Atomic and Molecular Physics
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Lecture - 34
Quantum mechanical treatment of Hydrogen like atom (Contd.)

So, what we have learn from last class about the radial wave function and radial distribution of hydrogen like atom ok.

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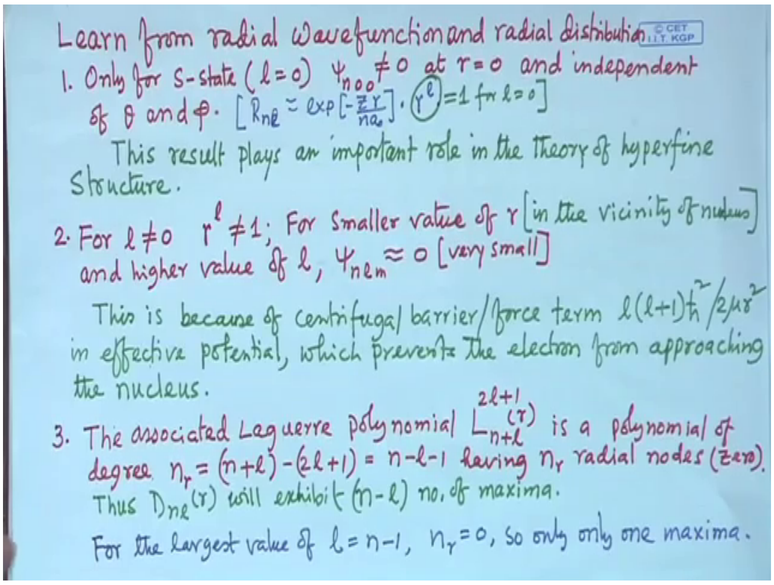

So, so we have learn from radial wave function and radial distribution is basically what we have seen for only for S-state means l equal to 0, this wave function is not equal to 0 at r equal to 0 and also it is independent of theta and phi right.

So, this is important information we got from the wave function and this result plays an important role in the theory of hyperfine structure ok. Second information we got that for l is not equal to 0 r to the power l, which is in wave function radial wave function. So, is not equal to 0 ok so, for smaller value of r means in the vicinity of the nucleus and the higher value of l so, psi n l m so wave function is very small it is it is almost 0 ok.

Why it is so, that I mentioned that this is because of centrifugal barrier or force terms. So, probably remember this kind of term can in the in the when we are solving the wave function ok, Schrodinger equation. So, their one term was there energy term one energy term was there right e and another term was there this potential energy b r ok.

And there another term this l l plus 1 h cross square by 2 mu r square this another term was where can there. So, this 3 term was there ok. So, this term is equivalent to a potential energy you know. It is a potential energy is a basically barrier ok, kinetic energy is helps to overcome it overcome the barrier.

So, this term came with the in the in the same way as the potential energy ok. So, so this because of this barrier is basically because of centrifugal force the effect. So, it is effective this is the effective potential this term together with the potential between the nucleus and the electron ok.

So, what was the potential z e square by r z e square by r and with the term another this l l plus 1 h cross square by 2 mu r square. So, that term also comes. So, this together it is called the effective potential. And this in that effective potential because of this effective potential where this term centrifugal barrier term is there, and that prevents the electron from approaching towards the nucleus ok. And then another information we got that associated Laguerre polynomial this is a polynomial of degree n r, n r is basically n l n plus l minus 2 l minus 1 a plus 1.

So, this basically equal to n minus l minus 1 that equal to n r we have written. So, it is the, this n r signifies that the number of radial nodes ok. Means this wave function will be 0 at yeah higher that is that is called the nodes when we plot wave function as a function of r.

So, that we have seen and we have also seen that this density probability that is a D n l it is the, it will exit it will exhibit n minus l number of maxima ok. So, what does it mean? So, you will have n r number of means n minus l minus 1 number of nodes then you will have antinodes or maxima that is just whatever the number of nodes plus 1, n r plus 1 number of maxima on node antinodes you will see ok.

So, that was that is what we have seen number of I think just yeah square number of antinodes or maxima.

