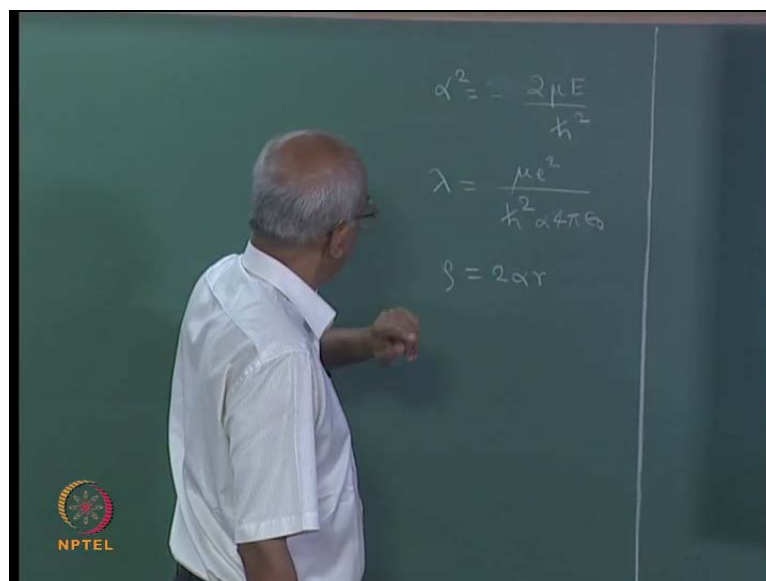


Introductory Quantum Chemistry
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Lecture -26
Atomic Orbitals – Part I

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The material that we need from the previous lecture is written here. We had the definition of alpha square by this equation then, remember a lambda was define to be equal to that, and of course rho the new variable which is related to R by this relationship. And then we found that you get acceptable solutions we have to impose the condition.

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$$\lambda = n$$
$$\alpha = \frac{\mu e^2}{h^2 n 4 \pi \epsilon_0}$$
$$\frac{1}{n^2} \left(\frac{\mu e^2}{4 \pi \epsilon_0} \right)^2 = - \frac{2 \mu E}{h^2}$$
$$E = - \frac{\mu e^4}{2 h^2 n^2 (4 \pi \epsilon_0)^2}$$
$$\alpha^2 = - \frac{2 \mu E}{h^2}$$
$$\lambda = \frac{\mu e^2}{h^2 n 4 \pi \epsilon_0}$$
$$\rho = 2 \alpha r$$

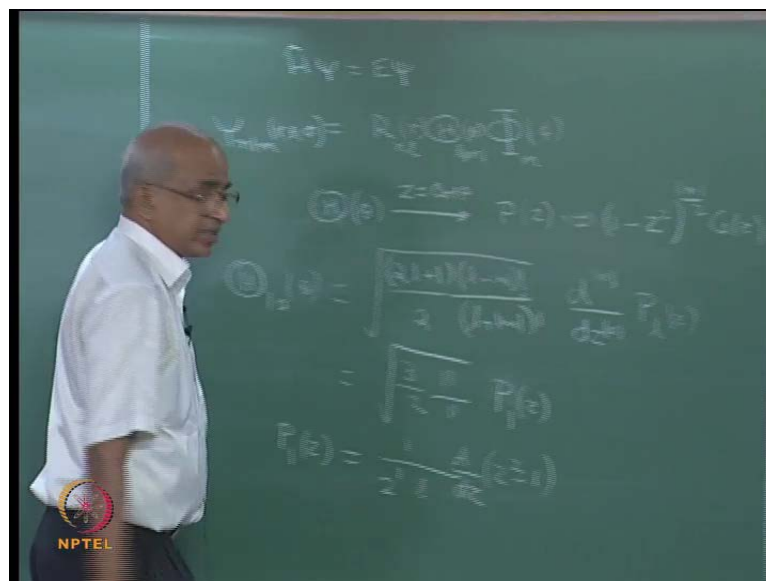
That lambda is equal to a number n, we also found that n should have the minimum value 1. Then impossible values are 2, 3, 4 etcetera and we were in the process of eliminating lambda and alpha, so that you will have an expression for E. So, let me do that lambda is equal to n. So, I am going to put here n and I should get an expression for alpha. So, what will be alpha then, going to be mu e square divided by h cross square n 4 pi epsilon 0 this will be your alpha. So, alpha square I can easily calculate it is going to be mu e square divided by 4 pi epsilon 0, the whole square 1 divided by n square h cross to the power of 4, and that should be equal to minus 2 mu e divided by h cross square because alpha square must be equal to minus 2 mu e by h cross square.

