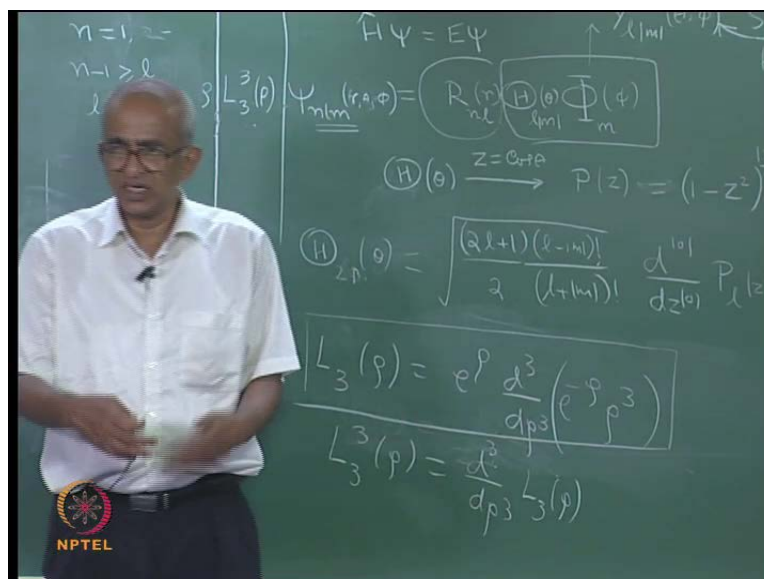


Introductory Quantum Chemistry
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Lecture - 27
Atomic Orbitals –Part II

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Well, before I continue with what I was talking you will see there was fine where I wanted to evaluate L_3^3 row and that we would defined as d to the power of 3 by the ρ to the power of 3 L_3 row itself involves differentiation. So, L_3 row is, so it is given by this expression but this there are 3 differentiation of this object, it is, it t d s and therefore I can do it in the lecture.

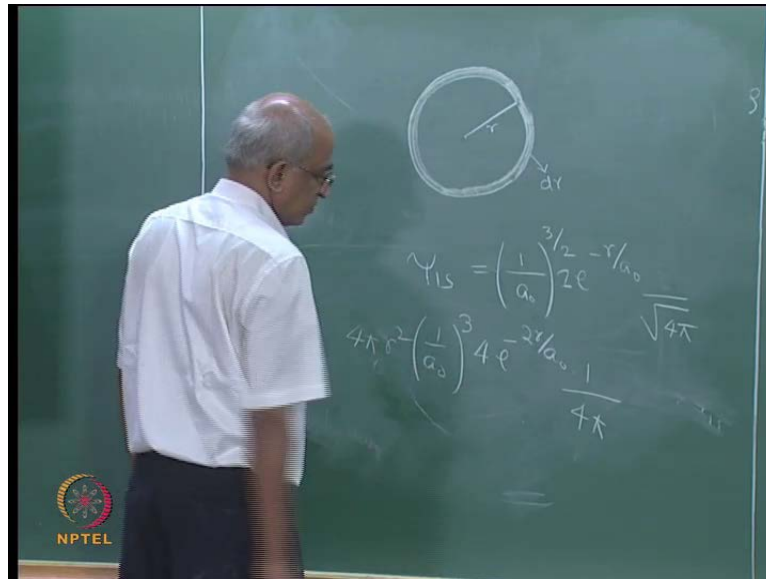
But, I can get a software like mathematicate to do the differentiation and all that you have to do is write this simple commands and I get the answer, the answer is actually 6 minus 18 ρ plus ρ 9 ρ square minus ρ cube. So, this I will you will have to go to here, so this is actually 6 minus 18 ρ plus 9 ρ square minus ρ cube, so that is this object and then you have to carry the 3 differentiation of that. When you carry 3 differentiations you will see this is going to be 0, that is going to be 0, this also will be 0 only this term will give you non 0 contribution and that is going to be minus of 3 into 2 into 1 that is all.

Therefore, what is the answer minus of 3 into 2 into 1, it is minus 6, so this objects if a valuated using all this formula which looks complicated you get the simple answer this is known as 6. So, this minus if you will have to put into the expression for the wave function that is all, so coming to the question that I was asking you. What is the probability that that the distance of the electron with from the nucleus is between 5 and 5.01 Armstrong, again I discussed that you say I disposable for make to use mathematical. To get produce this kind of density plots, for the wave function and that I have clear in this picture this is the density plot it is not exactly done, the way I have told you the mathematics I have put its own color.

But, if you look at the plot you will see that there is a concentration of density in the middle and as you go away with this is actually color coded. So, far away you will realize blue actually corresponds to 0 in this picture, so far away the wave function almost is very small and as you approach the from infinity. Let us we can see the value, here if you see where the value is actually 0.047, value of the wave function and, here it has increased the value is twice the previous value. Then when you get further that closer you find that the value goes on increasing and not only that anywhere along this circle what will happen the function is spherically symmetric.

So, it has big sizely the same value and as you approach the nucleus you will see that the value of the function goes on increase, so that is what I was telling you. But, now going back to this question I want to generalize and I want to ask what is the probability that the distance of the electron from the nucleus lies between r and $r + dr$, how will I answer such a question. Well if you say that the distance of the electron is equal to r where will the electron be, it can be anywhere on the surface of a sphere having radius equal to r . If you said that the distance is r equal to $r + dr$ then that means that you have to think of this slightly larger sphere let me just draw this two spheres on the board.

