Atomic and Molecular Physics

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Lecture – 32
Quantum mechanical treatment of Hydrogen like atom (Contd.)

So far, what we have achieved from Schrodinger equation for hydrogen like atoms? We have achieved that that energy expression n equal to minus mu z square e to the power 4 divided by 2 n square h cross square.

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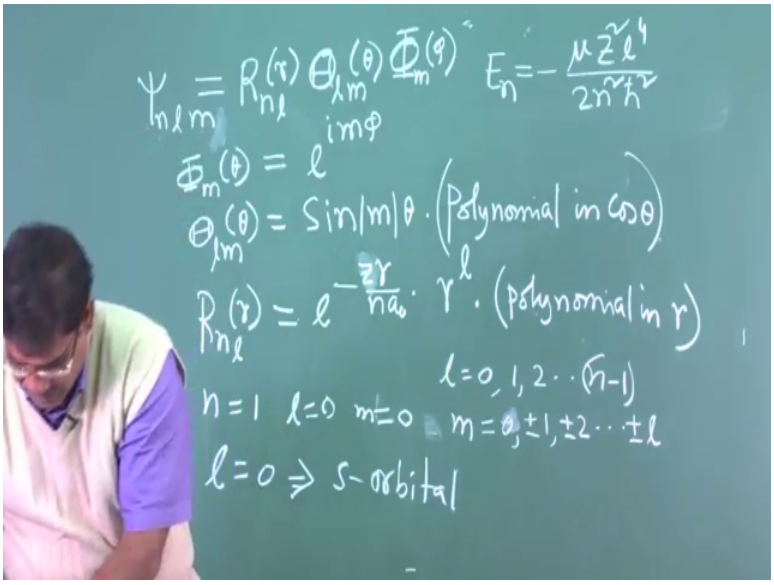

Which is sent from has we have achieved from the Bohr model. But additionally we have got this Eigen function psi n l m.

So now I will not write m l ok, just write I will write simply m ok. In case of m l, I will just write m ok. So, we got the wave function Eigen wave function solving the Schrodinger equation for hydrogen like atom is basically in this form R n l it is function of r, then theta l m function of theta and phi phi m function of phi. Where theta sorry phi m form of phi m is basically e to the power i in phi and form of theta it is l m it is theta this form is think is from is like sin m theta. So, this is the model mod m means positive value, because m value is plus minus value here just. So, positive value.

And this and this then some polynomial in cos theta ok, polynomial in cos theta ok. What is this basically you know this Legendre polynomial ok. So, that is that is so, has it is as a whole means in general it is looks complicated, but for different value of l and m l. So, I am this form are readily available so that we will use whenever we need to ok.

So, and then R n l R n l function of r; so, here just I am not using that part this normalization part. Here 1 by square root of 4 5 etcetera ok. So, these are constant term. So, only I am using this theta phi and r dependent part. So, here in this case on exponential term is there. So, that is basically e to the power it is r dependent basically, I think some constant, I think that is z ah, I think I should write it is basically r by n. N a 0, this I think z some constant terms are there.

But it is mainly e to the power minus r, r dependent part e to the power minus r, and then r dependent another part r to the power l ok, and then polynomial then polynomial in polynomial in r, right polynomial in r in r. So, this polynomial as I mention that what is the form of this polynomial that we know Legendre polynomial like associated Legendre polynomial. So, so these are the so, these are the wave function for hydrogen like, atom and their form is this ok.

Now, so, basically for increasing n and l so, this polynomials are there for increasing n and l. So, this polynomial form of this polynomials are basically complicated. But for first few values of n l and m so, these form of this polynomials are is simple. And let me, so far this first few values of n l and m. So, what are the values of this wave function? What the values of the; what is the polynomials wave function? So, that let me show. in a tell so, for first 3 values of n. So, in table I have shown you here the form of wave function.