So, you can this what will be the expression for E, we will find that E is actually negative because I take the negative sign to the other side. Then you find that it is equal to mu e to the power of 4 divided by 4 pi epsilon 0 square n square h cross is that correct, that is not completely correct I have a two missing I shall suspect. So, I have a 2 here, correct me if I am wrong, but I think I am correct this time at least. So, we find that we find that allowed energy levels are dependent up on this number n, that we had introduced. Only if allowed energy levels are given by this expression are you able to get an acceptable solution.

Otherwise we are not going to get an acceptable solution to the Schrodinger equation. And you also notice that e is dependent up on this quantum number n. So, I want to make

this explicit by putting a substitute n, and not only that when lambda is equal to n you look at this equation which I have shown on the board, when a lambda is equal to n, we can replace this lambda with n and it. So, happens that this equation again is very well known to the mathematicians, they were already studied earlier and therefore, again for these things we do not have to actually make use of recursion relations to find the functions, but we can use the knowledge from mathematics and just I use those functions. So, they turn out to be the functions which are which were discussed by Laguerre and you will come that there is the functions.

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And now let me recollect what we were doing we had the Schrodinger equation for the hydrogen atom. Remember this is the equation appropriate only for internal motion, we also had an equation describing the translation motion which we got rid off that I am not writing. So, this is just internal motion we have the equation $x \psi$ is equal to $u \psi$, what is it that we have done we have assumed that ψ may be written as a product if you remember, capital R capital theta and capital phi. And we solve the equation for capital phi we will see this solution in a few seconds.

We will see this solution once more, but we if you remember the quantum number m a rows in connection with that solution by imposing, the condition that the wave function is acceptable we got the quantum number m the... So, called the magnetic quantum

number, then we looked at the equation for capital theta, we found the capital theta the equation actually contains m. If you remember, I can show it to you once more.

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The Θ Part


$$\left(\frac{1}{\Theta(\theta) \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} \right) = -\beta$$

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \left(\beta - \frac{m^2}{\sin^2 \theta} \right) \Theta(\theta) = 0$$

$$z = \cos \theta$$

$$P(z) = \Theta(\theta)$$

$$\frac{d}{dz} \left\{ (1 - z^2) \frac{dP(z)}{dz} \right\} + \left\{ \beta - \frac{m^2}{1 - z^2} \right\} P(z) = 0$$

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This here is the equation for capital theta and you notice that it contains m right. So, the solution is going to depend up on m and further we have acceptable solutions only if this constant beta is equal to l in to l plus 1, this is something that we have seen. So, the solution actually depends up on the quantum number l, as well as the quantum number m. In fact it depends only up on the magnitude we will see that magnitude of m not one the actual value, but only on the magnitude of m.

So, therefore, we will explicitly say that theta depends up on l and m, it is a function of small theta and then we today we found the solution for capital R. Capital R has an equation which for example, its shown here right and you find that the equation contains l it also contains the energy, but energy is dependent up on the principle quantum number n. So, therefore, you realize that capital R actually will depend up on the values of n and l right. So, this is the general nature of the solution this is how the solution appears.

So, I wave function psi it depends up on all the 3 quantum numbers, again I would also like to specify there are only 3 only 3 quantum numbers that they come out of the solution, only 3 n l and m. And the allowed energy levels are given by this expression is written here and it is the expression exactly the same expression that was obtained by

Bohr according to his theory, but now you see we do not we are not assuming any particular orbit Bohr assumed that there are certain orbit's only those orbits are allowed and. So, electrons were following specific pass around the nucleus, but there is not what we are saying. Now, we are saying that this electron is characterized by its wave function and what we have obtained here is the wave function. Let me now talk about these function a little bit capital phi we have actually studied them in detail.

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The Φ functions

$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$ <p>$m = 0, \pm 1, \pm 2, \pm 3, \dots$</p> $\Phi_0 = \frac{1}{\sqrt{2\pi}}$ $\Phi_1(\phi) = \frac{1}{\sqrt{2\pi}} e^{i\phi}$ $\Phi_{-1}(\phi) = \frac{1}{\sqrt{2\pi}} e^{-i\phi}$	$\Phi_{m,c}(\phi) = \frac{1}{\sqrt{\pi}} \cos(m\phi)$ $\Phi_{m,s}(\phi) = \frac{1}{\sqrt{\pi}} \sin(m\phi)$ <p>$m = 1, 2, 3, \dots$</p> $\Phi_0 = \frac{1}{\sqrt{2\pi}}$ $\Phi_{1,c}(\phi) = \frac{1}{\sqrt{\pi}} \cos(\phi)$ $\Phi_{1,s}(\phi) = \frac{1}{\sqrt{\pi}} \sin(\phi)$
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So, these are the forms of capital phi, capital phi in general it would have the form one by square root of 2 pi e, e to the power of i m phi. This is the general form of capital phi and there that quantum number m takes the values is 0 plus or minus 1 plus or minus 2 plus or minus 3 etcetera. We can take all those values specifically if you say that, if you say that if you say that m is equal to 0 then if the function is just a constant 1 by square root of 2 pi. If you say m is plus 1 or minus 1 if it is plus 1 you have that solution while it is minus 1 you have that solution.