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So, here is my first sphere it has a radius equal to r and, here is my second sphere I mean this is not such a nice second sphere, but this is the best I can do and this has the radius equal to r plus dr . Therefore, the thickness of this part, this is how much it is dr obviously and, therefore we will see if you say that the difference of the electron is between r and r plus dr . It actually means that the electronic is anywhere inside this spherical shell, it is inside anywhere inside this spherical shell I want to mark that spherical shell.

So, if it I will raise any where inside this spherical shell its differences between r and r plus dr , so if you wanted to calculate the probability that the electron is in that region what should you do. Well first of all you will have to evaluate the wave function I think inside this spherical shell at any at any point inside the spherical shell what will happen the distance is the same from the nucleus. Therefore, the value of the wave function, here or there it is going to be the same and r the distance of spherical shell because dr is a very small amount.

Therefore, what is going to happen is that the r this distance, the wave function is not going to change much it will change slightly, but I am going to neglect that? So, anywhere inside this what is going to happen I will have valuate the wave function what is the wave function it is actually $1/a_0^3$, I do not remember it exactly. Now, I will draw it from my memory you can correct me if I am wrong this is my wave function this

is my ψ^2 , I understand that is the ψ^2 , here this is my wave function. So, with in this spherical shell I can evaluate the wave function anywhere it is going to be the same, so what I will do, then is I will take the wave function.

But, I am interested in the probability therefore I will calculate the probability density which is square of this function, only density is a square of the function and then what should I do I have to multiply by the volume of this spherical shell. Thus, the more the volume is the more is the probability, so what is the volume of the spherical shell, well that you can easily realize by remembering that see a spherical shell as only a small amount of thickness. So, if we multiplied this surface area of the inner sphere by the thickness of the spherical shell you will get the volume of the spherical shell surface area of the inner sphere is how much it is, $4\pi r^2$.

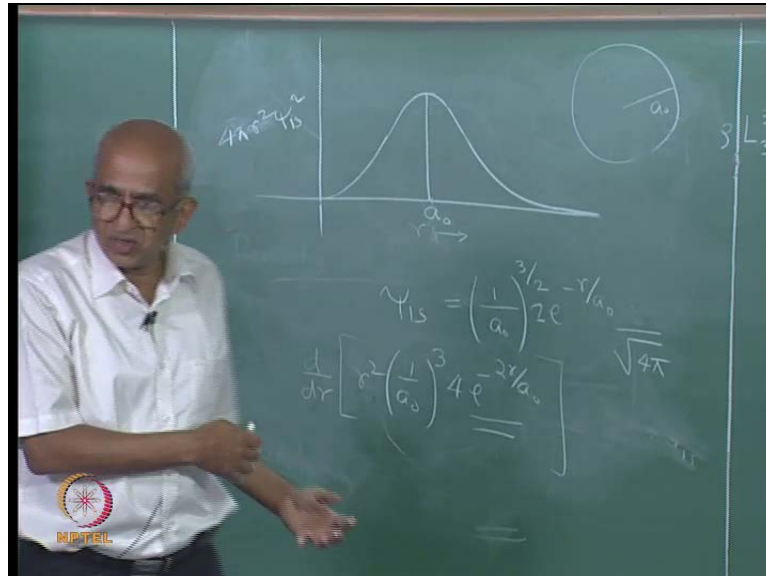
So, you take this multiply this by $4\pi r^2$ and then the thickness of the spherical shell as I have told you is dr , therefore this is the surface area of the inner sphere and thickness of the shell that is dr . So, multiply these things, you are going to get the volume of the spherical shell and this product is what you refer to as the probability. This is your probability that the distance is between r and $r + dr$ it is not surprising that there is dr because if the spherical shell thickness, increase the probability has to increase, therefore it has to be dr and dr has to be there.

So, what I am going to do is I am going to say I am going to define some function what do I call it some by some name that thing multiplied by dr is actually equal to $\psi^2 4\pi r^2 dr$. Therefore, I can define this object to be a function that is interest it actually tells you what the probability is that the distance of the electron from the nucleus is equal to r gives an idea how probable each distance is. So, this object is referred to as the radial distribution function and suppose I made a plot of this radial distribution function what does the radial distribution function give you it gives an idea of how probable a distance r from the nucleus is that is what it says.

So, if you make a plot of this object what would be the result let us look at that result what is it actually you take this square it, when you square it you are going to get $1/r^3$. Then you will get this square of this which is going to be $4e^{-2r} 4\pi r^2$ this is the square of the whole thing. You have to multiply this by $4\pi r^2$, you can actually this $1/r^3$ and that $4\pi r^2$ will go, so the

function actually is quite simple it is just this and suppose if you make plot of this against their the distance r .

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What are you going to get, this is the radial distribution function which is actually nothing but $4\pi r^2 \psi^2$ this is what the object is. So, if you look at this function you will realize that the small distances from the nucleus r is small, so what will happen the function will have a value which is very small why is it was small. Well, the answers you see you have to remember, suppose I asked you what is the most probable position for the electron what it would be.

The answer the most probable position is the position where the wave function has the largest value and that actually in this case is at the nucleus that is the most probable position for the nucleus for the electron. Now, what I am saying is that I am asking what is the probability that the distance of the electron from the nucleus is equal to r , I should say probability density that the distance is equal to r .

Then what you find you find that you have this r^2 , so because of this r^2 what will happen when r is very small, the function will have a small value and when you increase this value of r this function r^2 is going to increase. So, it will increase like this, but the increase cannot go on forever because you have this e^{-2r/a_0} . So, that exponential term, what it will do it will cause the function to decrease,

so eventually what will happen the decrease in the function will become very important and you will have such a behavior.