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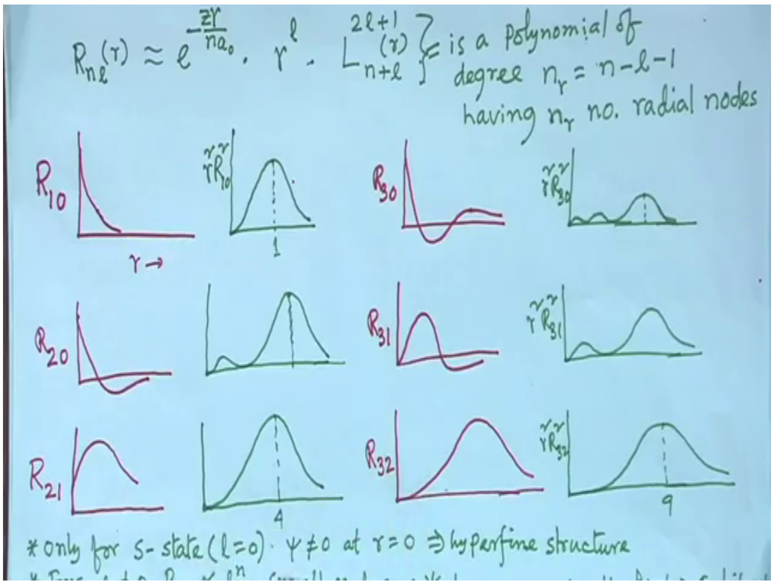

In this case it is the n r is 0 ok. So, this maxima is 1 n r plus 1 so, this 1 so, 1.

So, n r here in this case 1 so, this nodal point is 1, but maximum will be n r plus 1 so 2. So, here we are getting 2 maxima, in this case we are getting 3 maxima, n r is basically in this case n r equal to 2 n r equal to. So, 2 nodal point so, maxima you will get 3 because n r plus 1. So, you will get 3. So, as I mentioned that if you know the number of nodes.

So, then you can draw the wave function and this probability density you can basically draw the nature of the curve ok, without looking at the exact form of the wave function. So, these are the information we got.

So, now will study the will see the angular dependence of the wave function angular dependence of the wave function.

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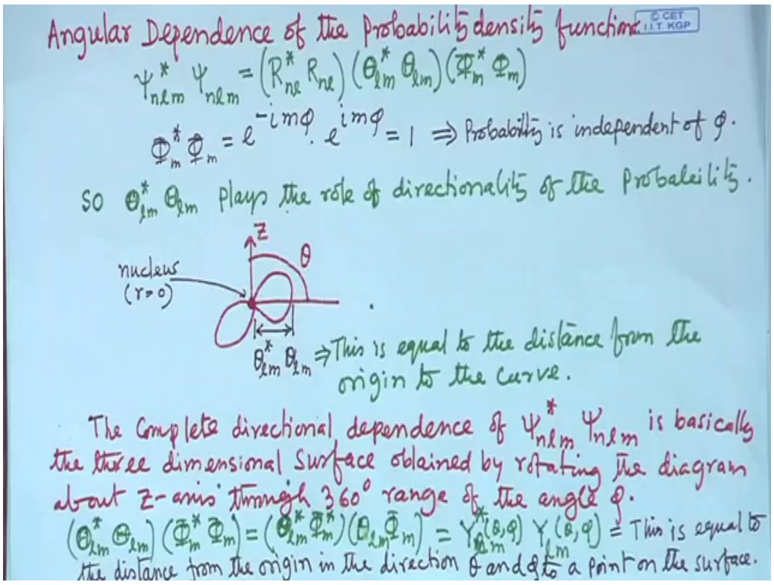

So, for so radial part we have seen radial probability density, now angular dependence of the probability density. So, probability density is as we have seen this defined like this so, here phi that we have seen e to the power i m phi ok. So, phi star is basically 1. So, this probability basically will be independent of phi. Now on the left for angular dependence left this theta part. So, theta l m star theta l m the plays the role of the directionality of the probability ok.

