Atomic and Molecular Physics

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Lecture – 31
Quantum mechanical treatment of Hydrogen like atom

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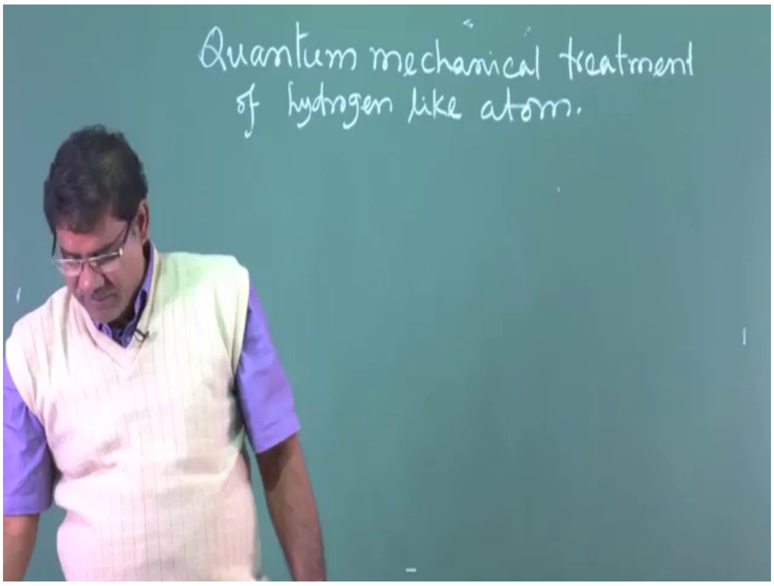

So, we are studying quantum mechanical treatment of single electron system or hydrogen like atom. So, in last class, we have shown how to solve the Schrodinger equation for hydrogen like atom and whatever result we got that today; I will discuss on the result. So, what we have seen basically one has to write Schrodinger equation in spherical coordinate.

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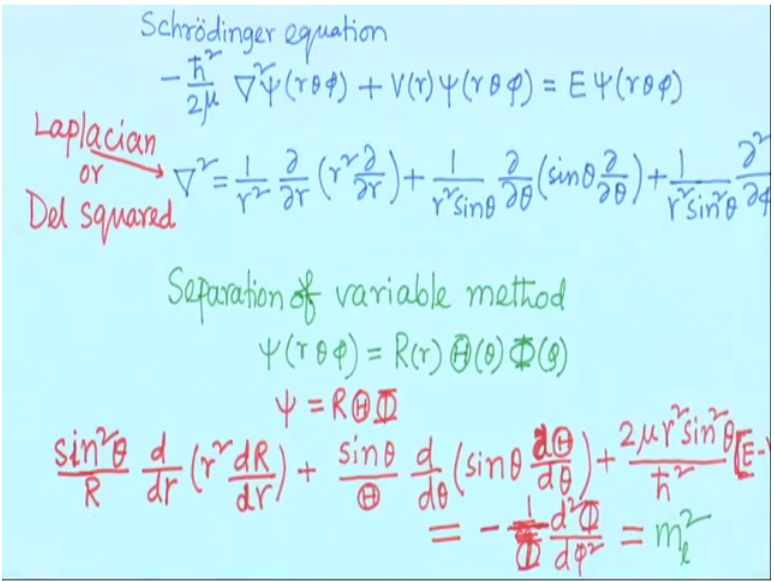

In spherical coordinate and then we have to use separation of variable method. So, this Schrodinger equation these are wave function of r theta phi and then separation variable method. So, this we have taken three independent functions of r, theta and phi. And then using this separation of variable method, one has to separate the equation and we will get three equations.