Now, in this region what is happening is that you remember you are calculating the surface area of the sphere surface area of the sphere is $4\pi r^2$ and the smaller, the sphere is the smaller, the surface area. That is reason why this r^2 is actually occurring in that correct and because of that if you made a plot of the radial distribution function $4\pi r^2$ by $1/S^2$ against r . What do you find you find that, near the nucleus it has a value which is very small, but as you go away from the nucleus the value increases it reaches a maximum?

But, then of course the wave function has to decrease so eventually the probability density probable density that the distance of the electron is equal to r decreases it become 0 at infinity distance. So, there is a most probable distance and this most probable distance is this one and I want to find the most probable distance, how will I find that you can use methods of calculus, how will you use the methods of calculus. It is actually extremely simple this is the plot this is the function that you are plotting you have to differentiate this with the respective r put the derivative equal to 0 and find that value of r at which the function is a maximum simple exercise in calculus.

You will find it and I am not going to do it because it is quite simple you will find that this most probable distance of the electron to the nucleus actually is equal to a 0 radius of the first bore orbit. Now, here again I want to tell you something you see according to the bore theory what was happening is that the electron was actually moving in a circular orbit and that the radius of the circular orbit was actually equal to a 0 that is what bore searched. Now, this is very unsatisfactory if you think about it as a chemise because have to imply that the hydrogen atom is like a plate is it not, I mean it is plain up if you had a circle when the electron was moving in the circle.

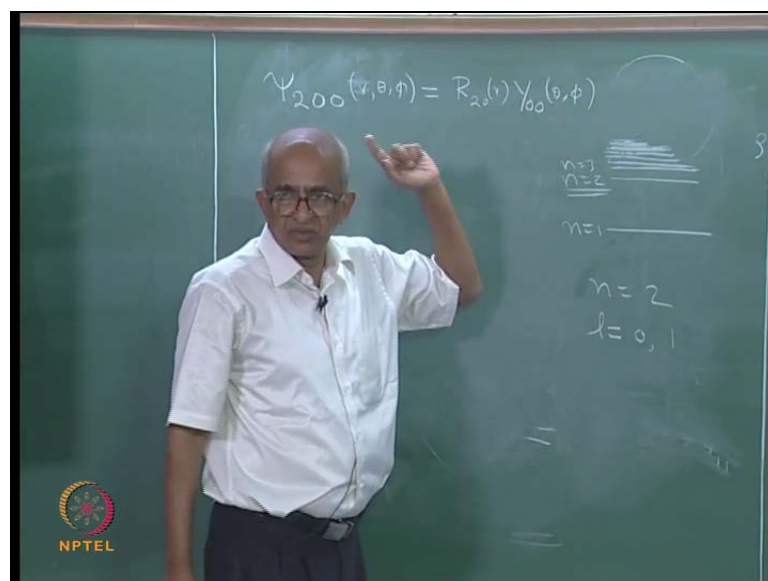
It is actually like a it is a completely a planner thing and I mean suppose you are a chemise you say I have 2 hydrogen atoms approaching thing of the reaction I mean suppose this is one hydrogen atom. This is the other hydrogen and the two approaches, they can approach like this they can approach like that then things will be different. But, there is not what is happening in the in the in this picture, in this picture I take each hydrogen atom, suppose you think of the hydrogen atom the electron is sitting in the

ground state. Each sitting in once atomic arbitrary, each electron once atomic arbitrary you have seen is spherical.

So, it is something resembling as sphere and those sphere is approaching each other right is whether they approach in this fashion or whether they approach in that fashion it is all the same. To do that, this is a much nicer picture of course and of course also the correct picture, but coming back to the bore theory. The bore theory was saying that the orbit is may be a circle like this and I can drawn this a circle of this form and the radius actually is equal to a 0, this is what the bore theory says. But, according to this what happens is that the a 0 is the only most probable distance if you, if you ask what is the most probable distance of the electron from the nucleus it is a 0.

But, there is a chance that the distance will be less than that and there is also a chance that the distance will be greater than that that is what the Schrodinger's wave equation is telling. Now, we will look at other wave functions we will look at the k is where is n is equal to 2, if you have n equal to 2 what will happen if you want to calculate the energy of the system it is very simple you just have to put n equal to 2. Here, that is all right and you will find that the energy is higher than previously in the previous case you had n equal to 1. So, therefore this is higher state, in fact it is the, what is referred to as the first exert that in fact I maybe, I should draw a picture.

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If we put n equal to 1 you will get this as the energy n equal to 1, if you want to calculate the energy you just have to use this expression just put n equal to 1 in there then n equal to 2 is somewhere. Here, n equal to 3 will be somewhere, here n equal to 4, 5, 6, 7, 8, 9 and so on as the value of n increases what happens you see, you have this $1/n^2$. So, what will happen is that the energy actually the levels get closer and closer and closer until n is equal to infinity, if n is equal to infinity what will happen the energy actually according to this will become 0.

Therefore, what happens is that the energy levels actually approach each other, sorry they get very close in the limit and tend to infinity the separation between the allowed energy levels is actually becoming very small. If you tend to 0 as the value of n approaches, so below 0 you have how many levels infinity numbers of levels are there for the hydrogen atom infinity number of levels are there.

Infinity number of atomic orbitals are there in the case of hydrogen atom remember my discussion of how many normal notes of motion for a string I told you that there were a infinite number of normal notes of motions for the string. It is exactly that what is happening, here this I remember this are all actually stationary states are standing wave patterns formed by the electron wave in space this are that is what it is. So, if you ask how many standing wave patterns are possible the answer is infinity and that is precisely what follows some solving these equations.