So, phi part will not it is the, it will not participate in the in the angular dependence of the probability density, because it is it is one. So, only we can look at this phi not phi theta l m star theta l m. So, this will tell us about the angular dependence of the probability density. So, angular dependence are so, this is the probability density ok, angular probability density and this is basically it is defined like this.

So, what is theta? So, theta is basically angle between the angles of a direction with the z axis right. So, if this is a nucleus now from the nucleus means r equal to 0. So, if we take z axis ok.

Now, now if you if you if you change that angle if you change the angle if you change the angle. So, means if you change the theta. So, at so, you are going a different direction, now in different direction what is the probability to find the electron? So, if I draw like this if this is the probability this curve is showing the probability. So, then what does it mean? So, when this angle theta angle theta this is 0. So, this it is 0 the probability 0.

Now, I am changing angle. So, this is say this is angle. So, at this angle so, this distance or here if you take this one in this case it looks 90 degree, but it is not necessary to be 90 degree any other angle ok. So, distance from this nucleus to that point on the curve ok. So, that is basically phi yeah theta l m star theta l m ok. So, this meaning of this probability density is defined like this. So, this is this probability density is equal to the distance from the origin to the curve ok.

So, these are the distance defined that the distance will tell about the probability of angular probability of finding the electron. So, here the complete directional dependence of this whole wave function is this ok, it is basically 3 dimensional surface obtained by rotating the diagram about the z axis through 360 degree range of the angle phi.

So, it is independent here we have seen that it is this probability angular dependence that is the probability is the, if independent of phi it is independent of phi means, if we phi which angle is phi angle is basically if you take the projection of these r on the x y plane ok. So, that projection it makes angle with the x so, that is the phi ok. So, that is the phi angle with x axis it is on a x y plane ok. So, phi can change from 0 to 360 degree ok, where theta can change with z axis it is 0 to 180 degree ok.

So, when will change theta from 0 to 180 degree so, if it is varies like this if it is varies like this density probability with theta is varies like this. Now it is independent of high means, now if you if you rotate if you rotate it with respect to this z axis with respect to z axis if you rotate it ok. So, you will get 3 dimensional view ok.

So, you will get the theta and phi independence ok. So, that will be the probability complete directional dependence of this of the wave function of this one ok. So, so this angular dependence of the probability that can be written in a new form. So, here I have written. So, Y l m theta phi star Y l m theta phi. So, Y l m is basically here Y l m is basically theta l m and phi l m ok. This 2 angular dependence this part one can write in this form Y l m theta phi. So, this Y l m theta phi is basically call the spherical harmonics is called the spherical harmonics, and this is basically this will tell us if we this Y star Y ok.

This will tell us about the probability from the origin in the direction theta and phi ok, up to the point on the surface ok. Whatever this we are getting and this after rotation by 360 degree, whatever this will get the surface ok; From the centres from the centre and the from the nucleus distance from this distance at a point on the surface.

So, that distance is basically the probability density angular probability density, which depends on angle theta and phi Y l m. So, we tell it is spherical harmonics it is a function spherical harmonics.

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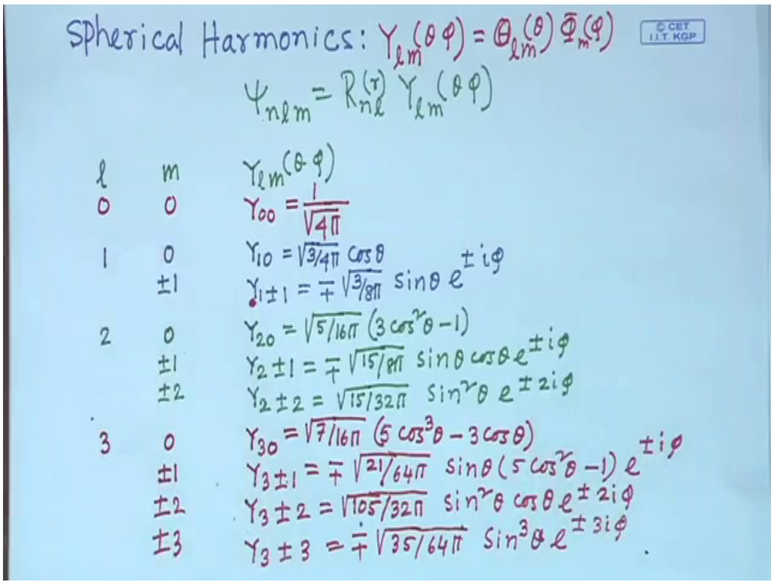

So, spherical harmonics Y l m theta as a function of theta phi so, this is basically theta 8 has 2 part one is theta part and another is phi part. So, in combination in combined way it is Y l m.