Similarly you can go and write in other solutions it is very straight forwards, but you should notice that if m is plus 1 or minus 1, what happens is that the solution is actually a containing square root of minus 1 right i is there, this is quite fine there is absolutely no problem with this. But it is rather difficulty visualize a wave function which contains both real and an imaginary part is difficult because you have to plot the real part, then you have to plot the imaginary part and then thing of its magnitude and so on.

So, chemist actually do not make use of this function these two functions, they do not use this is something that I have already told you, what they do is they combine these two for instead of they can combine these two and get a get solutions, which are of this form. For example, you can say get a solution which is of the form $\cos \phi$ than that we will have a normalized section factor of 1 by square root of pi over we can get a solution, which is of the form $\sin \phi$ and the normalization factor is again 1 by square root of pi right. Not only for this case when m is equal to plus or minus 2 you can do exactly the same thing, and you will get solutions which are of the form $\cos 2 \phi$ over $\sin 2 \phi$.

Let me make it a little bit clearer if you had m equal to plus or minus 2 you are going to get e to the power of $i 2 \phi$ over e to the power of $-i 2 \phi$, but e to the power of $i 2 \phi$ actually contains the cosine of 2ϕ plus $i \sin 2 \phi$, we know this result from mathematics e to the power of $i 2 \phi$ actually contains both cosine and sin. So, what you do is you actually combine this two, so that you will get only the cosine or only the sin. The advantage is that the solutions are then real and you are able to visualize it; chemist, usually prefer to have functions which they can visualize. So, that is regarding the ϕ functions and then if you think of theta functions.

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The slide is titled "The Θ Functions" in blue text. It contains three equations:

$$\Theta_l^{m_l}(\theta) = \sqrt{\frac{(2l+1)(l-|m_l|)!}{2(l+|m_l|)!}} P_l^{m_l}(\cos\theta)$$

$$P_l^{m_l}(z) = (1-z^2)^{|m_l|/2} \frac{d^{|m_l|}}{dz^{|m_l|}} P_l(z)$$

$$P_l(z) = \frac{1}{2^l l!} \frac{d^l}{dz^l} (z^2 - 1)^l$$

In the bottom left corner, there is a circular logo with a star-like pattern and the text "NPTEL" below it, with a small arrow pointing to the right.

I have told you these solutions how they are obtained and I have also told you that you can get this function by using recursion relations. And if instead of doing that we can

make use of knowledge available from the mathematicians. Remember how we went about the process of a doing the solution, actually we said that we have the function theta and that we change the variable to z was defined to be $\cos \theta$, if you remember we change from $\cos \theta$ we will write small variable θ to something called z is defined to be $\cos \theta$.

And then remember we had put $1 - z^2$ will I may be I should write this let me just remind you the process of solution, we had the function θ of small θ . We made this change of variable z is equal to $\cos \theta$ and function was then denoted by the simple p , p was a function of z . And then what we did we do we substitute it p is equal to $1 - z^2$ to the power of m by 2 in to g of z and then we found an equation for g .

See if you look at the things that are return see you find that that $1 - z^2$ to the power of m by 2 there, and this is actually your g , right this is your g , but return in a notation that is familiar that is borrowed from mathematics. So, therefore, what happens is that this is actually your g and if you wanted to calculate the g , what should you do? It says that you have to take the m th derivative of P , that is what this equation says. And what is P , P is define by this equation P is define to be well there are this derivatives maybe I will use this definitions to calculate one of the functions.

For example, let me imagine that I am interested in θ , 0 of small θ , suppose I am interested in that the formula will give me that is that square root sign, why do you have this factors square root of 2 plus 1 in to $1 - m$ factorial divided by $1 + m$ factorial. And there is a 2 here you should recognize that this is nothing but a constants, which multiplies the function why do you have the such a constant answer is I extremely simple, this is the normalization factor. Any wave function would be multiplied by certain things. So, as we ensure normalization. So, the normalization factors for these functions I have been calculate and it is just that.

And in this equation if you are interested in the in this particular function you will have put l equal to 1 and m equal to 0 that is how you will proceeds. So, put l equal to 1 and m equal to 0 we will do that and then this is multiplied by d to the power of 0 by z to the power of 0 of P z . And specifically if you say l is equal to 1 is equal to 1 you are going to get 3 by 2 , it should be 1 factorial divided by 1 factorial square roots d to the power of

0 by d is said to be d to the power of 0 is just now operation, you will get P_1 of z that is all this is fairly straight forward.