So, this is how the allowed the under levels are and as I told you I am going to look at n equal to 2, n equal to what will happen I would have ψ_2 if n is 2 our conditions implies that l has to be 1. So, l will be 1, sorry what are our conditions n is equal to 2, l may be 0 or 1, n equal to 1 equal to 2 is not allowed. So, let us think of this possibilities n is equal to 2 and let me say l is equal to 0 and if l is equal to 0, m is 0, so this is the function that I want to look at and obviously this is going to be $r^2 e^{-r/2a_0} \cos^2 \theta$ where it is because l is 0 and m is 0.

So, the function the angular part is just Y_{00} , but Y_{00} is something that we are already familiar with because in the case of the 1 S atomic orbit we wrote this down. We found that this is actually $1/\sqrt{\pi}$ or $1/\sqrt{4\pi}$ and R_{20} , you can evaluate using the formula that.

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The Hydrogen Atom - Radial Wave Functions

n=1, K shell:

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

n=2, L shell:


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

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

n=3, M shell:

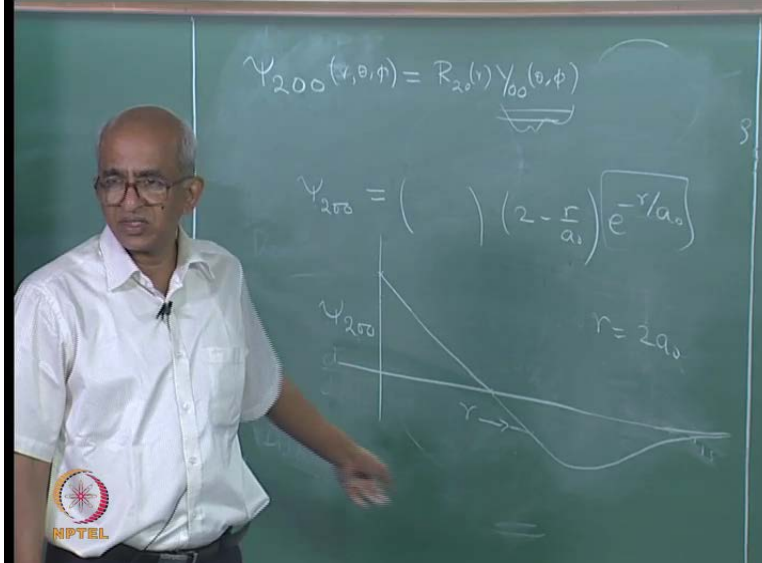
$$l = 0, 3s \ R_{30}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \frac{1}{9\sqrt{3}}(6 - 6\rho + \rho^2)e^{-\rho/3}$$

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

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


We have for example R 2 0 0 is written, here R 2 0 0 is written there you can make use of that and what will happen you will get the total wave function. So, I think the total wave function is there in the right, this is the wave function that is appropriate for the, for the 1 S we have already discussed this I will not discuss this. But, if n is equal to 2 and n is equal to 0, this is the function we have determined the angular part, we have determine the radial part multiplied them together you get this as the answer.



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$\Psi_{200}(r, \theta, \phi) = R_{20}(r) Y_{00}(\theta, \phi)$

$$\Psi_{200} = \left(\frac{1}{4\sqrt{2}}\right) \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$r = 2a_0$

But, what is most interesting is that you find the function Y_{00} and what is that it is $1/\sqrt{4\pi}$ and this obviously or in middle it helps you that this function has more direction dependence. So, this function also is going to be spherically this particular function not only this function if you, if ever you had a case where l is equal to 0, if l is 0 what about the value of m , m has to be 0.

The function that will occur as the angular part will be just Y_{00} and, so it will be $Y_{00}(\theta, \phi)$ and it will always be this $1/\sqrt{4\pi}$, it will not be anything else. So, whenever l is equal to 0 you find that the function is spherically symmetric and it is not necessary for me to discuss the angular dependency, so we have already done it. So, what is left is to discuss the radial part and if you look at the radial part it does obvious that it has this form and this part is a constant and you have the r^2 minus r by a e to the power of minus r by 2 a 0 that is the function.

So, how will they plot of this function look like ψ_{20} is equal to a constant, well we are not terribly interest the exact value of the constant, but what is more interesting is that 2 minus r by a 0 into e to the power of minus r by a 0. This is the object that is of late interest because this tells you how the wave function changes as you go away from the nucleus.

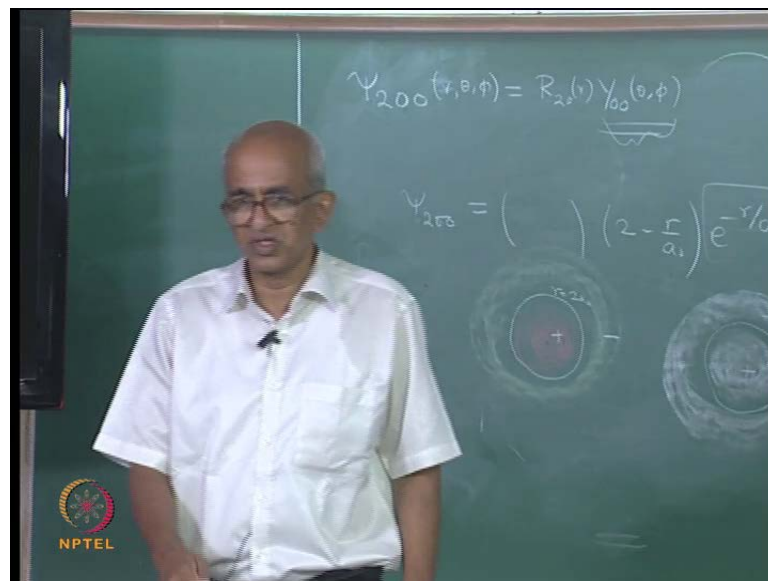
So, first we will make a plot of ψ_{20} against r , what will you find well this part is a constant it occurs for all values of r . So, this we are not terribly interest in this part when you look at this part if r is equal to 0 what will happen this is equal to 0 and this is equal to 1, so the function will have the value 2. So, the function is actually non zero and it will start somewhere here and as you increase the value of r from 0 what will happen to $2 - r$ by a 0 is going to be decrease and this also is going to decrease.