So, now wave function then we can write psi n l m equal to R n l radial part and this angular part. So, that is angular part is Y l m ok. So, now, few like radial part we have we have we have shown this few wave function for few value of l and n and l ok.

So, in this case for spherical harmonics so, what is the form for different value of l and m. So, for first few values of l and m here I have shown you. So, when l equal to 0 m equal to 0. So, this Y l m means Y 0 0. So, function is this one and then for l equal to 1 m is 0 plus minus 1 ok. So, corresponding spherical harmonics Y 1 0 and Y 1 plus minus 1.

So, these are the form. So, here it is the is the independent of for l equal to 0 and m equal to 0 it is independent of theta and phi and this l equal to one m equal to 0 it is it depends on theta only theta it is independent of phi, because m equal to 0. So, it is independent of phi so, other 1 plus minus plus minus 1. So, e to the power plus minus I phi that term has come and yeah similarly for l equal to 0 l equal to 2 m equal to 0 plus minus 1 plus minus 2 and corresponding spherical harmonics is given here ok. So, sin and cos terms are included their square. So, this they have some particular form that I have shown here ok.

So, for other l equal to 3 and different value of m these are the thing. So, here you can see for yes. So, now if you know Y l m this form is like this. So you will get the angular probability density taking Y Y star. So, if I now plot it in graphical form if you want to see, then angular probability density for small value of few value of l and m.

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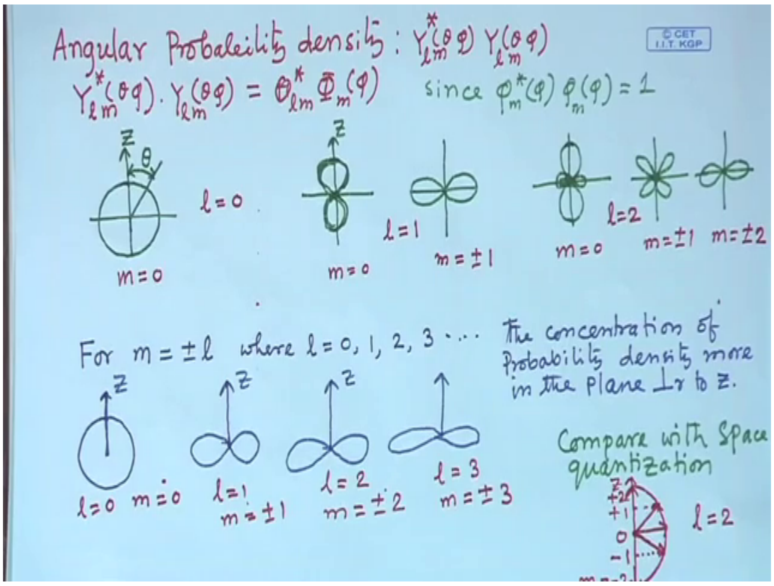

So, here so, phi star will be 1. So, only we have to concentrate about the about the about the theta so, for m equal to 0 and l equal to 0 if we plot probability density. So, it is the as a as we have seen wave function is independent of wave function is here independent of theta and phi this constant. So, constant means it will be spherically distribution. So, it is this and if you rotate it by 360 degree so, it will be sphere basically so this for m equal to 0 l equal to 0.

Now, for l equal to 1 m equal to 0 what was the wave function m equal to 0 l equal to 1 m equal to 0 ok. So, this is the wave function. So, cos theta it is the function of cos theta now square of it will be cos square theta right. So, probability density will be square of it means cos square theta ok. So, it is it is it is it is like this. So, distribution will how it is coming how it is coming. So, let me let me tell you. So, so what we have seen.

