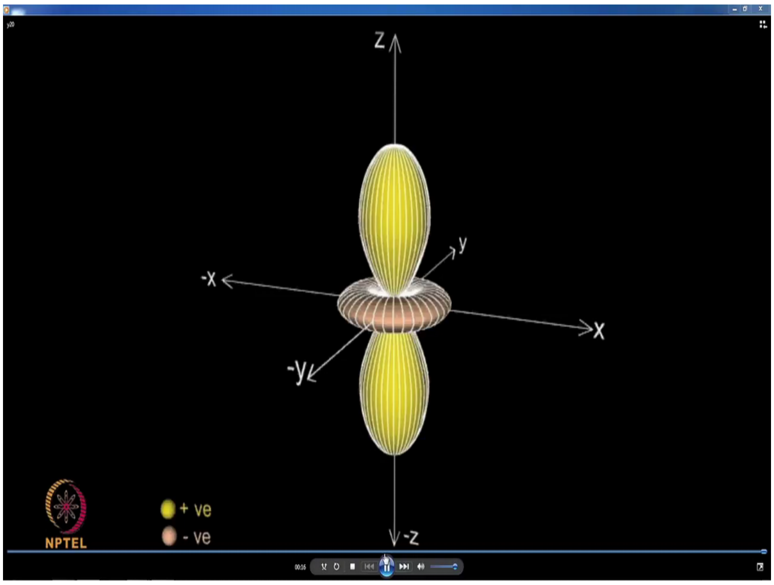

Therefore, it is the same plot for all values of phi, because the function is phi independent. Therefore, for 0 to 360 degrees, you get the familiar picture of the d orbitals with two balloons connected to each other by the torus that the ring in between. And, in some pictures you might see that the ring is standing out, and the balloons are not touching the ring, but that is wrong.

This is the mathematical representation the ring is tangential at 54.74 to the plus part and also at the bottom 125 at the bottom 125.26 it is tangential. Therefore, you see that this is a continuous surface this is the d orbital, which you call as a d z square orbital sometimes as you might find in textbooks. But it is essentially 3 z square minus r square and we have not considered the r we had only worried about the fact that 3 cos square theta minus 1. So, it is easy to visualize.

And let us take m is equal to plus minus 2, and find out what this picture is plus minus 1 you can in a similar way you can find out yourself. Plus minus 2 contains an imaginary that is a complex part. So, let me, get my function into real and imaginary parts. And let me leave the 15 square root of 15 by 32 pi for the moment, we do not need to worry about that. So, we have sin square theta e to the plus or minus 2 i phi, which is sin square theta cos 2 phi plus or minus i sin 2 phi. And the real part is sin square theta cos 2 phi, this is the real part of Y 2 2 theta phi, the imaginary part is leaving the i out, obviously the imaginary part is sin square theta sin 2 phi.

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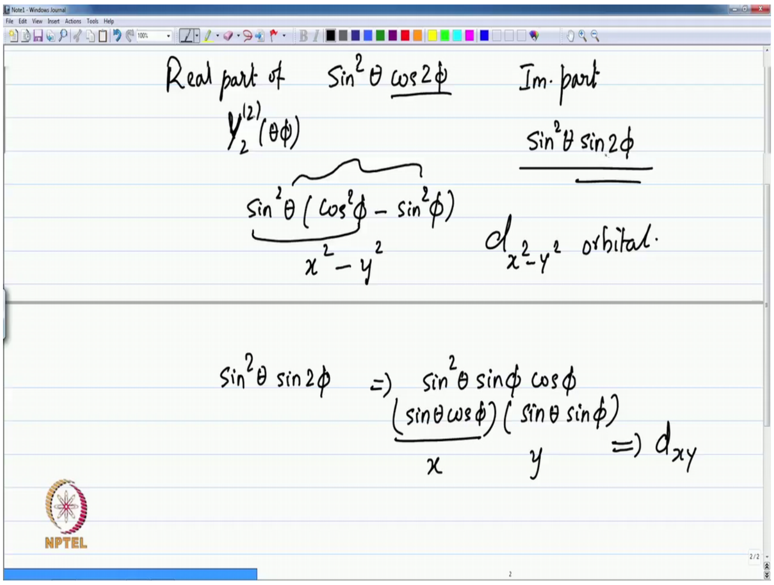