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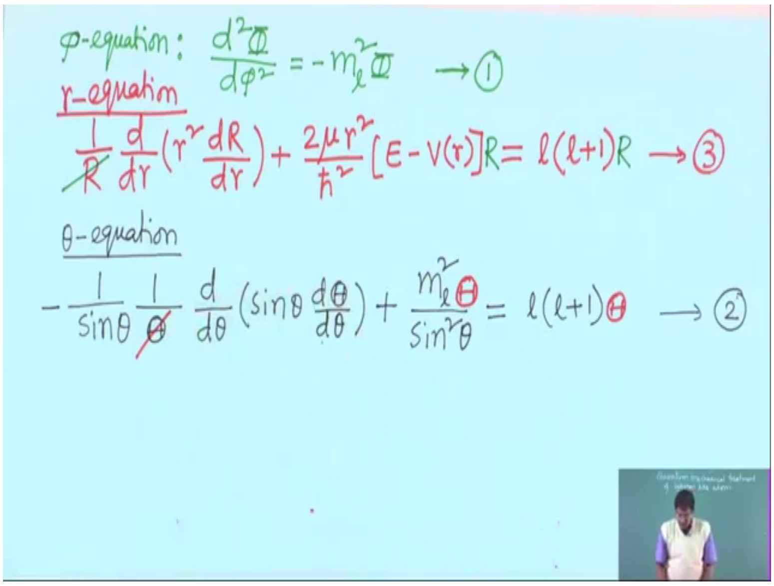

So, one is phi-equation. One is phi-equation; another is r-equation, and theta-equation. So, we have these three equations. Now, we have to solve this equation and we will get the wave function phi, r and theta.

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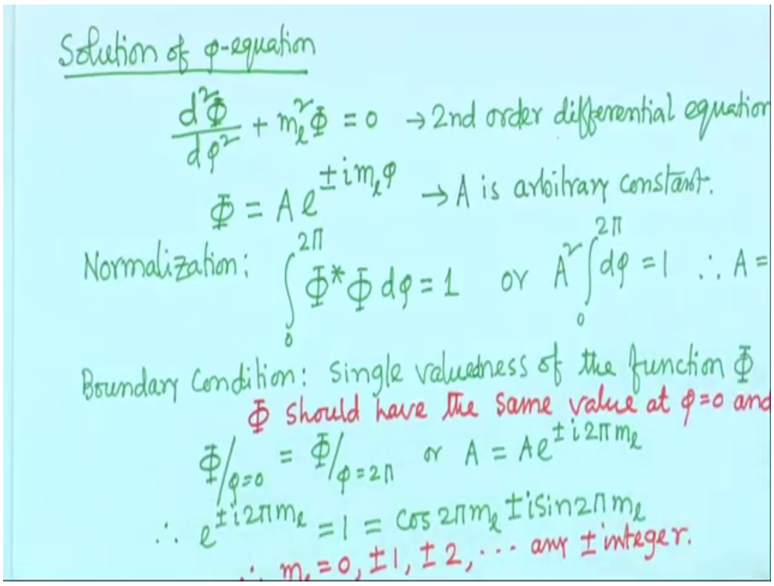

So, how to solve that without details calculation I have shown you that solution of phi equation. So, these the standard second order differential equation. And it is generally solutions standard solution is this. And for normalisation one can find out this value of A. So, this A value is 1 by square root of 2 pi.

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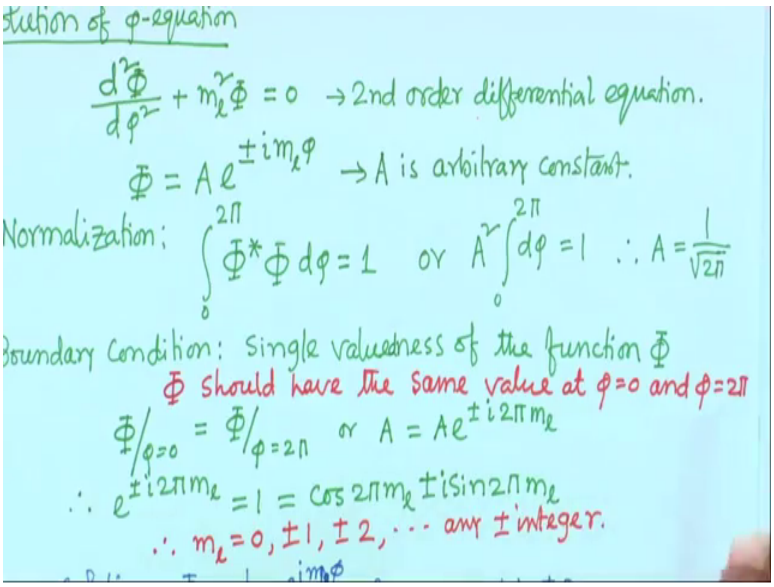

So, here we can see that is one constant m l it has come during separation variable method; and this m l is basically it from boundary condition 1 can show that m l can take value minus l to plus l. And what is l that has come from the next theta equation.