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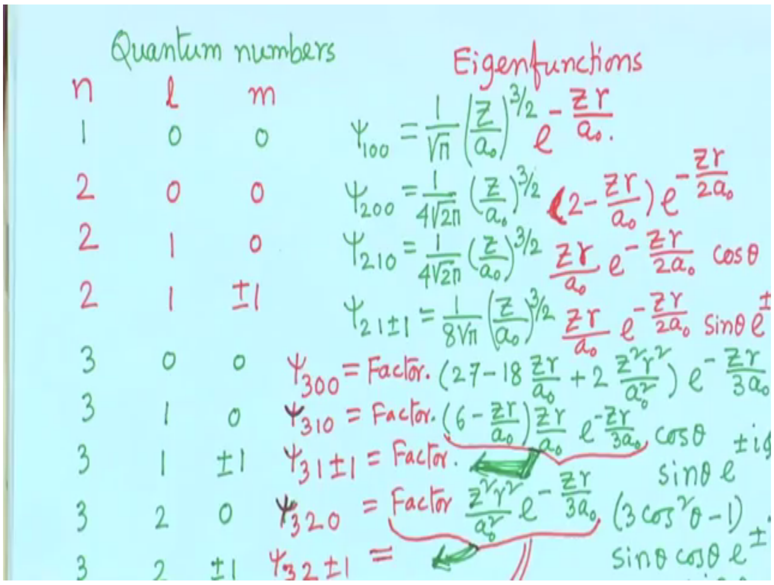

So, what is the form of wave function? Psi n l m? So, what is the complete wave function for first 3 values of n means, automatically for values of n, what will be the l value and m l value that will know. So, that already know that for n equal to for n l is basically 0 1 2 up to n minus 1. So, minimum value of a l is 0 and maximum value of l is n minus 1. And for ` a particular value of l is basically n value is basically yeah. So, 0 plus minus 1 plus minus 2 up to plus minus l ok.

So now, first 3 value of n means, n equal to 1 n equal to first few values n means n equal to 1, what is the value of l and m l? L equal to 0 and m l equal to m m equal to 0 ok, is equal to 0, m equal to 0. So, so far that what will be the wave function? For that what will be the wave function? So, m equal to 0. So, this is 1. So, this part is 1 ok, and for l equal to 0, l equal to 0 ok, for l equal to 0, and corresponding m equal to 0. So, this theta 0 0 theta. So, what will be the; that will be also, it will be 1, if I see thus whatever polynomial I have shown you earlier. So, this form of polynomial, I think I have yes, yes. So, polynomial this the Legendre polynomials.

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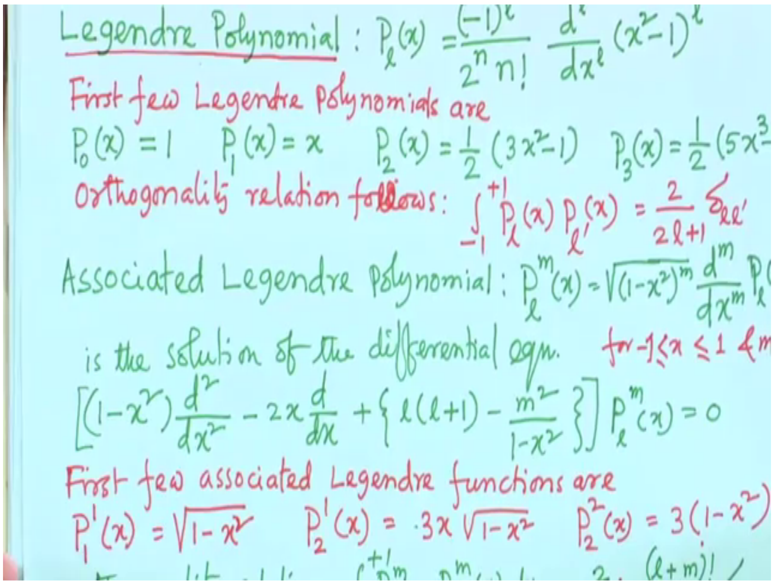

So, first few yeah so, here I have so, Legendre polynomial. So, associated Legendre polynomial. So, P 1 1 is given here. So, P 0 say ok, P 0 there is one basically P 0 P l l equal to 0; so, automatically n equal to 0 n equal to 0. So, that this form of associated Legendre polynomial is is it is get it with this P l P l ok.

