Atomic and Molecular Physics
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Lecture – 33
Quantum mechanical treatment of Hydrogen like atom (Contd.)

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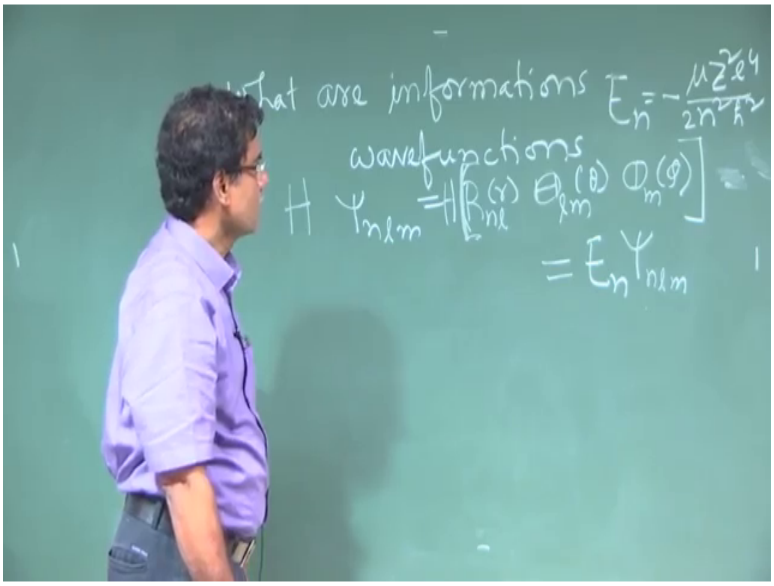

So, we are discussing basically, what is the information one can get from the wave function. So, from solving Schrodinger equation, for hydrogen like atom, we have we have got basically the Eigen value, Eigen equation where, Eigen function Phi n l m, that is in terms of R n l radial part and the angular part l m theta and phi m function of angle phi. So, this is the Eigen function and if you apply operator say Hamiltonian on this. So, we will get Hamiltonian on this.

So, we will get basically Hamilton on this. You will get E n Phi n l or we can write this one. So, this is the Eigen equation. This Phi n l m, this is the Eigen function and n is the Eigen value. In this case it is energy, because we applied operator on these that is energy operator Hamiltonian that is energy operator.

So, for that n, the specific value of this n, we have seen E n equal to minus mu z square e to the power 4 by 2 n square h cross square, which is same; yes we got from the Bohr model and now, that what we are discussing what else benefits we can get from solution, from solving this Schrodinger equation for the same hydrogen like atom. So, as I mentioned that we get this wave function, we get this wave function, this Phi m l m Phi n l m. So, this gives a lot of information about the system. So, what is the information we can extract from this wave function that I was discussing? So, for that I have already shown you that this is basically wave function..

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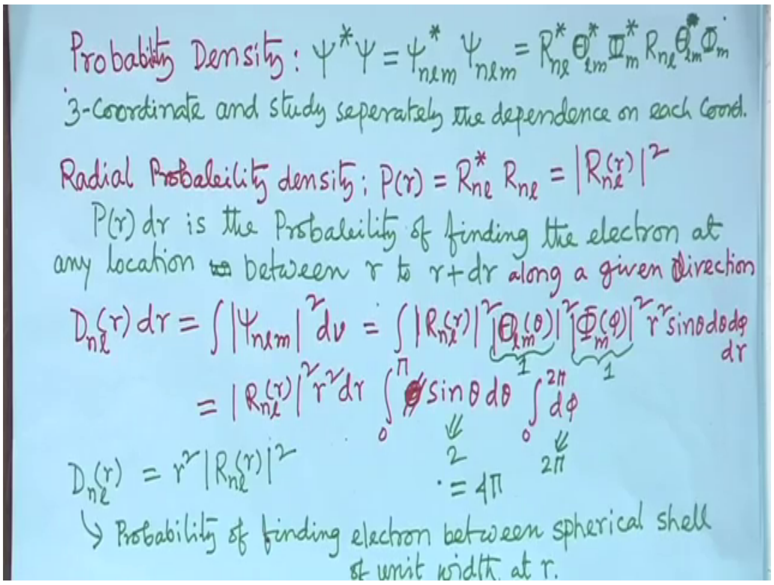

So, to extract information we have to take probability density. So, that Phi star and here, we are getting this radial probability density that is basically R dependent R n l star R n l. Right?