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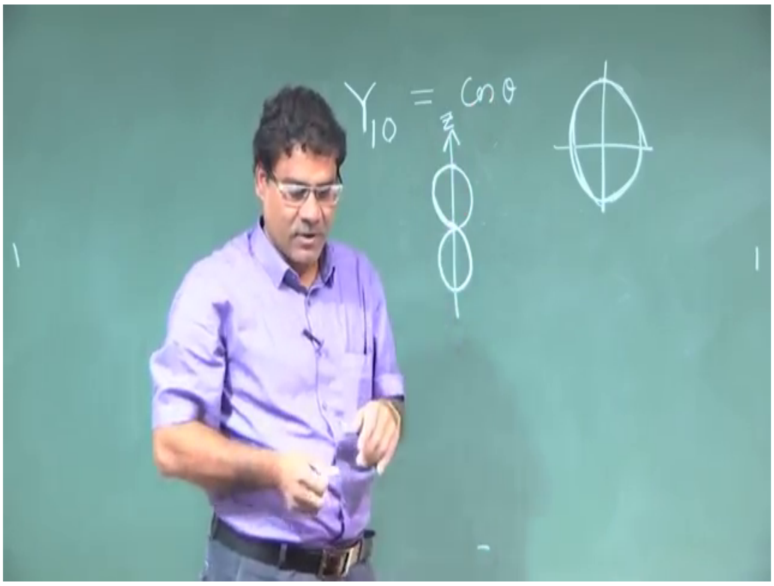

So, Y l equal to 1 and m equal to 0, now this term is basically is having cos theta ok. Now probability will be square of it ok. So, if I plot it this wave functions if I plot it. So, this is z axis this is z axis.

Now our theta is basically changing with this with this angel change from this z axis. So, it will make angle defined angle. So, now, you see if I plot cos theta what I will get if I plot cos theta cos theta term you know this is the, what is the term cos theta. So, in this direction what is the value it is 1, means theta equal to 0 it will be 1 ok. So, I will get it is the one. So, it is the one probability is this square of it will be square of it also it will be one right.

So, now when it is 90 degree this means it is like this 90 degree in this direction ok. What is the probability in this direction 90 degree to be 0 right? So, it will be 0 ok. So, at other direction say 45 if it will be this value is 1 by root 2.

So, square of it will be half. So, it is varies it will vary like this 0 to 90 degree it will vary like this. So, it has basically we have 4 quadrant right 0 to 90, then 90 to we have basically this first quadrant. So, 0 to 90 90 to 180 180 to 363 180 to 270 and then fourth quadrant is 270 to 360. So, here just one so, but in case of cos theta or sin theta it will follow the same symmetry right. So, basically for 4 Quadrant we will this for one quadrant if it is. So, for other 4 Quadrant it is the same ok.

So, for in it is for whole range of angle although it is we tell this theta varies from 0 to 180 degree right why we tell, because 0 to 180 degree if you take 0 to 180 degree and then if you rotate by 360 degree, then it will basically it will convert the whole space it will be sphere right.

So, so; that means, basically you are covering this whole angle. So, this angle and this angle and also one has to go this other angle so, anyway. So, these are dumbbell shape is coming because of this function ok. So, that is why I have drawn here like this I have learn drawn a like this cos theta term ok, when l equal to one and m l equal to plus minus 1.

So, in this case what is the wave function in this case wave function is sin theta term, in this case wave function is sin theta term ok this cos theta term and other m equal to plus minus 1, it is sin theta term is there right. So, this sin theta term is there right. So, for sin theta and this will go square it this will go. So, sin square theta. So, basically so, it is will be sin square theta, because this is the plot this for sin square theta and for whole for 4 quadrant. So, at angle theta equal to 0 means in this direction went z direction. So, probability it is 0 right.