So, P 0 that is basically l equal to 0, it is 1. So, this part also will give you, this part also will give you the 1. This part also for theta 0 0, it will be 1, this is 1, and for n equal to 1, l equal to 0. So, r to the power l r to the power 0 this is one ok. So, basically this e to the power minus z r n a 0 ok. And from this polynomials it is one has to seen it comes one basically I can show you, it also comes one if you see this table. It is also comes 1.

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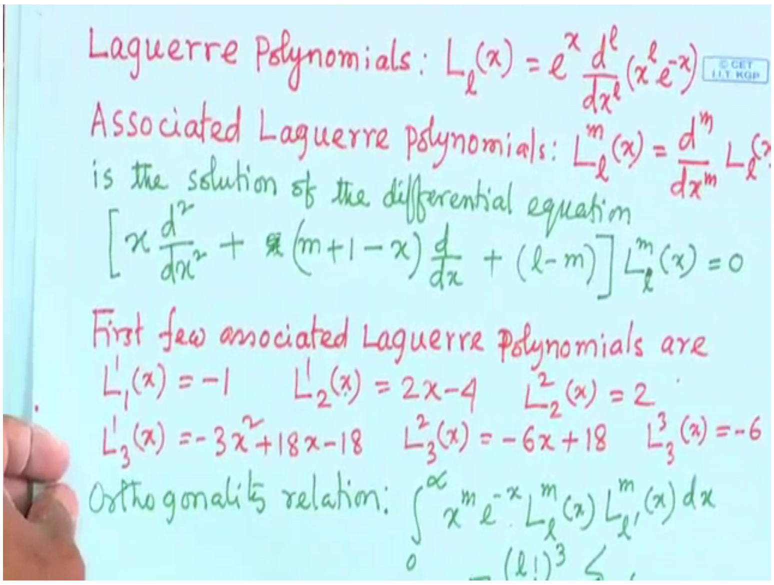

This is Legendre polynomials L 1 1. So, this is the 1 or minus 1 ok. So, so this is the psi 1 0 0 psi 1 0 0. So, this one, this part one this is also one or minus 1. So, only this part list. So, that is why, it is here one can see this psi 1 0 0, it is the so, this is the normalization form normalization part it comes. So, I am not giving takes on that, but exhibits the exact normalized value for this wave function. So, this is the only r dependent part is left. E to the power minus r ok. So, it is changes exponentially with r this psi value psi 1 0 0.

So, similarly we have this we can for n equal to 2 n equal to 2 n equal to 2. So, we will have l equal to 0 and 1 0 and 1 ok. And corresponding m l m value will be or l equal to 0, this is 0 and for l equal to 1. So, this will be 0 and plus minus 1. So, 0 and plus minus 1. And for that you have wave function now psi 2 0 0 psi 2 1 0 and psi 2 1 plus minus 1. And it is form is like this ok. So, these are constant term forget them, but here you can see this, this the it is 2 minus r z r by a 0 of course, and exponential e to the power minus r z r by 2 a 0. Because it was n a 0. So, this part n equal to 2, 2. And here it is for 2, 1, 0. So, this term is there, this now it is this z r. It is basically r e to the power minus r only r dependent minus r, and now cos theta term is there.

Similarly, for psi 2 1 plus minus 1. So, here this term r e to the power minus r, this in this case sin theta. So, this is the this is the theta dependent theta part, and then there will be 5 part because e to the power i n pi. So now, here m equal to plus minus 1. So, that is was it is e to the power plus minus e to the power plus minus 1. So, plus minus i phi ok. So, these are the few wave function Eigen wave function for hydrogen like atom. So, this for n equal to 1, and then n equal to 2 now for n equal to 3 n equal to 3. So, l will be 0, 1 and 2. And for each l again they have you have n value ok. And now, we will get psi 3, 0, 0. Here I have not written this factor and just mention here some factor. This is the r dependent part, this is the r dependent part ok. And here psi 3 1 0 factor this is the r dependant part ok, and this is the theta dependant know phi dependant. But because n equal to 0; means e to the power i n pi. So, that will be 1 ok.