And what is P_1 of z that is define their P_1 of the z according to the last line would be given by 1 by 2 to the power of one factorial d by d z right its says to the power of 1 , but I have put 1 equal to 1 in to e z square sorry operating up on e z square minus 1 . This is your function and what is this, you can carry out the differentiation d z square minus 1 . If we differentiate you are going to get $2 e z$ and that $2 e z$ and this two are going to cancel. So, you will simply get the answer z right.

So, what is θ_1 that may be this value of p z may be put back here. So, of the answer is going to be square root if 3 by 2 in to e z , when the answer as we can say it is fairly simple square root of 3 by 2 $e z$ what is $e z e z$ is nothing but $\cos \theta$ because $e z$ is our variable that we had introduce. And therefore, θ_1 of θ is actually simply square root of 3 by 2 was this right.

So, in a similar fashion if you are interested in any particular solution in any particular θ that is a 1 is equal to 2 and m is equal to 0 , you can just use this formulae. I do not think I will need I will do other examples, but it is fairly straight forward all that unit is if θ if 1 is equal to do just put two here and may be 1 is equal to 2 and m is equal to 1 . That means, you see you will have to put 1 equal to 2 here instead of that 0 you will have to put one there. Then you go ahead and do the calculation you will get the function right. So, the functions which are calculated in this fashion I think they are probably there. In the next few slides, but before I do that let me look at the capital R the function capital R .

Capital R depends up on n and l and it is a function of small r and it is a little bit, I mean this is more messier than the previous one, the previous one itself you may say it is little messy, but if you look at it, it is not that figure you can for any given values of l and m you can easily calculate the function using the formula. So, capital R in a similar fashion can be calculated using this formula, you look at this expression well there is a constant here that f naught yet introduced, but I will introduce, what is the constant?

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$$R_{21}(r) = - \left[\frac{2}{2a_0} \right]^3 \frac{(2-1-1)!}{4 \times 3^3} e^{-\rho/2} \rho L_3^1(\rho)$$

$$= \left(\frac{1}{a_0^3} \frac{1}{27 \times 4} \right)^{1/2} e^{-\rho/2} \rho L_3^1(\rho)$$

$$L_3^1(\rho) = \frac{d^3}{d\rho^3} L_3(\rho)$$

$$L_3(\rho) = e^\rho \frac{d^3}{d\rho^3} \rho^3 e^{-\rho}$$

Well we have defined rho to be equal to 2 alpha R, what was what was alpha? Alpha is equal to mu e square divided by h cross square 4 pi epsilon 0. So, let me do that let me write that. So, rho is equal to 2 times mu e square divided by n h cross square 4 pi epsilon 0 in to r gradient. Now, this constant this whole thing I am going to call it 1 by a 0, that whole thing is 1 by a 0. So, that I would have 2 divided by n a 0 in to r to be equal to rho.

Now, you may ask why did I do that that step, why did I introduce this 0? The reason is that a 0 is something that is very physical. Remember the Bohr theory, in the Bohr theory you are saying that the electron follows circular orbits, and there is its first Bohr orbit with the quantum number n equal to 1 and that has a specific radius. If you remember that radius is nothing but this a 0 right, if you looked at the expression you can go back and look at the expression you will find that this. What is the definition of a 0? A 0 is define to be define by this equation 1 by a 0 is equal to mu e square divided by h cross square 4 pi epsilon. So, we if you define a 0 to be this then it is just the radius of the first bore orbits.

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The R-functions

$$R_{nl}(r) = -\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n(n+l)!^3}} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho)$$

$$\rho = 2\alpha r = \frac{2\mu e^2}{n4\pi\epsilon_0\hbar^2} r = \frac{2}{na_0} r$$