Because sin theta is theta equal to 0 it is 0 right and maximum value is 1 sin theta when theta equal to 90 degree when in this direction. So, it is the direction it is the with z axis in 90 degree. So, we will get maximum value 1. So, sin theta 1. So, sin square theta also 1. So, this is the maximum ok. So, this is the at 0 angle this is the minimum and 180 degree that is the maximum sorry 90 degree is the maximum. So, you are getting 0 to 90 degree. So, this so, for other quadrant also from symmetry one can draw like this.

So, it will be like this distribution angular dependence. So, maximum probability to find out the electron in at the direction of 90 degree in case of m l m equal to plus minus 1 ok. Similarly for l equal to 2 now when you are going for higher value of l. So, things becoming so, this your wave function also becoming slightly more and more complicated, but one can plot it and if you plot. So, it will be it will be like plot will be like this ok.

So, here one thing you can see that from this plot 1 can see that for smaller value of smallest value of m this m equal to 0. So, contribution is along the z direction ok. Maximum probability to find the electron along the z direction right and for highest value of l for highest value of m that is basically m is plus minus l. So, this probability is maximum along the in on the plane maximum probability is basically on the plane which is perpendicular to the z axis means x y plane to find the maximum probability find the electron in the on the x y plane right.

So, here you can see so, for m equal to 0. So, maximum probability along the z direction m equal to 0 maximum probability is along the z direction and l equal to way when m is maximum that is plus minus l. So, in this case plus minus l so, maximum probability on the on the plane perpendicular to the z axis means x y plane. So, this can be x axis or y axis whatever so, that I will discuss.

So, in basically for m equal to plus 1 if it is x axis then m equal to minus 1 it will be along the y axis ok. So, it is basically that how we have written m equal to plus minus one it is basically on the x y plane. So, because z is perpendicular z is perpendicular and z is perpendicular to the plane x y plane, now I am moving from the direction z to the x y plane ok.

So, now variation when m equal to 0 so, maximum probability along the z direction, when m equal to maximum that is plus minus l this then this maximum probability is on the plane and in between value of l m that is less than plus minus less than less than l, but greater than 0. So, there it to this to find the electron the probability maximum probability will be in between these 2 between this z direction and the x y plane ok.

So, that is what is happening here in this case when m is plus minus 1. So, this is the maximum value this is the minimum value and in between this is the value and this it is the it is it is neither along the x axis neither along the neither on the x y plane it is in between ok.

So, here another things also as I already described that for m equal to plus minus l where l equal to 0 1 2 3 ok so, this concentration of the probability density more in the plane, which is perpendicular to the z. So, that is why when l will be value will be higher and higher this you will get the more and more probability along on the x axis on the on the x y plane ok, which is perpendicular to the z plane z axis. So, so from here m equal to l equal to 0 so this is the probability and now l equal to one and this from maximum value m equal to plus minus 1.

So, it is on the plane on the plane. So, this it is also on the plane, but here just I have I have I try to show you or tell you that this for all value of m which is equal to plus minus l. So, all only you can find the so the probability to find the electron or direction dependencies basically only on the x y plane or the plane perpendicular to the z axis ok. And this with higher value of l this extends. So, up to longer up to longer the probability becoming higher and higher on this on a particular direction.

So, so this of now image in now what we are seeing what we are seeing or thinking that these or what we what we got from this analysis that, about the about the z axis, now probability to find the electron at different angle ok.

So, in case of in case of m equal to plus minus l, we have seen that this density angular density or probability density is maximum on the x y plane right. And along the z axis is probability is to find the electron probability 0 right, for maximum value of m that is equal to plus minus l and for minimum value of m that is the basically 0 m equal to 0. So, this we are getting the, we are this maximum probability is along the z axis and 0 probability to find along the on the on the plane ok.

So, now we are so, now we remember this space quantization in Bohr modal and after that this Rutherford model. So, they actually not Rutherford this Sommerfeld; he introduced the space quantization what is space quantization? Space quantization basically so, this orbit whether it is rotating in a orbit. So, that orbit it is on a plane. Now this plane, now it can be this plane is again in space it is quantized ok.

So, this plane basically it can be in any direction means theta can be any value, but it was restricted because of postulate of space quantization so; that means, only this plane can be at the particular orientation ok. So, that is the space quantization ok.