So, similarly psi 3 1 plus minus 1. So, it will have are dependent part, then cos theta term. And then factor no, no, cos theta this factor, this factors it will be repeated. But it will be sin theta dependent, and is it will have phi dependent. So, similarly psi 3 2 0 is the same factor will be here, and then theta dependent term sin theta cos theta e to the power plus minus i phi and psi 3 2 plus minus 2, it will be same this factor, but this theta dependent for sin square theta, and phi dependent for e to the power plus minus I 2 phi. So, from here what we are see, what are the important? What are the remarks we can we can do from this wave function ? That for l equal to 0, for l equal to 0 ok.

So, m l automatically m l will be 0 n n will be 0 ok. So, l equal to 0. So, that is basically s, s orbital l equal to 0, this is basically s orbital s orbital from different orbits; means, from differ different n value for different n value n equal to 1, 2, 3 whatever we here we have shown ok. So, l equal to 0. This is s orbit, and in case of s orbit so, this is basically s orbit. It is independent of theta and phi, only depends on r. Then this is s orbit ok, and here also we can see it is independent of theta and phi ok. But this one is P orbit l equal to 1 ok. So, P orbit depends on theta, it has r dependence it, but it depends also on theta, but independent of phi ok.

And then other part also this when m l equal to plus minus 1. So, it has theta dependent as well as it has phi dependent also. So, here we can see that for l equal to 0, it is independent of theta and phi, for l is not equal to 0, l is not equal to 0. It depends on theta, as well as in some cases is phi. And here also we can see this is l equal to 0 l equal to 0 psi 3 0 0. So, it is also independent of theta, but other all other s s, l is not equal to 0 in depends on theta l is not equal to 0 means P state etcetera. And so, if I plot this wave function so, one can find out is how this wave function varies as a function of r theta and phi. But it is it synthesis 3-dimensional 3 coordinate r theta phi. So, it will be slightly complicated drawing will be complicated ok. So, instead of a draw drawing this plotting this psi n l m, if we plot if we plot just individual wave function of that is R n l, then theta l m, and then phi phi m. So, then it will be more convincing more easy to understand.

So, let us see if you plot wave function R n l as a function of l, as a function of r, how this wave function varies with r so that will see next. So, I think this table will be. So, for plot in so, I can the so, this basically, the plot I got then, next I will this is the polynomial I do not need them basically. So, before plotting this psi or R n l so, you are let us see about the probability.

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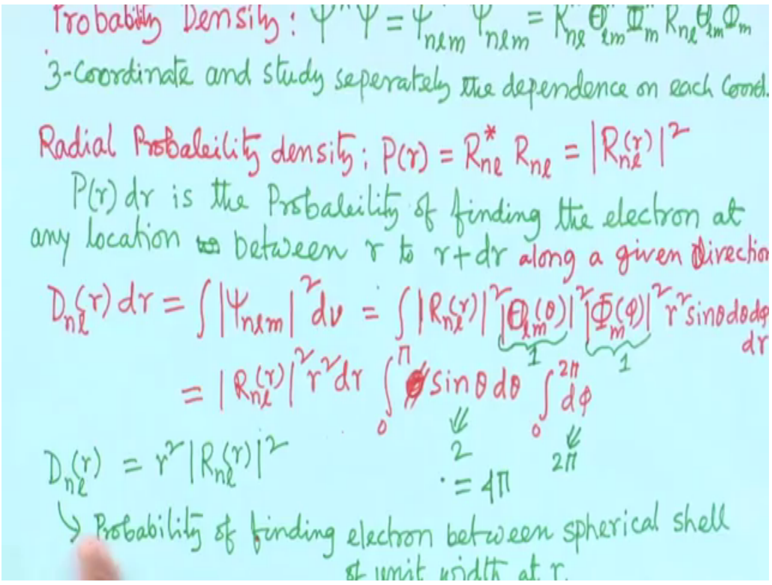

So, as I already mentioned in quantum mechanics, this it is it is difficult to tell the definite value of a of an observable. But one can tell in terms of probability, possibility to find a particle as a at a position or to find the momentum of the of the particle or energy of the particle.