Therefore, the function will start decreasing and in fact when r is such that it is equal to $2a_0$ of course 2 times the radius of the first bore orbit what will happen you will have $2 - 2$. So, the function will be 0, so this will actually decrease to 0 at this point and beyond this point. If you take r to this side what will happen r is actually greater than $2a_0$ which means that this object is going to be negative, so the function becomes negative and as you go further what will happen. Well, you see this is how definitely going to decrease to 0 as r tend to infinity, therefore cannot go on decreasing like this eventually it has to turn around and become 0.

So, this will be the plot, this will be the plot of the wave function against these terms, so what do you find at a distance of r equal to $2a_0$ the wave functions becomes identically equal to 0. So, you say that there is a node for the wave function where is that node is just the point or a point where the wave functions becomes 0 you say that is a node. So, r is seconded $2a_0$ is the node, so when is it that r is equal to $2a_0$, answer is you think of any, sorry not any sphere. But, you think of a sphere having radius is equal to $2a_0$ send at the nucleus anywhere on the surface of the sphere r will be equal to $2a_0$ and down the surface of that sphere.

The wave function will be identically equal to 0 and within the sphere what will happen the wave function will be within the sphere r will be less than $2a_0$. Therefore, you are in this in this region, within the sphere you may be somewhere here, so the wave function will be positive while outside the sphere you are in this region. There the wave function will be negative and, therefore if I wanted to represent this wave function by shading how will I represent the function.

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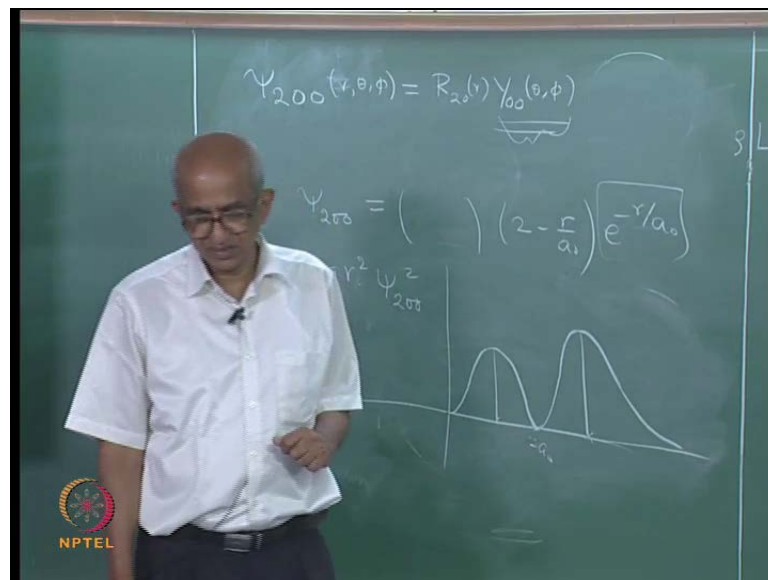
Let me, let me say, here is the nucleus and this is where the function is positive region I will indicate with this color instead of putting plus and minus I will also put plus and minus let me put this color. So, this is how the wave function is, in fact as you will realize the wave function has a non zero, large value at the nucleus as you go away from the nucleus the constant decreases. Here, is the sphere having radius is equal to how

much $2a_0$ r equal to $2a_0$, there the wave function actually becomes equal to 0 inside the wave function is actually positive what about outside.

Outside the wave function is negative and I will indicate that with green color and as you go away from the nucleus what will happen the wave function will steadily go on decreasing that of 4 say it will become 0 earlier. So, in this region the wave function is negative, so this function has a node the node is actually the surplus of S sphere of radius $2a_0$.

Now, if you want you can take this square of this function say that that is the probability density and make a similar plot how will it look like. Well, when we have taken the square the square is going to be positive everywhere, therefore I will just use chalk of white color this is the surplus of the pure of the radius $2a_0$ outside. Again, the wave function has a, I mean the square has a positive values, therefore this is positive because it is density I mean, I do not have to put plus or minus sign it is positive always so. But, the thing is on the surface of the sphere again the square also will become 0, I can also make a plot of the radial distribution function.

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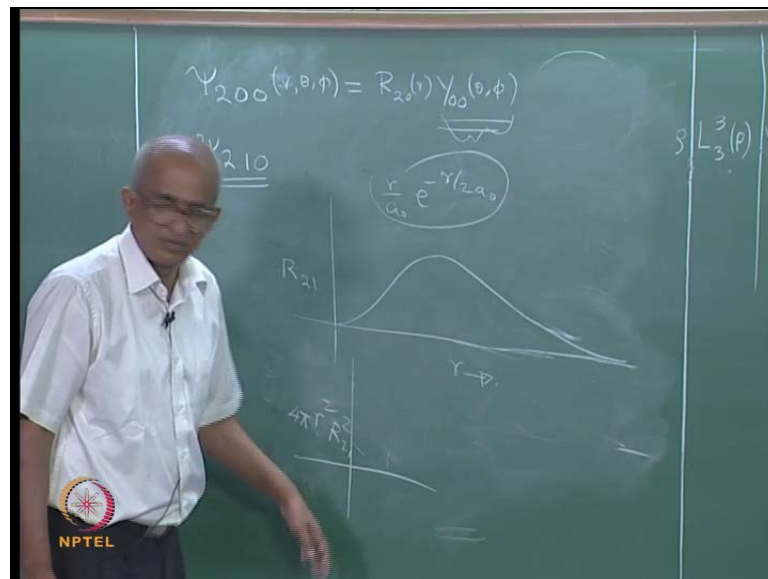