So, this probability density, we have seen that P r that is this probability, to find the electron in along a given direction, at location between r to r plus d r. So, that is basically P r D r P r D r. So, but another probability density parameter, we have defined that it D n l r d r. So, that is we have integrated over the theta and Phi, so; that means, this D n l r, it is equal to r square D n l square.

So, this is how it comes, that I have described. So, this is the probability to find electron between spherical shell of radius r n r plus d r. So, between r and r plus d r to Fe 2 sphere 2 spherical shells. So, between these two spherical shells, what is the probability to find the electron? So, varying the r we can get probability at different radius at different distance from the nucleus. Ok?

So, that is what I was discussing and if as I mentioned that, when n l m that value increases. So, these wave functions become complicated, but first few wave functions for smaller value of quantum number. So, this I have shown you.

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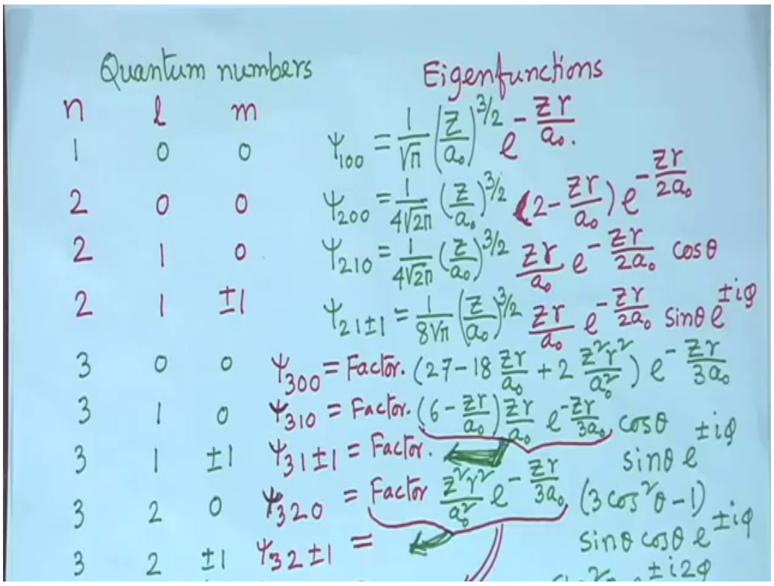

So, here we can see for n equal to 1, 2, and 3. So, corresponding l that is if n equal to 1 l equal to 0, m equal to; obviously, 0. So, this wave function form of wave function is this. So, for n equal to 2, l equal to 0 and 1 and corresponding m equal to 0 plus minus 1 and this is the wave function that I have described; here we can see that for l equal to 0 and m equal to 0. So, it is independent of this wave function, it is independent of theta and Phi, there is no term of theta and Phi here l equal to 0, m equal to 0. So, in these two cases there is no theta and Phi term, but for l equal to 1 and m equal to l is not equal to 0 and m is not equal to 0. So, in that case, this wave function depends on theta and Phi, here also; 3, 0, 0 this also independent of theta and Phi. Ok?

Now, if I take just radial part. So, it is r dependent part. So, then you know already I have shown you that radial part basically R n l R n l.