So, so, what so, here I have the form so, here as I mention that will instead of plotting this wave function as a whole. So, will plot this R n l, who is basically it will tell the r dependence of the wave function. So, if we plot this one. So, it will tell about the theta dependent part of the wave function, and this will be phi dependent available. But this so, the behaviour of wave function as a function of r theta phi, that is one thing. It give some information ok. But to get to get more information, that basically we get the from the probability density, and that probability density is defined probability density is defined psi star that is the probability ok, is psi is the wave function psi psi star is the probability ok, 2 2 find the particle at a particular position, or 2 find the momentum of the particle in a in a particular position etcetera ok.

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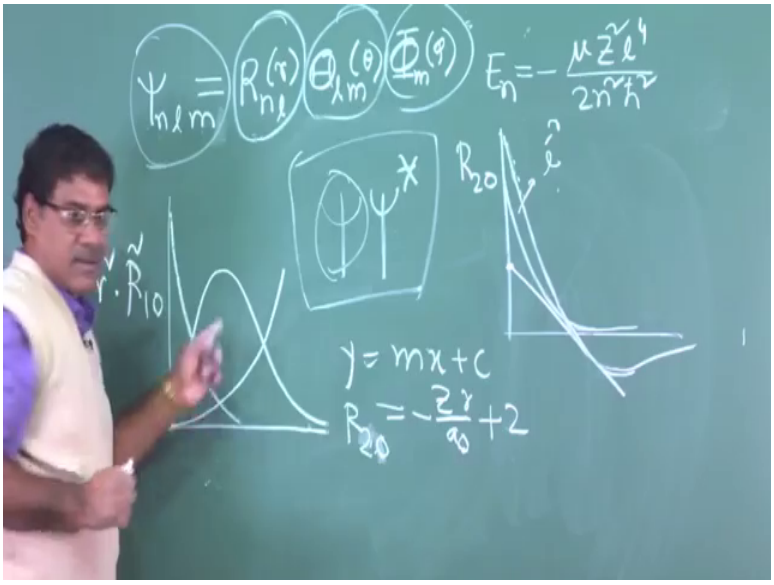

So, this instead of this plotting psi. So, will plot it, it will give some what it will give that will see, as well as this also more important psi psi star one has to plot psi psi star. So, that is the basically probability of probability density. So, so, that is the probability density also one has to plot to get information ok. So, this is the probability density for hydrogen like atom, this is the probability density ok, probability density is depend psi star psi ok. So, that means, we have Eigen function psi n l m. So, this star psi n l m. So, that is basically in terms of we are getting this 3-part R n l, and R n l star theta l m star phi m star ok. So, psi star means this, and then other part is psi ok.

So, basically here we have getting R n l star R n l ok, theta l m star theta l m, phi m star phi m. So, so this probability density for 3 coordinate ah, we can study separately ok. So, one is radial part, one is radial part. So, we are telling that radial probability density. That is, P r we have written here P r ok, radial probability density P r equal to R n l star R n l equal to 1 can write this also R n l R square ok. So, P r what is P r then? Or P r, d r is the probability of finding electron at any location between r to r plus d r along a given direction, r to r plus d r along a given direction. So, radial probability density P r ok, it is basically to find a particle along a particular given direction at distance r, at distance r. So, that is basically P r. And P r d r is is basically at a given distance given direction, what is the probability to find the particle at any location between r to r plus d r ok. So, that is the P r d r ok. So, this is the radial probability density.

Now, not radial probability density. So, it can be expressing other way also. Now this is this P r d r we have written along a given direction between r to r plus d r, what is the probability ok. Now if I if I define other another parameter, that what is the probability to find a particle between 2 spherical shell this spherical shell of radius r and another space sphere sphere of radius r and another sphere of r plus d r. So, what is the problem to find the electron between these 2-spherical shell?