Recall that cos 2 phi, so this function is sin square theta cos squared phi minus sine squared phi. And remember sin theta cos phi is like x, therefore this is x square, and sin theta sin phi is like y and therefore this is minus y square. So, this part is often referred to in your textbooks as d x square minus y square orbital. And in the same way, if you look at sin square theta sin 2 phi, this is borrowing the numbers out I mean the there is a 2 here, but what is important is it is sin square theta sin phi cos phi, which is sin theta cos phi and sin theta sin phi multiplied to each other.

So, remember this is x and this is y. So, this is often the d x y orbital that you see. And you see the difference between the two functions is essentially the difference between cos 2 phi and sin 2 phi. Cos 2 phi and sin 2 phi differ by pi by 2 or pi by 4; if you change phi by pi by 4, cos 2 phi becomes a sin 2 phi. Therefore, you see that there the whatever the shape that you will have for d x square minus y square will be only rotated by 45 degrees to get the shape of the sin square theta sin 2 phi that is the d x y we will see that.

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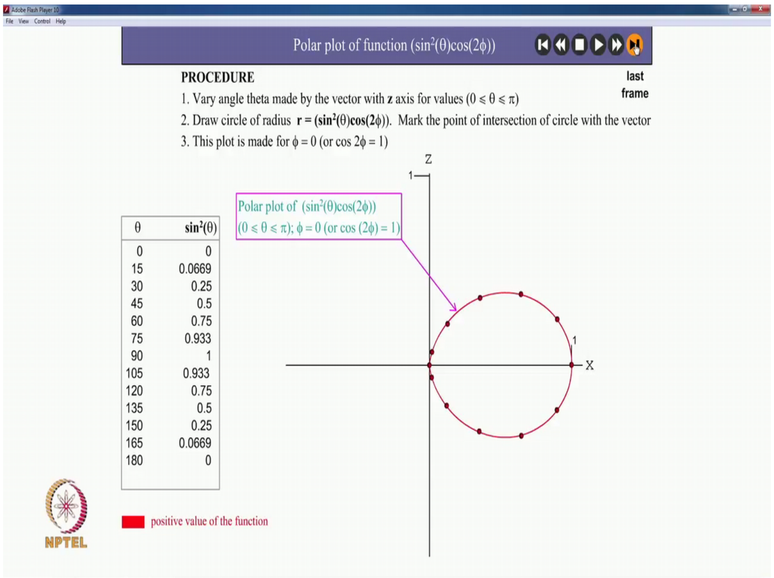

So, let us start with the real part for the d orbital the sin square theta cos 2 phi, and since phi is equal to 0 gives you cos 2 phi is equal to 1. And therefore you get the maximum value for sin squared theta Let us, plot it along the x axis, and then plot it for various values of phi in going around, so that for each value of phi the cos 2 phi multiplying sin square theta will change the shape to get you the full 3 dimensional picture. This is sin square theta with cos 2 phi equal to 1. I do not have to go through this, let me go to the last frame that is what you will get ok. If you want to play around to see and stop, and see that it plots the writing this is sin square theta.