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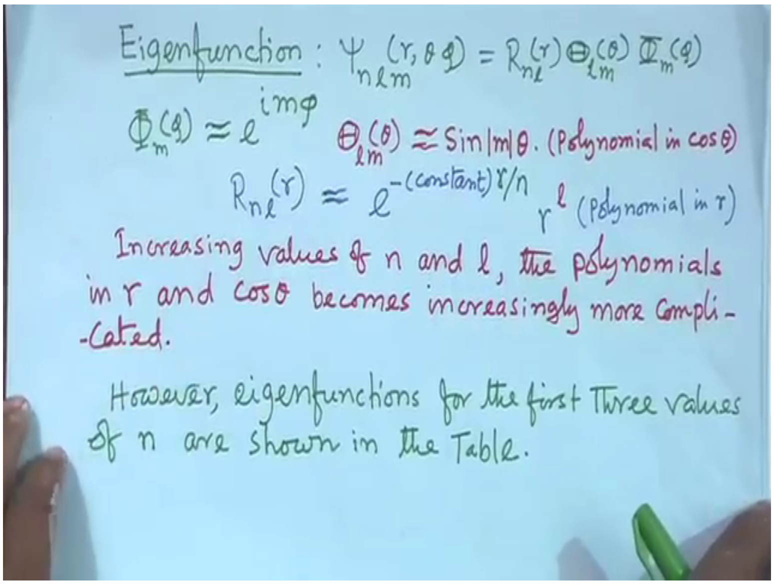

It is the form, is like e to the power minus r some other constant and n is there. So, it depends on r. So, exponential term, another is r to the power l and polynomial in r. Ok?

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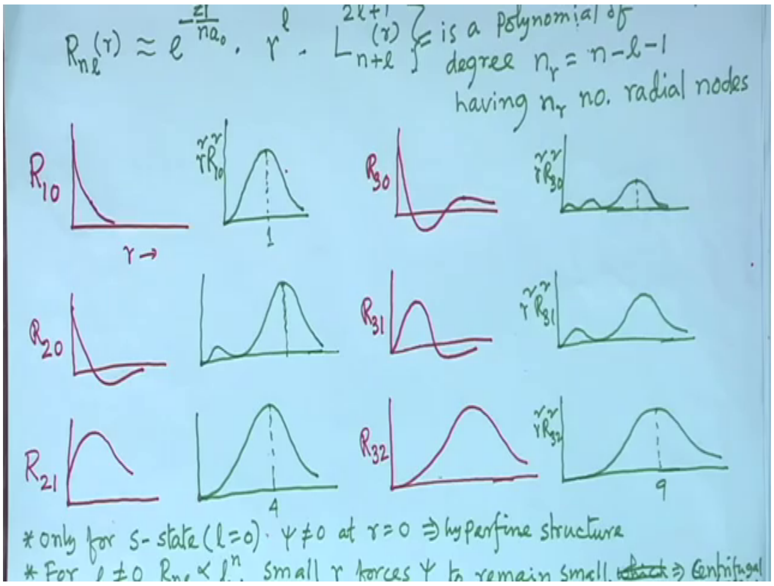

So, now if you consider this radial part, this I was discussing. So, R n l is e to the power. So, just I have neglected this normalisation factor. So, here e to the power exponentially e to the power minus z r by n a 0 r to the power l and this is a polynomial. So, this polynomial, this laguerre polynomial associated laguerre polynomial, it is called a polynomial of degree n r. So, n r is basically here n plus l minus this 2 l minus plus 1. So, this is basically n minus l minus 1. So, this is the degrees of, it is called the degrees of this polynomial. So, this number is what is the degree? It is n r. So, this is the number degree of polynomial. So, this basically, this degree of polynomial, it signifies that the number of radial nodes.

So, I already have tried to. So, this one, if I plot them as a function of r. So this wave function radial, with this e to the power minus z r a 0 for R 1 0 for R n l. So, 1 0 for 1 0, this is the exponential, I have drawn exponential curve, I have drawn exponential curve, this one. Fine?.

Now, the probability density, radial probability density R square R n l square here, 1 0 R 1 0 square. So, it will be like this. So, how it is? It comes that I tried to explain you here actually this exponential term that you have.