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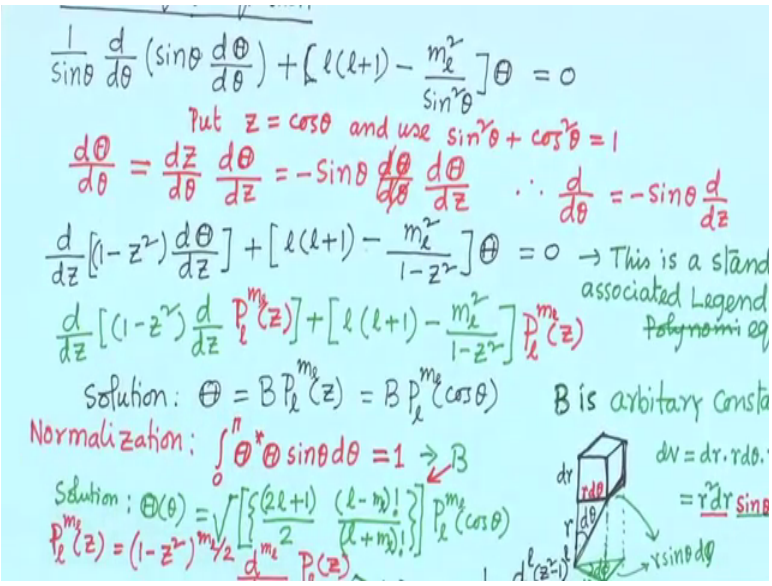

So, this during solution of theta equation; so this variable l constant not variable; constant l k mean; and the solution of theta equation is basically in terms of this is in terms of associated Legendre polynomial and this Legendre polynomial that is form of this Legendre polynomial is basically this is associated Legendre polynomial and this Legendre polynomial.

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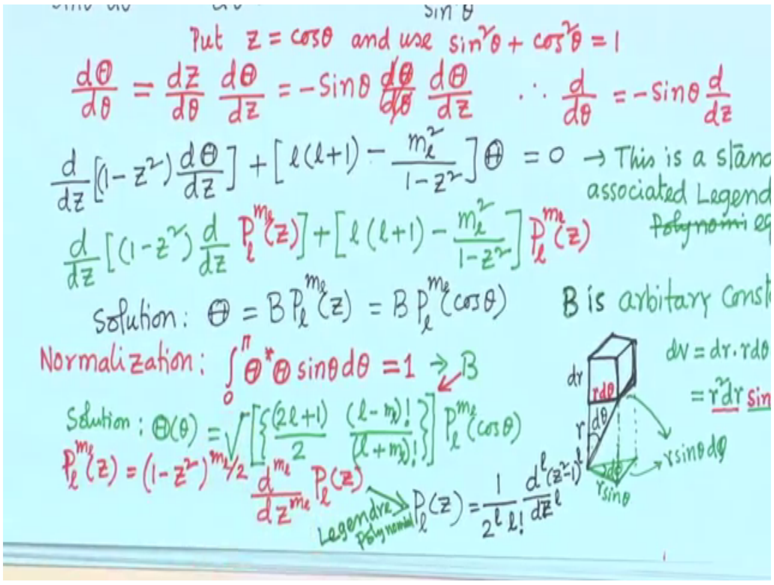

So, when P l Z, P l function of Z, so then it is the Legendre polynomial then it is associated with m l, so that is the associated Legendre polynomial. So, here these polynomials are basically this is standard form of different kind of polynomials. So, Legendre polynomial is one of them. So, I will tell you about these polynomials. So, here we have got this theta equation their theta solution in terms of Legendre polynomial are associated Legendre polynomials.