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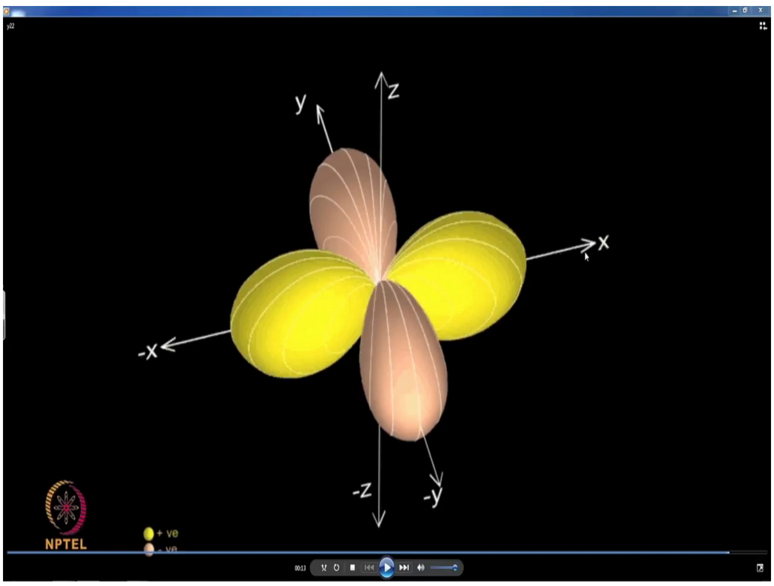

And then, what you have is this is modulated by cos 2 phi it is modulated by cos 2 phi with cos 2 phi being 1 at x, where phi is 0 cos 2 phi being minus 1 at y, where phi is 90. So, in between cos 2 phi goes to 0, namely at phi is equal to 45. Therefore, the graph goes to 0 at 45, and then it increases, but becomes negative, because cos 2 phi is negative in that quadrant in that part of the range of in that range of phi. And then when it comes to minus x axis, this is 135 somewhere around again cos 2 phi goes to 0 at 135, but when phi is greater than 135, and 180 and 22 cos 2 phi goes through positive values, see it for yourself so that is essentially how we picture.

So, you see the picture of the d x square minus y square, which is your pair of lobes along the x axis as well as along the y axis, but with the opposite signs, because of the cos 2 phi modulation 2 phi modulation. And this is an even function you can see that the plus x and minus x plus y and minus y they both have the same sign.

Now, what about the other function the other function is sin theta sin theta cos phi sin phi cos phi sin phi, therefore it is sin square theta. So, the plot of sin square theta is the same as what we had before, but since it is cos phi sin phi we do not want to plot it along the x axis, because it is obviously 0 at phi is equal to 0. You can see that it is a maximum at phi is equal to 90 sorry at phi is equal to 45 not 90, because that phi is equal to 45 cos phi is 1 by root 2 sin phi is 1 by root 2 they both have the same value. Therefore, you see this function actually is between the two axis, it is not split by the axis. At both the axis the function is actually 0, because phi is 0, phi is 90, phi is 180, and then phi is 270. So, on all the axis, the function goes to 0, but between the axis the function goes through a maximum from 0 to 45, and then it goes to 0 from 45 to 90 and so on.

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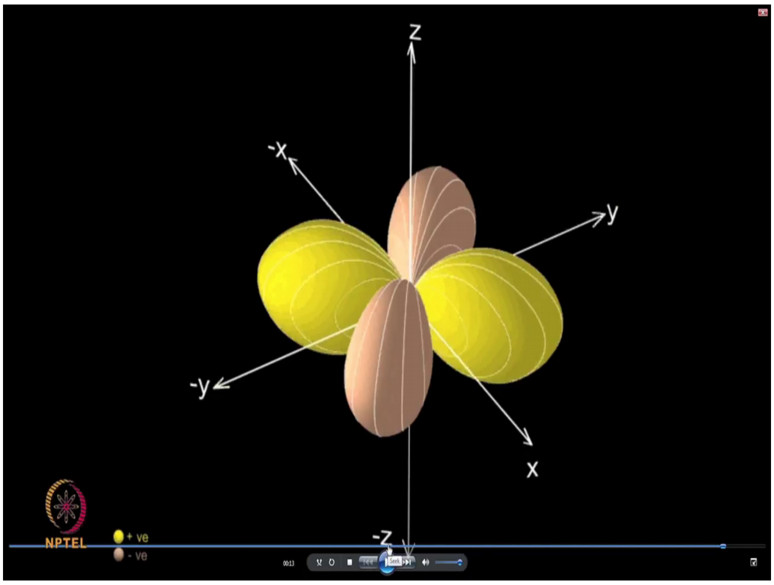