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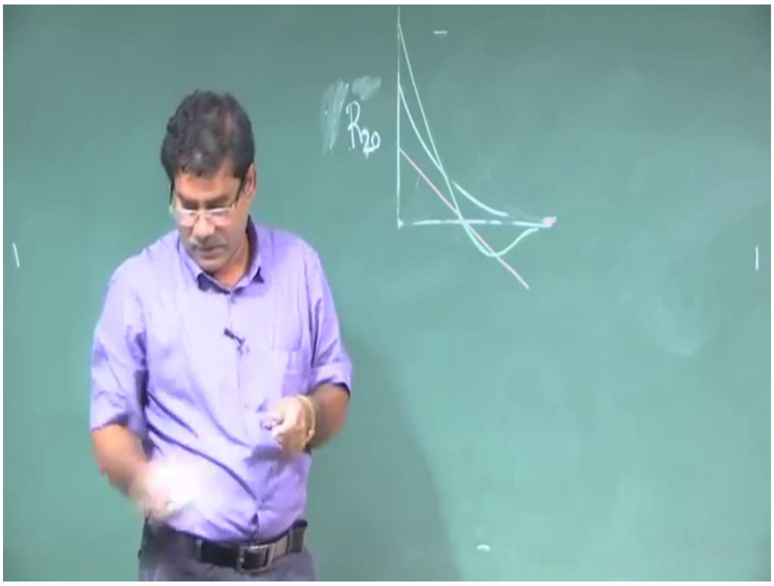

So, I have shown you, R 1 0 - R 1 0. So, exponential term is there and in addition. So, when I am making its square and this R square. So, it means this R 1 0. So, what are the exponential terms? So, it will be more sharper, because it is square. Now, it is e to the power minus 2 r minus e to the power minus 2 z r by n a 0. So; that means, its shape will be like this and additional another term R square is there. So, that is if you take Y equal to. So, these I have done y equal to e to the power minus x kind of things and another part is there, y equal to r square or x square. So, it is basically hyperbolic, sorry parabolic. So, it is parabolic function like this. Ok?

Now, you if you multiply them, if you multiply these two curve. So, here it is 0, here summary will get maximum and it is going towards 0. So, at the end also, you will it fallow this curve. So, if we multiply them, basically you will get this kind of curve. So, this tends to 0. So, this is now your probability curve. Here probability curve if I.

So, this is the here, just this R 1 0 - R 1 0 and corresponding the probability radial, probability density r square, R 1 0 square. So, this one can plot, similarly R 2 0, also I have shown you that it has it exponential term. Another linear term is there. So, in this case; so exponential term, it will be I think this is R 2 0, R 2 0, R 2 0, it has exponential term. So, if I just R 2 0, if I plot R 2 0. So, it will be R 2 0, it will be one exponential term like this. Ok?

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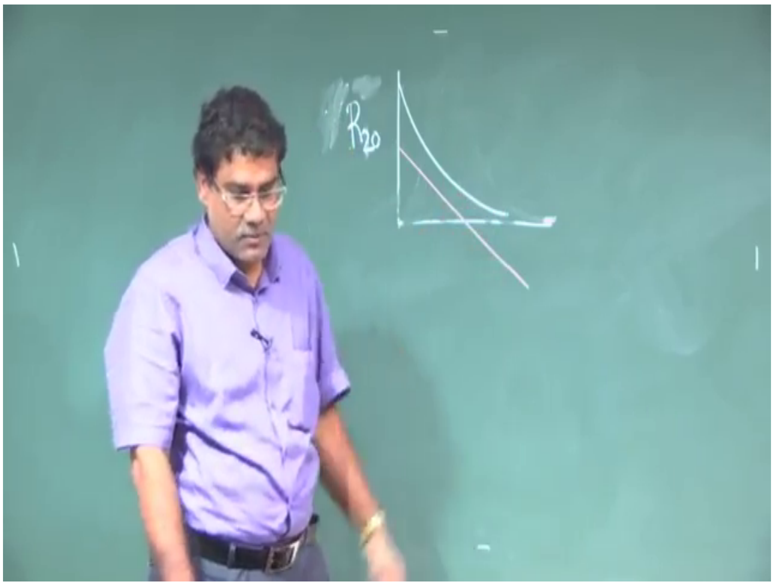

E to the power minus z r by 2 a 0, another is y equal to m x plus c. So, this curve will be like. So, it is C is plus two. So, it can be, say like this. So, negative slope, it is a negative slope minus z a 0 r. Ok?