$$L_p^s(\rho) = \frac{d^s}{d\rho^s} L_p(\rho)$$

$$L_p(\rho) = e^\rho \frac{d^p}{d\rho^p} (\rho^p e^{-\rho})$$



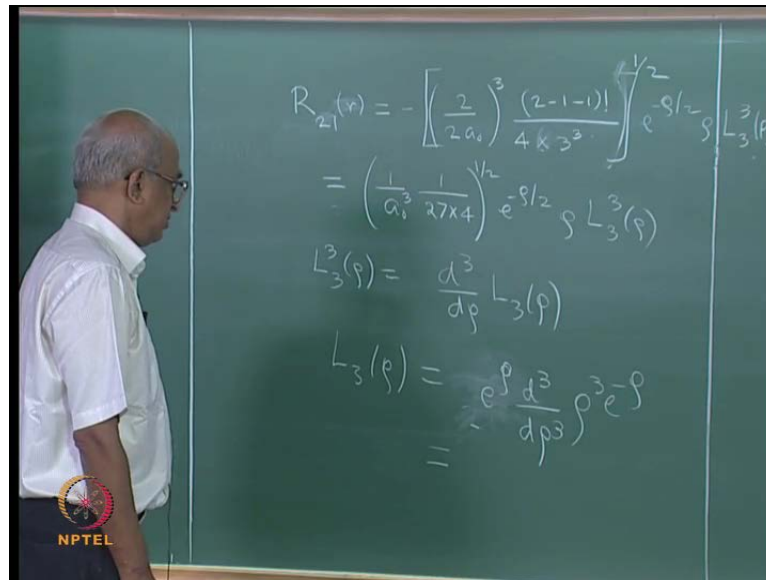
So, now if you look at this expression you have rho equal to 2 divided by n a 0 r and what is capital R, capital R is defined in terms of rho, rho we have already defined. As well as a 0 as well as the principle quantum number n right which we have encountered. So, this is the definition and why do we define why do you have this part here, this part answer is extremely simple you want the wave function to be normalized. So, this is the just normalization factor, and then remember in our method in our solution solving process we had actually introduced e to the power of minus rho by 2, remember in the solution we had said that is the c to the power of minus rho by 2. And then we had introduced the rho to the power of s and found that that rho to the power of s is actually a rho to the power of l because this is equal to l.

So, therefore, rho to the power of l then the remaining part is written here these are actually known as Laguerre polynomial. So, the Laguerre the name is here it is a French name I do not exactly know how to pronounce it French names are not usually pronounced the way they are written then follow the spelling and pronounce it, but there is what I have done Laguerre polynomial. So, how do you calculate Laguerre polynomial?

The prescription also is given here, this see you have to follow this definition, it depends up on two numbers, p as well as s let us say L p L s sorry L p and s, where you see here for example, l capital L depends up on n plus l and 2l plus 1. So, you have to imagine

that $n + 1$ is written as p and $12 + 1$, temporarily we can write it as s then $L_p s$ is actually defined to be a derivative of L_p and what is L_p ? L_p is defined by this equation, maybe I shall demonstrate this by saying one particular case. We do not have the time to discuss all cases, but one particular case.

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Let me take where should I take may be not the simplest possible case, let me say R_{21} . So, that it will be a little bit complicated. So, if you think of R_{21} what is going to happen is I am going to have minus 2 by n is 2, so $1 - 2 = -1$ to the power of $3 - n - 1$ minus 1. So, $2 - 1 - 1$ factorial divided by 4×3^3 right I am jumping some steps and just substituted the values of n and l in this in this expression right in this expression, I substituted it the values of n and l n is equal to 2 and l is equal to 1.

And then what would I have left I would have e to the power of minus ρ by 2 ρ to the power of 1, 1 is one. So, $\rho^3 L_3$ and $12 + 1$ is how much 3. So, that is my function, what is it simpler count to be 1 by 0 to the power of 3 this is 0 factorial which is 1 divided by 4 in to this is 27 to the power of half e to the power of minus ρ by 2 ρ L_3 , 3ρ , this is what I have.

Now, what is the $L_3^3 \rho$, well I realize as now taken one of the easiest, this may be a little bit difficult let see $L_3^3 \rho$ is actually a third derivative of $L_3 \rho$, how did I get that? You just look at this expression you just look at this expression a p is 3 and s is 3.

So, you just use that you will find this and what is $L^3 \rho L^3 \rho$ is 1 by 2 to the power of 3 , I am using the does not correct it is equal to the e to the power of ρ d cube by d rho cube rho cube e to the power of minus rho. I realize this is a little bit difficult for me to perform I can do it, but it will take time.

I think I will work it out I may actually work it out using a computer program called mathematic here, but I do not think I will do it now, it's fairly easy if I use the mathematical programs. So, what would be the answer, I think I shall give it as an exercise I shall work it out and show you in the next lecture. So, this is how the calculation will proceeds.

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The Hydrogen Atom - Radial Wave Functions

n=1, K shell:

$$l = 0, 1s \quad R_{10}(r) = \left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0}$$

n=2, L shell:

$$l = 0, 2s \quad R_{20}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{2\sqrt{2}}(2 - \rho)e^{-Zr/2a_0}$$


$$l = 1, 2p \quad R_{21}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{2\sqrt{6}}\rho e^{-Zr/2a_0}$$

n=3, M shell:

$$l = 0, 3s \quad R_{30}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{9\sqrt{3}}(6 - 6\rho + \rho^2)e^{-Zr/3a_0}$$

$$l = 1, 3p \quad R_{31}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{9\sqrt{6}}(4 - \rho)\rho e^{-Zr/3a_0}$$

$$l = 2, 3d \quad R_{32}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{9\sqrt{30}}\rho^2 e^{-Zr/3a_0}$$



So, once you have if I determine these things, you give me any value of n l m , I have given you how to calculate phi we know how to calculate phi that actually is very simple. We know how to calculate theta and we know how to calculate R, like this only the question of substituting the values and doing this steps at we have seen just now and. So, you will get the total wave function. So, let us look at this function so 1 by 1.