So, the picture you can see that the picture starts with the middle of the axis at x it is 0; and at y also it is 0. So, the bulk of the picture, bulk of the shape is in between the axis. And it is only a 45 degree tilt, because the difference between the d x y and d x square minus y square is a 45 degree angle. So, their shapes are determined by the way we represent the mathematical functions, and then the way we plot them in a spherical axis system or in the spherical polar coordinate system. So, these are for the big orbitials. I will show 1 f orbital as I mentioned in the last lecture. And then we will leave the rest to be seen by you.

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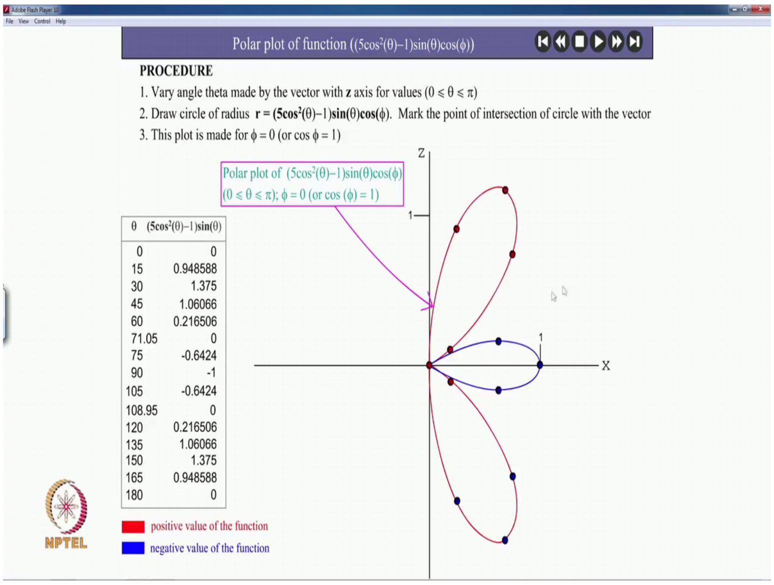

The function y 3 1 is 5 cos square theta minus 1 times sin theta times cos phi. This is a trigonometric function homogeneous function of order 3, because one is nothing but sin square theta and cos square theta. So, it is 4 cos square theta minus sin square theta times sin theta so everything is cubic times cos phi. And therefore for phi cos phi and therefore, for phi we have chosen the value 0 that this is maximum. And so what you see is the plot of phi cos square theta minus 1 times sin theta on the polar coordinates.

You can see that it goes to 0 at 3 place 3 places phi cos square theta minus 1 that is this is minus 1 when cos theta is 0. And this is again phi cos square theta minus 1 that is 0. And at 180 degrees also it is 0, because it is there is a function sin theta. Therefore, the plot looks like the shape. You start from 0 as the theta value goes this way the function increases to this point. And then as the theta becomes more and more, the function comes to 0, then the function goes through this value and it comes back to this. And this is multiplied by cos phi and therefore, the actual representation and again you can see that there is a plus part there is a minus part and there is a plus part multiplied by cos phi phi.