So, now if we multiply this two, so what you will get? You will get, I think if you multiply them. So, it will follow this. So, it will have some higher value and then, it is going towards negative. So, if we add this curve. So, it will be like this, I guess I have any other colour, yes I have another colour. So, if we add them. So, we will get basically, sorry it should be exponentially I think I have to. So, here we will get negative and this exponentially it is going towards 0. So, it will multiply them. So, it is very small value.

So, it will be like this. So, negative value, it will be negative. So, I think it will be 0; it is 0, multiply 0. So, I think it has to be like this. Ok?

So, that is what I have drawn here. So, I have drawn here and corresponding it, is make square of it. So, you will get this type of. So, this way just taking the wave function as we have shown one can plot, but as I told you when this a n and l value is higher and higher n value is higher and higher. So, things become slightly complicated, but one can plot for higher value also taking help of computer programming. Now, one can plot them. So, anyway, so here without seeing this wave function, I can also plot this, if I know the degree of polynomial that is n r, if I know that one.

So, so for n l in this case, n is 1, l is 0. So, what will be n r n r? It is equal to n minus l minus 1. So, n equal to 1, l equal to 0. So, 1 minus 1 is equal to 0. So, number of nodal point will be 0 for R n l number of nodal point will be 0, means it will not cut R axis and that is what is happening, for this n equal to 2 l equal to 0 n equal to 2 l equal to 0. So, n r equal to 1. So, number of nodal points is one. So, it will cut R axis only once. So, that is what is happening right one similarly for R emu R n l n equal to 2 and l equal to 1. So, n equal to 2 l equal to 1. So, here n r n r will be 0 right? So, number of nodes will be 0.

So, this wave function, if we plot, it should be like this. So, from wave function explicit form of wave function as just as an example, I have shown this to know other wave function, also this nature of the wave function, one can draw just knowing the degree of polynomial from higher you will get the number of nodal points. So, one can draw ok, and corresponding if you make them square.

So, so here, yes if I square it, I have shown that how it is coming similarly for others. If you take square of this wave function and R square, basically probability density. So, it varies, it will vary like this, other one varies like this. So, here also you can see this n equal to 3 l equal to 0. So, number of nodal point is two. So, it will cut at this point and this other point. So, nodal point at 2.

Similarly, in this can nodal point is one. So, it will cut once, others one n equal to 2 n equal to 3 and l equal to 2 n equal to 3 l equal to 2. So, n r equal to 0, means, number of nodal points are 0. So, it will not cut these, it is varying like this and corresponding variation probability, density variation radial probability, density variation is like this. So, so if you plot the probability density, radial probability density. So, you are getting this.

What does it is mean? It is this meaning is that, that this probability to find the electron is maximum at this point, at this radius R it can. So, so in Bohr model, what we have seen in Bohr model? We have seen that electron only can be found in on an orbit. So, there are different orbits. So, in between there is no possibility to find the electron, but in quantum mechanics, what we have seen that is not correct. So, it is basically electrons, it is not a particle, it is period. It can be found everywhere, basically it can be found everywhere, but in some places the electron has maximum probability. So, this curve is telling, this is the radius R, where this, it has maximum probability and other you can see, this it has here tiny P cut there. So, small probability there, but this negligible basically, but higher probability to find the electron for this state, it is at this position. Ok?

Similarly, for this state it is the probability to find out this way. So, here you can see what we are seen that l equal to 0, that is a state basically l equal to 0, that is a state, n equal to 1 B state l equal to 2 D state. So, for only a state where l equal to 0, l equal to 0, here l equal to 0, here l equal to 0, here for this case only this wave function is not 0. It has some finite value, it has some finite except l equal to 0, for other value of l, this probability to find the electron at the at r equal to 0, it is a 0, right a 0! So, means r equal to 0, means it is at easily in nucleus position at nucleus the probability to find the electron is basically 0, but it is only exceptional case, we have seen in case of l equal to 0 for l equal to 0.