So, here this orbit it is on the plane, now this angular momentum that is basically l is l related angular momentum. Now this direction of angular momentum is perpendicular on this plane where this orbit is situated right. So, that is the direction of the angular momentum ok.

Now, here so for space quantization for a particular l value so, here I shown you l equal to 2 for l equal to 2, I have shown this space quantization l equal to 2 space quantization m value will be 0 plus minus 1 plus minus 2 ok.

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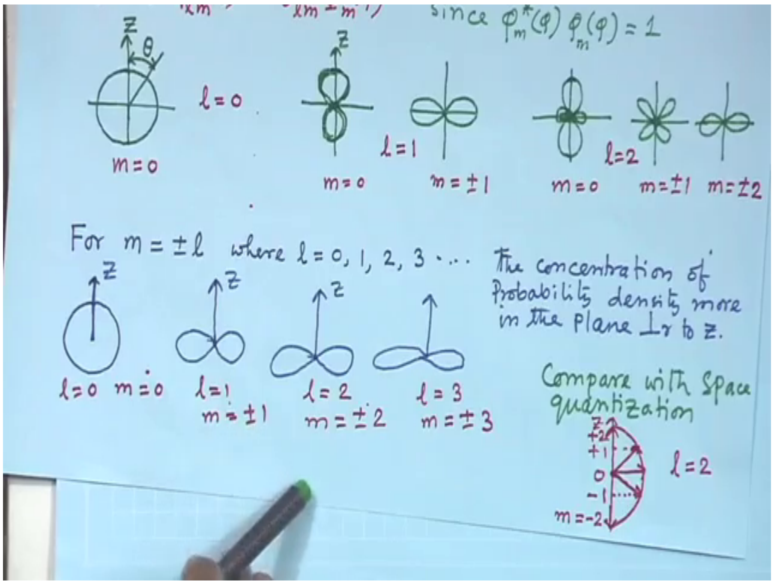

So, basically this for so, it will be quantized in such a way it will be quantized in such a way that m l value will be 0 plus minus 1 and plus minus 2 um. So, 0 means m l 0. So, that is the projection of the angular momentum it will be this is this direction. So, what is the value of the projection along a fixed direction that z direction so, for this projection is this. So, this projection will be this value will be integer value. So, plus 1 or plus 2 or 0 or minus 1 or minus 2 ok. So, these are the 5 possible.

So, now in this case l when l equal to m equal to plus 2 means is equal to l is equal to l. So, in this case this the projection is maximum this; that means, this direction of the angular momentum direction of the angular momentum is along the z direction, that is why we are getting maximum projection.

So, for m equal to l either plus l or minus l only it is the parallel anti parallel to z axis so; that means, in that case this direction of the direction of the angular momentum is along the z direction. Means orbit you will be on the plane orbit will be on the plane x y plane, if orbit is on the x y plane, then direction of the angular momentum will be along the z direction right. That means, for m equal to highest value that is l m equal to l plus minus l in that case the orbit the orbit will be on the x y plane because the direction of angular momentum is along the z the z direction ok.

So, probability to find the electron along the z direction is; obviously, 0 because this orbit is on x y plane. So, the probability will be maximum to find the electron on the x y plane. So, that is what from our analysis of the wave this wave function angular part of the wave function is telling us ok. So, this is on the so, this perpendicular this circle. So, this is on the x y plane this is on the x y plane there maximum ok. So, l so, for maximum value of m, which is equal to plus minus l.

So, this is the so, this wave function probability angular probability density is telling this maximum probability is on the x y plane. So, which is nothing, but just one can compared with the space quantization of Sommerfeld. So, this is the this is all information basically we are getting from the wave function and this is coming in natural way, but in case of Bohr Sommerfeld model this everything also correct, but concept was introduced on Ad hoc basis.

So, just on assumption this called basically postulates and this same things we are getting when we are analysing this wave functions which we got from the from the Schrodinger equation for the for the hydrogen like atom ok. So, I think I will stop here.

So, thank you very much.