What will that be, it is going to be $4\pi r^2 \psi_{200}^2$ how will you make a plot well it is squarely symbol all that you need to do is take this function, put it there calculate $4\pi r^2$ into that square and make a plot. Well, we can think about it you see we have seen this is the point $2a_0$ there the wave function will become 0.

So, naturally x^2 also will become 0 in this region, what will happen the wave function is positive and non zero, but at the at the origin $4\pi r^2$ then will make the product equal to 0. Therefore, it will start with 0, here it will increase to some value then it has to decrease to 0 at this point because there the wave function is 0 and then beyond that what will happen, the function still is positive. So, it will increase to a larger value perhaps and then it will decrease, so this is how the plot of $4\pi r^2 \psi^2$ for this particular case is going to be.

Then suppose you are ask the question what is the most probable distance of electron from the nucleus what will, what will be your answer well you can say it well you do it is calculus you will be able to find the maxima of this function. So, what you do you take this function differentiated with respect to r at the derivative equal to 0 find the answers till the two values of r will be this one, I do not know how much it is you can easily do, it is not a difficult thing.

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You can find this value as well as that value and say there are two most probable distances one is this one and the other is that and among the two which is most more probable and answer is this is, the second one. This is that is what actually happens, this is the one that is the most probable distance if you remember this plot that I have shown you this is for the 1 S atomic orbital I can make a similar plot. So, the true as atomic

orbital I think it is, here I will like to show you if it is, here no personally it does not seem to be here.

Now, in the, in the let us look at the case where n is equal to 2, n is equal to 2 and l is equal to 1, n is 2 l is 1 and what about m , remember m is constrain to be this is the condition. So, if l is 1 m can be 0 that is a possibility or it may be plus 1 or minus 1, therefore you have $\psi_{2,1,0}$ as one solution, then you have $\psi_{2,1,+1}$ as another solution $\psi_{2,1,-1}$ as the that solution.

So, I am going to have 3 solutions, but then if you look at look that all the solutions, all of them have n equal to 2 if all of them have n equal to 2 what will happen. You look at the expression for energy does not depend up on the quantum numbers l and m , if depends only up on n , if it depends only up on n what will happen all this 4 solutions have precisely the same energy.

So, correspondent to that particular energy we claim that there are 4 difference solutions of a Schrodinger equation. So, we say that this particular energy level is 4 fold degenerate degenerates is 4 fold degenerate because there are 4 space and we will look at the states $\psi_{2,1,0}$ today. Then we will look at the other two later, so $\psi_{2,1,0}$ what is the form of $\psi_{2,1,0}$, I you can evaluate it using the formulary that are there on the board. But, he we will not spend time on that we will just look at the expression this is the expression this function wave already discussed and n is equal to 2 and l is equal to 1.

You can have the functions site $\psi_{2,1,0}$ and what do you find you find that various is this radial part of the function which is which is written here. There is the radial part, there is also the angular part and interestingly this time the angular part it is not a constant, earlier it was $1/\sqrt{4\pi}$. But, here the angular part is not a constant and you find that actually the angular part has the term cosine of theta, therefore what will happen you realize in medley that this is the function that is going to depend up on direction in space.

But, before you look at the direction dependence you can look at the radial dependence of the function the radial dependence is how you see the radial dependence there is this r , r and e to the power of minus r by 2 a 0. Therefore, the function expect for a constant the function was $f_1 r^0 e^{-r/2a_0}$ that is the that is how the function is. So, this is the radial part of the function this is actually r^2 , n is equal to 2, l

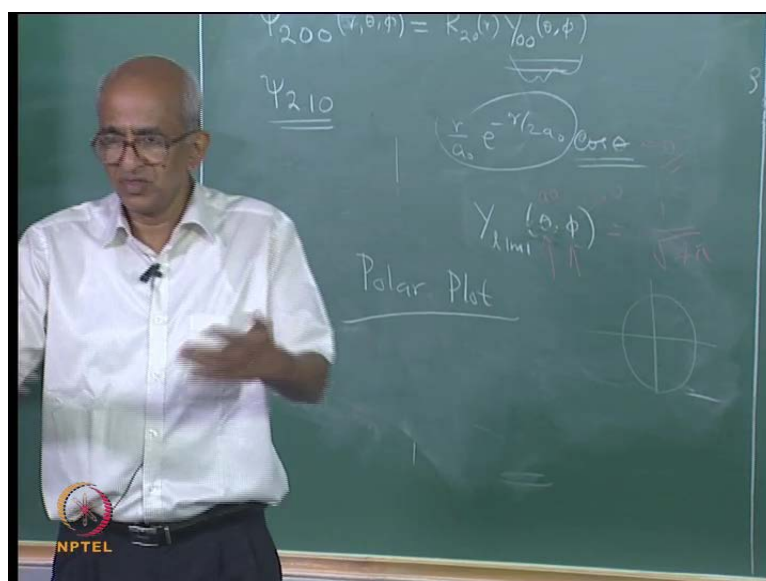
is equal to 1, so the function is proportional to this some factor here which I am not writing.