Now, again I should introduce a few definitions actually this work this part of the wave function, if you look at it that determines how the wave function changes as you go a wave from the nucleus. It is referred as the radial part of the wave function right, how does the wave function change as you change the distance of the electron from the nucleus. While the remaining parts they are dependent only up on the angles this is

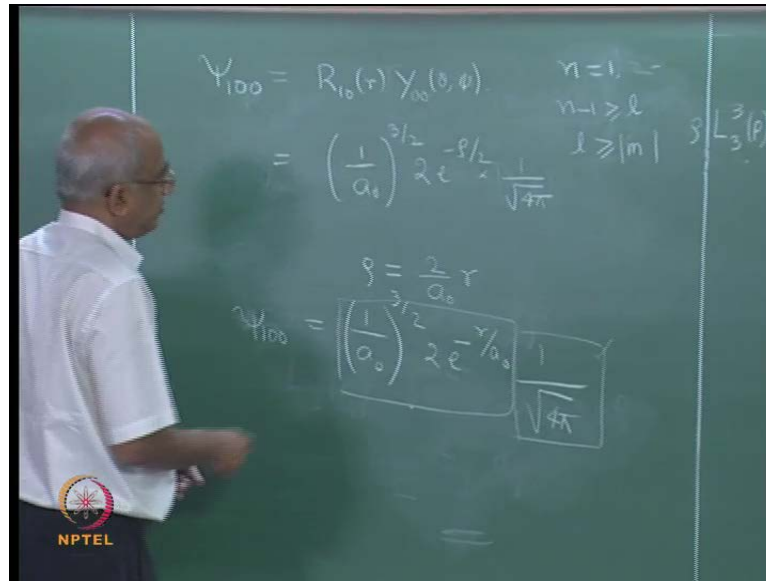
dependent only up on the angles theta and phi. And what do these angles determine? If you remember this angles actually determine different directions in space they do not say anything about the distance of the electron, but they say in which direction the electron is located right.

So, this is refractive of the angular part of the wave function, while that is refractive as the radial part of the wave function. And further usually this product, this product is denoted by the symbol Y with a suspect l and suspect m and it is a function it is written as a function of these two angle variables, which actually denote directions in space as I have told you. Again the reason is that this function were studied by the mathematicians this functions are known as spherical harmonics, this to together are not or denoted as capital Y and they are known as spherical harmonics. So, let us look at the wave the wave functions one by one.

If we looked at the expression for energy, where is my expression for energy the expression for energy is actually sitting here right. You find that there is this minus 1 by n square, this is actually of the form the energy is of the form minus 1 by n square in to something, which is a constant. That is of the form of the energy is, see if you put n equal to 1 remember n is a quantum number which can take the values 1, 2, 3, 4, 5, 6 etcetera. You would realize that n is equal to 1 will be the lowest possible state of the system because if you put n equal to 1 you are going to get minus 1 in to that constant.

Here you put n equal to 2 you will find a number, which is greater than the previous one because you see their it is a it is a same number, but multiplied by half multiplied by 1 by 4 over the same number multiplied by 1 by 9, when you put in n equal to 3. And therefore, the lowest possible state of the system which we usually as ground state of the hydrogen atom will be obtained by putting n equal to 1. So, let us say I am interested in that state.

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Wave function n is 1 and we had derived these conditions on the quantum numbers, whatever the conditions n has to be and integer greater than or equal to 1. So, we have taken 1, l n minus 1 has to be greater than or equal to 1, this is another condition that we have derived. And the third condition was with l has to be greater than or equal to magnitude of m , this was the conditions that we derived. And therefore, if n is one second condition implies that l can have the value only 0, that is what you find and if l is 0 m can have only the value 0.

So, therefore, the moment use a n is 1, l has to be 0 and m has to be 0 there is no other way and this is the only solution with n equal to 1, and that solution has energy which will be obtained by putting n equal to 1 here. So, that is the ground state of the system and what you find the ground state of the system has only one solution, we say that this is an energy level that is known degenerates. If you have more than one state you say it is degenerate, but here there is only one state having this particular energy.

So, what is the form of this function well it is going to be R_{10} of small r right, what am I using I am using this expression R_{10} and to the other part is capital Y , I will use the notation capital Y_{00} of theta phi. But what is the capital Y_{00} , this makes that l is 0 and m is 0. That is actually going to be theta 0 0 of a small theta in to phi 0 small pi, this is what it is and this we have already evaluated its value is 1 by square root of 2π . And this one I hope I have I have it in my tables, which we will make use of well it is not

given separately, but the I thought I all that happens is that θ_{00} is just $1/\sqrt{2}$ not in my tables, but the result is just if we calculated it you will find that it is $1/\sqrt{2}$.