So, here it is, one, there is a probability to find the electron close to the nucleus. So, this wave function does not vanish at for L equal to 0 and this is very important. Later on, we will see that this is very important to explain the hyperfine structure. So, as I described earlier, fine structure. Fine structure, that is because of l's coupling for l interaction between the l and S spin angular momentum and the orbital angular momentum and hyperfine structures.

Again, fine structure after that, this fine structure also, it is spirited. This spirit square, this energy diffraction very small, but one can see, one can measure this separation and that is very, there is very small, although it is very small, but it exists and what is the origin of these, of this fine structure, that is basically interaction with the nucleus of the electron. So, if electron is if, wave function does not exists near the nucleus. So, how this interaction will have in? So, so in that sense hyperfine structure for S, for this case higher r equal to 0, but this Phi wave function is, wave function exists and this gives chance to interact electron with the nucleus and as a result, we get some splitting of the fine structure and that is called basically hyperfine structure ok?

So, what else information we can get from here? So, for l is not equal to 0, l is not equal to 0. R n l is basically proportional l n, because this term is there, l n term is. So, when l equal to 0. So, this term will not contribute only, but when l is not equal to 0. So, this term will contribute and these terms, you see for higher and higher l value for higher and higher l value and for smaller and smaller r value means r tends to 0, when r tends to 0. So, this r is smaller value. So, smaller value less than 1, if it less than one then if you. So, then r square is greater than r to the power r q is greater than r to the power 4 S S. So, this power when increasing power.

So, this factor will be smaller and smaller. So, for higher value of l. So, this will make this wave function smaller and smaller so; that means, when r tends to 0. So, this existence of this wave function, it is a wave function, will be smaller and smaller and it will go to vanish. So, means for when r is not equal to 0. So, probability to find the electron towards nucleus is negligible and that is what is happening, that is what is happening for l is not equal to 0. So, wave function, it is negligible value, it is almost 0 for all cases it almost 0 for all cases except l equal to 0.

So, that is the thing and this is happening because and this effect is more and more when l values are higher and higher, these because of basically this, l is basically this angular momentum right? So, because of angular momentum, there is a centrifugal force and centrifugal force means, it is electron is rotating. Now, for higher and higher l, what will happen? So, this centrifugal force will be higher and higher, means it will try to because of this centrifugal force electron, this force will try to take away electron from the nucleus.

So, so that is why when l value is higher and higher, the possibility to find the electron towards nucleus, towards r tends to 0, is will be smaller and smaller. So, these are the some wave function, radial wave function. These are the information one can extract. So, these are very important information. So, one can also find out the expectation value, expectation value of the radius.

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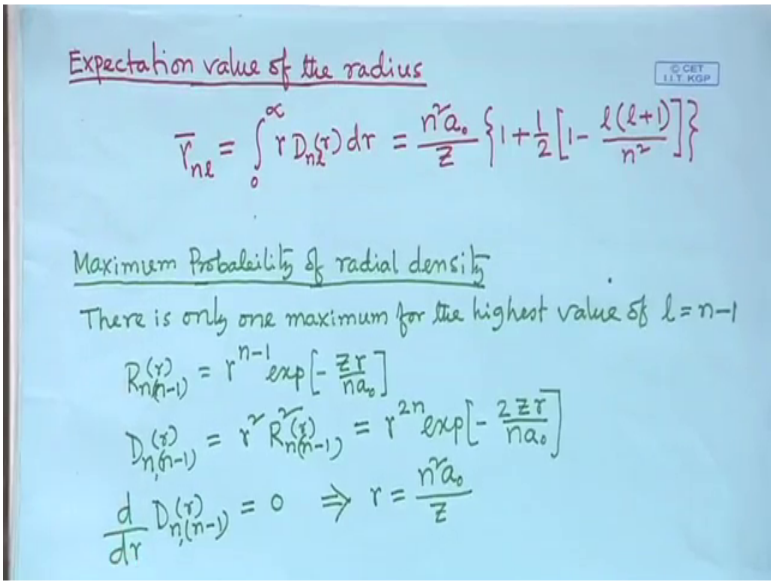

So, what is the expectation value, how to find it out? So, say position if we find also r Phi star, Phi star R Phi and then, you have to integrate over the range and then, you will get if it is normalize. So, that way one can write. So, then we will get the exponential value of that, of this position or in this case it is radius. So, if one calculate this one. So, D n l r. So, this is the probability to find the election between two spherical shells ok?