We can make a plot of this against r , how it will look like well if r is equal to 0 the function actually is 0 if r is equal to 0, the function is 0 and as you go away from the origin the function actually increases. Then it will reach a maximum and the eventually all wave functions when you are far away the wave functions will decrease to 0, so this is how the appearance is, so the most impression thing regarding this function is that the value at the nucleus is actually 0.

But, this was not the case with the S orbital we have discussed to 1 S as well as 2 S, in both the cases the function was non zero at the nucleus. It was 0, it is equal to 0 in the, in the case of l equal to 1 we will find that this in general case whenever l is equal to 0 the value of the wave function is actually non zero.

Only S orbitals, I mean non zero value at the nucleus all the other orbitals that we will see, we will have a value which is equal to 0 at the nucleus. So, the function is actually 0, here you can even plot $4\pi r^2$, but any way I do not think I will go that and doing that $4\pi r^2$ r^2 1 square if you want you can make it plot that is not good. Now, we want to look at the angle dependence you see angle dependence is interesting it contains this factor of cosine of theta in this case it is little bit with simple because there is only theta there is no pi that is how it is.

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So, how will I make a physical picture, how can I understand this function how it varies in different direction what I want to see is I want to understand how this function is in different directions in space. So, in general what is going to happens is that I will have $Y = l \sin \theta \sin \phi$, this is the angle dependent part in the earlier case this angular dependent part was just a constant, but now we have some functions and I want to understand the behavior of this function.

How will I do it and that method that I am going to adopt is referred to us making a polar plot of the function let us, let me imagine that I have the nucleus and I think of any particular direction in space? For example, these is my x axis that is a direction the positive x axis you say direction in space and that will have the value of theta equal to how much 9, 9 theta is 90 x direction theta is 90 and the value of phi is actually 0. Therefore, for a particular direction in space I know precisely what the value of theta is I know precisely what the value of phi, so I can take those values of theta and phi put it in.

Here, for example we just now show that for the positive x direction this is ninety and phi is actually 0, so what I will do is I know the functional form into that functional form I will put the value of 90 and the value phi which is 0. For example, in the, if you have this function $\cos \theta$ you will put theta equal to 90 degrees and phi is not there, so you do not have to worry about that you put theta equal to 90, what will happen this will be actually equal to 0. So, you can evaluate the function this function in any given direction in space correct, so when you evaluated what will happen that this in this particular I got the answers 0.

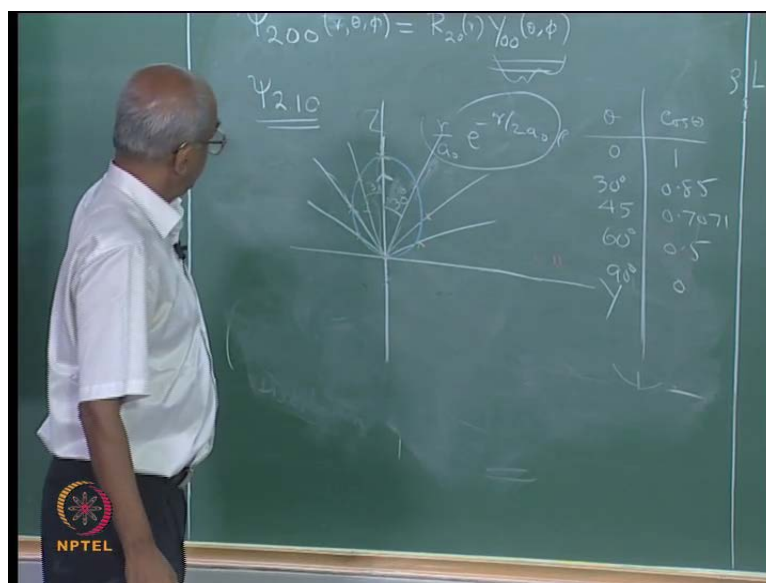
But, may be you will get an answer not 0 may you will get 0.5 for maybe you will get minus 0.5 that also is possible. So, then what I am going to do is this, let us say in this direction I evaluated the function, here is my origin that is where the nucleus is if you like in this direction I will evaluate the function. Suppose I get a value of 0.5 then what will do is in that direction I will find a point such that its distances from the origin is equal to that 0.5 you may ask what will happen if it is minus 0.5. Well, what I will do is I will forget the negative sign, so that the distance will be 0.5, now we will forget the negative sign I may say that well that is arbitrary that why do you that the answer is instead of saying forget the negative.

Then I will say if the function time outs to be negative, I will take the absolute value of the function and put a point such that its distance this equal to that absolute value. So, I will do that for each direction correct, so in this direction I will have a point in this direction, I will have another point and imagine all possible direction in each direction I put a point. Then I will join together all this points and the result is going to be a surface and that surface is what is referred to as polar plot, to illustrate suppose I made a polar plot for 1 S atom orbit for 1 S atom orbital.

This function actually is equal to 1 by square root of 4 phi, so in any direction you evaluate the function answer is going to be 1 by square root of 4 phi. Therefore, what will do you will put a point in space in such that its distances from the origin is equal to 1 by square root of 4 phi and then join together all this points what is the answer this nothing but a sphere surface of sphere. So, you say that the polar plot for an s orbital is what it is nothing but spherical it is a surface of a sphere this is to give you the idea and, now what should I do, I have this particular orbital.

We want to do that for that particular orbital the function is not a constant this not a 1 by square root of 4 pi, but it is actually cos theta may be multiplied by a constant. But, I will not worry about the constant I just need to worry only about cos theta, so what should I do I should make a plot of make a polar plot of this function how on I am going to do that will very quickly.