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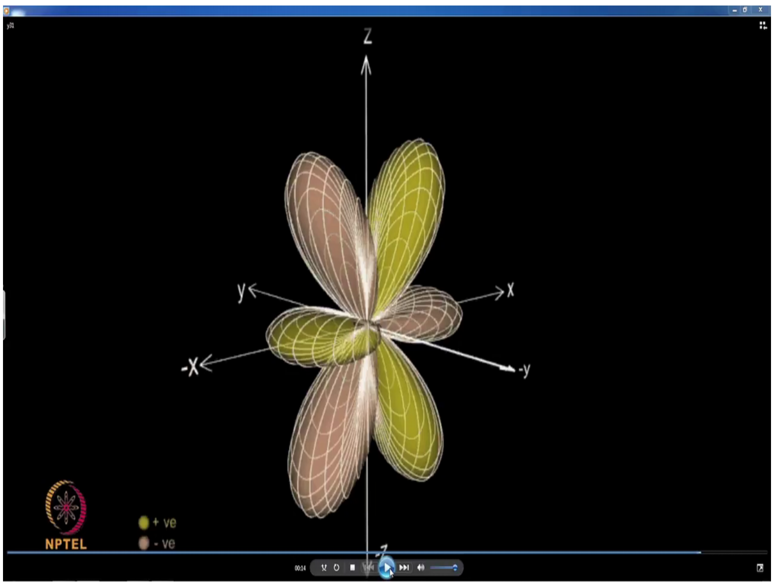

So, if we look at the cos phi part together, the modulation that you see is followed by that followed by that, but now in the whole 5 axis system therefore you see the plus, minus, plus, minus, plus, minus and this is an odd function. The f orbitals or odd functions of the in the three-dimensional coordinate systems. And you can see that whatever is here, it is opposite on this side is negative; whatever is here, it is opposite part is negative here and so on.

So, this is the shape of one of the f orbitals it has the value phi, it has the equation phi cos square theta minus 1 times the sin theta cos phi. The cos phi comes from the real part of exponential i phi, therefore what you see is this is Y 3 plus r this is plus 1, and if it is multiplied by sin phi, that is Y 3 minus 1.

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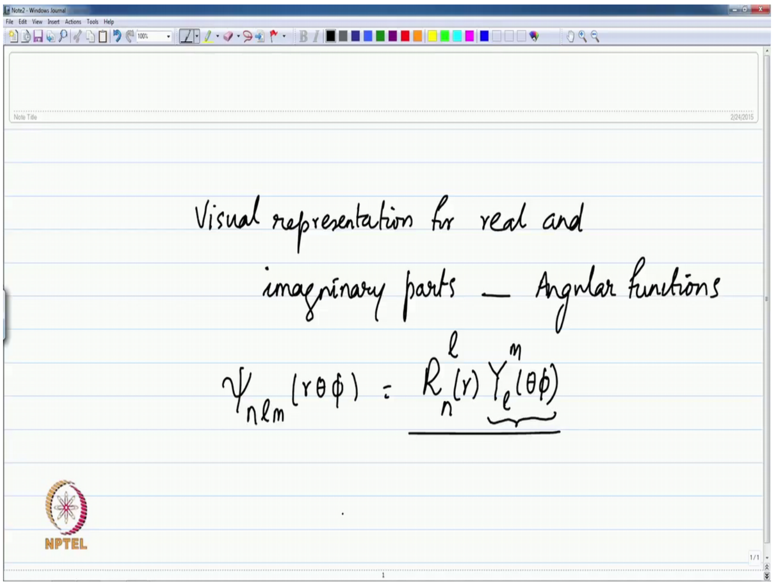

So, what we have is a visual representation for real and imaginary parts, but this is only angular function. We have not seen the angular function multiplied by the radial function because you remember psi n l m or theta phi is the radial function R n l of r for multiplied by Y l m theta phi theta phi. So, what you have seen is only the visual representation for these, but the radial functions bring in their own nodes along the radii r this sphere.

And therefore, the radial function multiplied by the angular function the three-dimensional visual representation is quite complex. In the next part, we will see the radial function, and the square of the radial function. We will discuss the probabilities the radial probability distribution. We will discuss the angular probability distribution and do a small bit of calculations involving the spherical coordinate system for the hydrogen atom. And with that the mathematical as well as the physical picture of the hydrogen atom that I wanted to give for this course is complete. So, we will do that in the next part.

Until then thank you very much.