Therefore Y_{00} actually happens to be $1/\sqrt{4\pi}$ and R_{10} itself is written here I told you how to evaluate this why will not go into its evaluation, if you look at this expression there is a small chance that you will get confused because there is a capital Z sitting there. I will tell you what it is, but there is a 0 which your familiar and then two the power $3/2$ and 2 into a to the power of $-\rho/2$ ρ is already defined. So, what is this capital Z said when you say this particular expression is valid not only for the hydrogen atom, for the hydrogen atom nuclear charge is unity. It is also varied if you remember, I said treatment that I am going to give you is varied even if the nuclear charge is 2 positive charges or 3 positive charges or any number of positive charges, but only one electron.

And say and this equation that is written there is valid for any value of the nuclear charge, where the it has been assumed that the nucleus as the charge of plus capital Z into e . So, imagine that the nucleus is actually having Z positive charges. So, that the net charge is Z into e and there is only one electron. So, this may this be valid for helium ion it will be valid $1/2$ plus for beryllium $3/2$ plus and so on. For helium $H e$ plus the value Z will be 2, but because we are interested only in the case of hydrogen atom all that I need to do is I will take this expression and say that because I am interested in the hydrogen atom this Z is simply equal to 1.

So, what will have R_{10} we know how much it is, it is it is actually equal to this is equal to $1/a^0$ to the power of $3/2$, $2e$ to the power of $-\rho/2$ and the multiplied by Y_{00} that we have found is $1/\sqrt{4\pi}$. And what is the ρ itself ρ is the define to be how much? $2\alpha r$ that is fine, but I have another expression here is this other expression sitting, in times of a^0 ρ is equal to divided by $n a^0$.

So, in this case n is 1 ρ is nothing but $2/a^0$ into r , combining all this thing I will get ψ_{100} to be equal to $1/a^0$ to the to the power of $3/2$, $2e$ to the power of $-\rho/2$ by a^0 into $1/\sqrt{4\pi}$ this is my final answer if I get all this things. Now, this remember this is radial part of the wave function and that is the angular part of the wave function, what as happened you see this is very interesting because the angular part even

though I say that is the angular part it is just say constant, correct it is just a constant. There is no θ over ϕ occurring in that expression, the radial part of course, it depends upon the distance of the electron from the nucleus which is smaller.

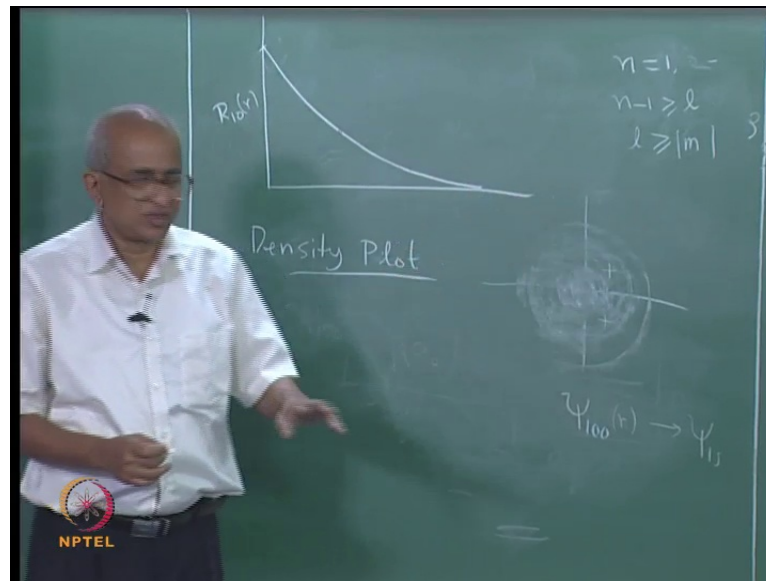
So, what is the conclusion regarding this wave function, see I want to understand this particular wave function and here also would like to introduce a very important word, which I am sure which you are very familiar with. This solution that I obtain represents what it is the wave function for the electron in the hydrogen atom that is an atom of course, as only one electron.

So, any one electron wave function is referred to as an atomic orbital. So, this is an atomic orbital, you give any possible values for n , l and m there is self is an atomic orbital and what we have found is the wave function for the ground state, this is wave function for the ground state. So, this is the atomic orbital for the ground state of the hydrogen atom it has the quantum numbers n equal to 1, l equal to 0 and m equal to 0. So, it is ψ_{100} and it is go it is actually your atomic orbital's one has this is the one as atomic orbital as we are going see.