So, that is the further to get the probability density for that type ah. So, that is if we write that is D n l r d r. So, here basically psi psi star d v. Because here theta and phi also that we have to consider this as a whole. So, within this volume between 2 spherical. So, within this volume, what is the probability? So, that I am coming later. So, here if I define this D n l r d r is defined as psi psi star d v that is volume elementary volume if I integrate over this whole volume ok. So, what will happen? So, here theta part is basically it it is angle if I change angle 0 to pi, theta phi part if we by the angle between 0 to 2 pi ok. So, it will have then the second write from here we have seen this R n l square theta l m square phi m square ok. And this elementary volume R square sin theta d theta d phi d r. So, that is already I have discussed earlier. So, here if I integrate over theta and phi not over r, then I can write this R n l square, it is basically R n l square R square from here R square this r theta R square d r. And this theta and phi for theta phi integrate 0 to pi and 0 2 pi ok.

So, this is giving with this, this is giving me 2 and this is 2 pi, this is basically 4 pi. And here normalise part I have not written ok, if I write the normalize part this 4 pi will go ok, here we have not taken normal normalize part. So, remember this for phi it was it was 1 by square root of 2 square root of 4 pi ok. So, if you if you square it ok, because phi m square. So, it will be 1 by 4 pi will come. So, this here 4 pi. So, it will go ok. So, that is the basically so, here D n l r R square D n l R square ok. So, what is the meaning of this D n l as a function of r? This is basically the probability of finding electron between spherical shell as I mention between spherical shell of r and r plus d r ok.

So, it is the theta among for all all theta and phi direction, but distance between radius between r and r plus d r ok, what is the probability? So, this is the P r difference between P r d r and d r d r d r. So, this is the in one case, along the given direction over is the probability between r, r plus d r. And another case D n l function of r d r, there is the what is that is the probability to find the electron between 2 spherical shell of r and r plus d r. Or if I lead this d r so, the D n l r is basically the finding the electrons, electrons between spherical shell of unit with ok, unit with d r is of unit.

Now, so, for unit with at r ok. So, these are the density probability, probability density ah. So, to find the electron what is the probability to find electron when we are going away from the nucleus? So, means at different distance from the nucleus, what is the probability find the electron? Ok. So, that is D n l tells that one ok. And D n l depends are R n l and R n l what is the form of R n l for different value of different value of n and l. So, that we have seen R n l it depends on what exponential term e to the power minus r, that is one part. And r to the power l and then Legendre polynomial ok. And first few polynomial from the table we have seen.

So, basically these are the r n R n l ok, this is the R n l ok, it depends it is so, first one n equal to 1 it depends some is basically exponential it changes exponentially. So, if I plot it as a function of r so, these wave function will be wave function, will be like this.

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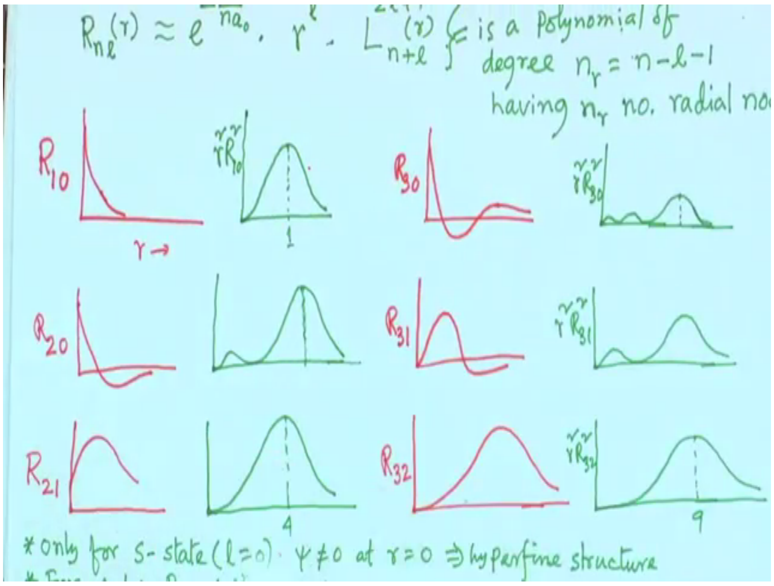