So, now, r if I take this and if I want to find out, the expectation value of radius. So, r takes r. So, then if we integrate, so if we evaluate, then you will get this type of expression, this is the expectation value of radius and here, you can see that this part if I just of this part. So, it is what is this n square a 0 by n square a 0 by 0 right? So, that is what. This is the same thing; this is nothing, but the Bohr radius right? This radius, we obtain from Bohr model. What we obtained n square a 0 by z a 0 is, I think h cross square by mu e square.

So, that was the 0. So, exactly from Bohr radius whatever, but in this case, expression values, it is not exactly the Bohr radius. What about radius we got from the Bohr? So, it is different and depends on the l expectation value is like this, but if we find out the maximum probability of radial density. So, for maximum probability, for radial density, we have seen that, that only for this, when l is equal to, only for these cases, where l, where l of the maximum value for a particular n l equal to n minus 1.

So, for a particular value of n, maximum value of l is n minus 1, for maximum value of l. So, here we can see, this is the maximum value of l n equal to 1. So, l equal to n minus 1. So, 0. So, it has only one maximum value, in this case it is the one maximum, in this case this is the l equal to 2 for n equal to 1. So, this is the l equal to n minus 1. So, maximum value of l for maximum value of l, we have seen this only one maximum. So, for other cases, this is not one maxima other maxima or so, there, but out of them. So, one is P dominate, other r negligibly smaller ok?

So, but in this condition, when n l is equal to n minus 1, if I, for this case for this case, basically I can write R n l l equal to n minus 1 r. So r to the power l. So, now, I have replaced n minus 1 exponential this term. So, this is the. So, for highest value of l, I can write this wave function, like this. Now, corresponding density, radial density, probability one can write this r square into this. So, this ultimately, you are getting this square means 2 n minus 2. So, this r square is there. So, r to the power 2 n exponential, it is square term 2 r there ok?

Now, how to find out the maxima for a particular value of a parameter? So, in this case of parameter is r. So, if you differentiate it with respect to r and make it equal to 0, then what about the value of r d we will get r, this parameter you will get. So, that is the value higher, you will get the maximum probability. So, if you evaluate this. So, we are getting r equal to n square a 0 z. So, this is exactly the same expression, as we got from the Bohr model. So, it is the Bohr orbit. So, here we can only tell.

So, that at this radius, at this radius, we will get this we will get this probability of the electron, I is maximum. So, that much we can tell, but in Bohr model, it solders only on this orbit, it will find out, but in this case, at the; in the orbit. So, they will be maximum probability to find the electron, but it will not be only there, it will be other places also, but its probability is very less compared to the R orbit. So, basically this from wave function, we are getting the similar information, whatever we got from the Bohr model ok?

So, so here you can see, this is the maximum probability and the expectation value is slightly higher than this one, because this part is there. So, plus some extra additional part is there. So, that depends on l. So, for l equal to 0, l equal to 0, this part is 0 so, but then, you are getting this is one plus half means 1.5 times of this radius or the orbit in the

Bohr model. So, expectation value is higher than the most probable value that is, because of the asymmetry of the probability curve. Asymmetry of the probability curve is now the probability curve asymmetry of the probability curve. So, expectation value and the most probable value, this is the most probable value, most probable value, but expectation value is taking the average kind of things on this curve and this, if this curve is symmetric then, we would get the same value, but seeing the curve is asymmetric, this curve is asymmetric because of that it extends longer towards the higher r value. So, that is why this expectation value is higher than the actual maximum probability value ok?

So, these are the information one can get from wave function. So, I discussed about the radial part about along the various distance from the nuclear and position, what are the probability to find the electron. So, that I discussed from the radial wave function. So, in next class, I will discuss angular dependence probability. So, I will stop here,

Thank you.