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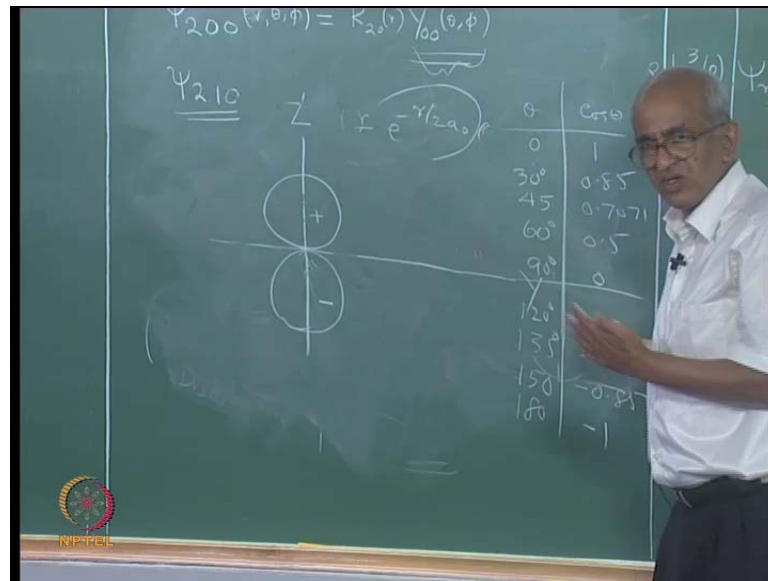
Let me say I have my coordinate systems, this is my z axis this is my y axis and the way it has been put we said that the x axis will like that pointing towards and I am not going to show that. So, what I will do, I will first think of this direction in space z axis and I know that the value of theta along the z direction is equal to theta what is the definition of theta. Theta is the angle between the direction and the positive direction we will see if your direction is this 1, then this is your theta remembers.

So, if I am saying that my point is alone I am think of a direction which is along the z direction then the value of theta will be 0 degrees and cos theta when theta is equal to 0 is 1. Therefore, what is going to happen is that I will have to put a point somewhere here such that its distance from the nucleus from the origin not the nucleus. But, from the origin not the nucleus form the origin is equal to 1 unit, this distance will be equal to 1 unit. Now, suppose you think of a direction something like that such that this angle is thirty degrees 30 degrees you have to evaluate cos 30 degrees, cos 30 degrees is actually a root 3 by 2 and root 3 by 2, maybe I will just write to table.

So, that I have a ready reference to the table I can have a ready reference to the table theta and cosine of theta if theta is 0, this is 1. Theta is equal to 30 degrees answer is 0.85 if it is 45 degrees it actually it is 0.7.71, actually this will turn out to the 1 by root 2 then 50 degrees turn out to be 0.5, 90 degrees is this will turn out to be 0. So, these are the values, so 30 degrees what will happen the point that has to put is at a distance of 0.85 which will be somewhere, here then 45. It will be somewhere here and the 60 degrees it will be somewhere here and I mean why should I concern myself to this side I can also do the same thing with other side because for this direction also it is 30 degrees, this direction is also 30 degrees.

So, theta is 30, so you will have one point, there you will have second point well I am in a hurry because I am finish then I will, here this one and this, what is this. So, I have marked this point and then what should I do, I have to go together all this point what will happen if you, if you think of this direction this 90 degrees, so that point that you will put actually coincide with the original, so going together this point. So, what is the result that you are going to get you are going to get a curve like this when I am not too happy with this figure as I always say that is because I put the points. Then I join them to form curve, what I should I have done is I should have drawn the curve and probably put the point.

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So, let me, let me modify this figure because I want the figure to look correct, actually I made this float what you get is nothing but a very nice circled it is actually a perfect circle. Even though it does not appear to be a perfect circle just touching the horizontal axis that is how the float is in the seminar fashion, you can continue downward, actually if you think of 120 degrees you will find there it is minus 0.5.

Now, you see the function is negative if you think of 135 degrees $\cos \theta$ is minus 0.7071, 150, 150 will find minus 0.85, 180 you will find it is minus 1. So, in all if the downward direction that means you are thinking directions downwards the function is negative and I remember what I told you if the function is negative I am going to take its absolute value. Put points in the downward direction such that the distance is equal to the absolute value, so then what will happen I will get another nice circle looking identical and these 2 circles what do they do.

They touch each other at the, at the origin and then of course in this upward directions the function is positive so I will put a positive sign here and the downward direction the function is negative. So, I will put negative sign there, but remember this plot I have compiled myself to a plain what is the plain it is why is it plain it is that why is it plain that I confined myself. But, suppose I did the same thing in the xz plain xz plain will be this plain at for the xz plain and the yz plain what is the difference between the two you see this plain would have.

Well, if you are on this side actually π is equal to 90° while if you are on the other side π is equal to 270° . But, if you think of the xz plane what will happen the value of ϕ will be different at all, but you look at the function the function has no dependence upon ϕ . Therefore, if you made this plot in the xz plane what will happen if the plot will appear similar, if in fact if I put my hand here and plotted. It is going to look like that and not only that even if you had a plane like that the function will look the same, therefore if you wanted get this actual 3 dimensional appearance of the plot what should we do.

You have to take this figure and rotate it about this is the axis if you rotate it this figure about the z axis you will get the actual 3 dimensional appearance of the polar plot and what is that. It is just 2 spheres having their origins along the z axis just touching each other at the origin, so that is how it is. In fact, we run out of time. So, in the lecture I will show you the polar plots that I have made using mathematics.

Thank you.