So, R n l basically it has exponential part, it has exponential part, and then after the l term and this Legendre polynomial. So, so, if I plot it what you will see n equal to 1 l equal to 0. So, wave function explain form of the wave function that we have seen that you have seen this it will vary like e to the power minus r, right? It will vary it will be the exponentially d k. So, it is exponentially d k with the it is ok. So, similarly for n equal to 2 l equal to 0, what is the form of R n l? So, what is the form of R n l n equal to 2 l equal to 0 ok. So, this is the different part R n l. So, it has this says exponential as well as this another term is says linear term is there ok.

So now so, basically if we plot this 2 term if we plot just to show u if we plot this turns one is exponentially d k term one is exponentially d k term. It is not 0, what is it is move like this. Another this term is basically e to the power minus r term. And another r to the power another 2 minus z r by a 0 2 minus r, another term is 2 minus r. So, 2 minus, r means y equal to m x plus c y equal to m x plus c right. So, in our case y is basically R n l. In this case, it is n equal to 2 and l equal to 0, n equal to 2 and l equal to 0 n equal to 2 and l equal to 0 ok.

So, this we are plotting R 2 0 R 2 0. And then your that is the y, now x is in our case r. So, r is here minus z r by a 0. So, minus minus z r by a 0. So, minus r so, m x so, this is the m negative slope is the negative slope, and plus c means here 2 plus here 2 ok. So, if you plot this one so, what will be the; so, it will cut positive at 2 it will cut positive this 2 right c. And a positive y axis it will cut like this starting from for r equal to 0 c c is 2. So, it is stay here or here somewhere ok, whatever depending on value with normalize value or not. And this negative slope, means slope is not like this it is negative slope, it is negative slope is the is like this I guess ok. Ok negative slope it is like this.

Now, if you multiply them, what will get? What will be the form? So, it is basically, I can show you. So, it will be like this so, it is following exponentially ok. Exponentially is high value. So, this negative r is just 2. So, it will have some value. So now, this plus this so, it will start from say here. So, here so, it is value is adding. So, going up slightly. So, it will be like this ok, and now here it is basically negative. So, here it will come and then it will it will be like this, you know it will be like this. So, it is say Is going to exponentially. So, it is it depends here I have been drawn this it can be like this also. So, depending on that vary is basically this way ok. So, that is why here it is the R 2 0 is like this ok.

Similarly, R 2 1 1 can see and one can plot ok. Now this probability, if I plot probability to find the electron between 2 spherical shell, there is the probability ok. So, one can plot one can get this why one can get this. From here what about the r so, so we have to make square of it. So, we will get basically because here why it is it looks like this. So, R 1 0 square so, this is basically this square is says this is more exponential because e to the power minus 2 r now ok. So, it will once happening, but with that R square term is there, with there the R square term is there. Now R square term means, is the it will give parabolic you know ok.

Whatever this we are getting, whatever this we are getting r 1 0 square. So, it will be more (Refer Time: 39:02) exponential because e to the power now square term is there e to the power minus 2 r, earlier e to the power minus r now minus 2 r. So, it will be first r ah, and then multiplied with R square multiplied with the R square ok. So, we will have another ah, I think parabolic term R square y equal to R square ok.

So, it will be parabolic. So, it is this kind of things will be there ok. Now if we multiply this 2. So, 0 and this if we multiply. So, it will be 0 ok. Now here 0 and this is value. So, it will be also for 0. So, that is why is is it will vary like this, it will vary like this. So, that is why I have drawn here ok, that is I have drawn here like this. So, so this way one has to plot, this way one has to plot this wave function and you can see this wave function is varying like this. But their density probability, radial density probability it is varying like this. So, I will discuss more on this issue, because you can get the physical information from this plot. So, let me stop here.

Thank you very much.