Now, you look at the angular part angular part is just a constant, this means that if I had nucleus here and I think of a point somewhere here, let us say distance is 5 atomic 5 a 0 right or may be let me make a little bit simpler by saying that the distance of the point is 5 Armstrong's right. So, you evaluated here or you evaluate at that they point somewhere there, whose distance also is 5 Armstrong's. Then you will find that the value of the wave function there as well as here is going to be the same because as per as this two point are concerned the distance is the same, only the angles θ and ϕ are different correct.

So, therefore, you can I can go further I am say that thing of any point on the surface of a sphere having radius equal to 5 Armstrong's, the function is guaranty to have the same value right. And therefore, we say that this is a function that is spherically symmetric, it does not depend upon direction and space it simply depends upon the distance of the electron from the nucleus it is independent of the direction. So, that is the reason, why we say this particular function is spherically symmetric. And further you will you take this part, I want to understand this plot this part how will I understand this part, well the answer is that I will make a plot of this part.

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Be very precise the thing of making a plot of R_{10} , R_{10} is actually a function of small r , I should be making a plot of it against R and this is the functional form. So, if you look at the functional form what does it contain there is a constant the constant is not is not dependent upon distance, what is dependent on distance is this portion will change as you goes the change, the distance of the electron from the nucleus and what happens to that function? Well it is actually e to power minus R by a 0 any exponential function you know of the form e to the power minus R by a 0 you would know that it is going to decrease exponentially, as you go away a form the nucleus.

And therefore, if you made a plot of this it will have its largest value at the nucleus right when R equal to 0 this function, will have the largest value as you go away from the nucleus the function will go on decreasing steadily, this is how the function is. And strictly speaking when is that the function becomes 0 , e to the power minus R by a 0 when is that the function because 0 we can put R equal to 500 Angstroms, still you will have not at 0 , but you will have e to the power of minus roughly 500 right this object is let me say it is 500 .

Then you will have e to the power of minus 500 which strictly speaking it is not 0 , but for all practical purposes of course, e to the power of minus 500 is 0 . But strictly speaking what will happen is that if you made a plot it will go on decreasing it will never

become 0 and unless you are at an infinite distance. So, this is the dependence up on distance, I have told you that the function is spherically symmetric.

So, what I want to do now is to combine these two information, I know how it depends up on distance I know how it depends up on the angles, if I want to combine these two information's and to make a plot, which will give you both the information's, how will I do that? Well the usual procedure is to make use of what are referred to as density plots.

So, if I have a function you see the function actually will have different values in different regions. Suppose, you have space the function is defined everywhere in space at each point it will have a certain value. So, what I am going to do is I am going to represent the function by shading, simply by shading using my chalk, but wherever the value of the function is large, I will put it large density of shading. While wherever the value of the function is small, I will have a very lesser density for shading.

And if the value of the function is 0 then actually I will not have any density there, and though you may run the problem, well if you suppose the function is negative, what you do there? Again I will just worry about the magnitude of the function and put shading, but then I have to tell you that in this region the function is it is negative. So, I will put a negative sign in that region. So, that is the usual procedure that I will adopt.

So, if I did that with this particular function what is going to happen? It is my nucleus varies if that this function has the largest value it has the largest value at the nucleus. So, therefore, the density of shading is going to be maximum at the nucleus and as you go away from the nucleus, the density of shading will decrease and eventually when you go further and further away, the density of shading will simply go on decreasing. And this is how you would represent this particular function this is ψ_{100} instead of writing ψ_{100} , I will also write ψ_{1s} because this is what we referred to as the 1s atomic orbit. So, this is the way in which I can represent this atomic orbit, the density of shading will be maximum at the origin and as you go away the function is going to decrease correct.

Now, this is the wave function, but I can or when the of course, I should also tell you that this particular function is positive everywhere right the function you look at it, it is everywhere positive. So, therefore, it you would also indicate that they become positive signs and you will see that this is the way one s atomic orbit it is represented in your textbooks. But then if suppose I am in you may say that well after all it is not the wave

function, but the square of the wave function that is interesting, you can say that definitely why because this square gives you probability density right.

So, if you like you can even make a plot of R_{10}^2 because this is the wave function you can take the square of that or you can take ψ_{100}^2 and construct a plot just like this. And I am not going to do that why the reason is simple the appearance is going to be just the same, it will have its largest value at the origin and as you go away from the origin the function will simply decrease right.

So, now, I want to ask a question, what is the probability that the distance of the electron from the nucleus lies between R and $R + dR$ or to be very much clearer. I want you to think of a distance of the electron being 5 angstroms and 5 point may be naught 1 Angstroms. So, I want to say what is the probability that the distance of the electron is between 5 and 5 point naught 1 Angstroms, this is something that we are going to calculate. I think I will stop here and continue in the next lecture with this question.

Thank you for listening.