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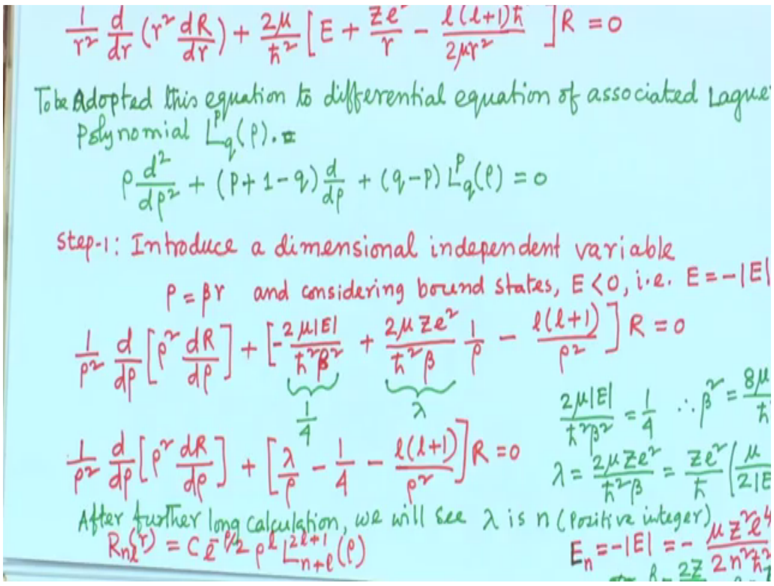

So, and finally this solution of r equation, solution of r equation, and in that case is a solution is in terms of associated Laguerre polynomial. So, this is another polynomial. It has it has standard form. And from basically from mathematical physics one learns this different kind of polynomials. And this here we have taken solution for e is less than 0, this is basically for bound state; if e is greater than 0, so this centre it is called scattering state is unbound state ok. So, but here we have only considered the bound state. So, solution is valid for e is less than equal to 0. And this solution we got that is R n l function of r is in terms of associated Laguerre polynomial. And in this during this solution, we got the energy expression n that is basically minus mu z square e to the power 4 by 2 n square h cross square.

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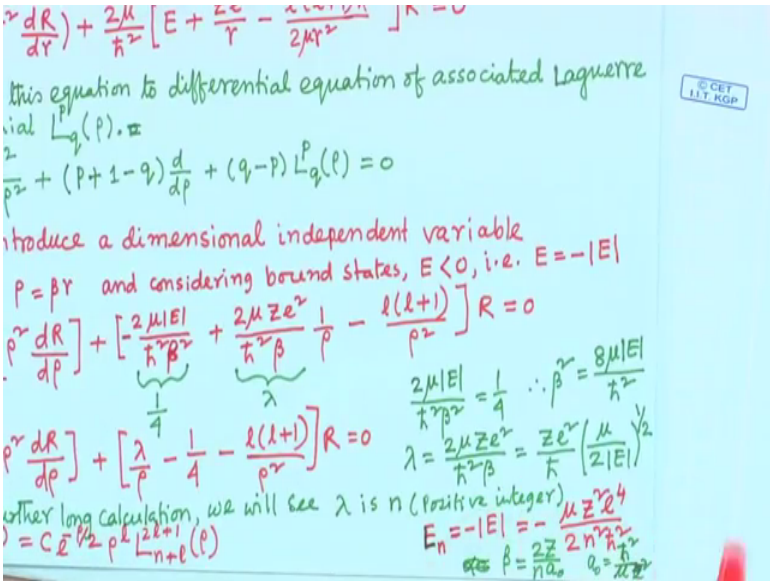

2 n square n s 2 n square h cross square, and which is exactly same as the as the as the Bohr as the energy we achieved from the Bohr model. And also here we have consider this a 0 this Bohr radius that is h cross square by mu is square ok. So, this result really one can we use this Bohr radius in terms of Bohr radius a 0, one can express this radial terms. And one has to normalize then one can get this value of c.

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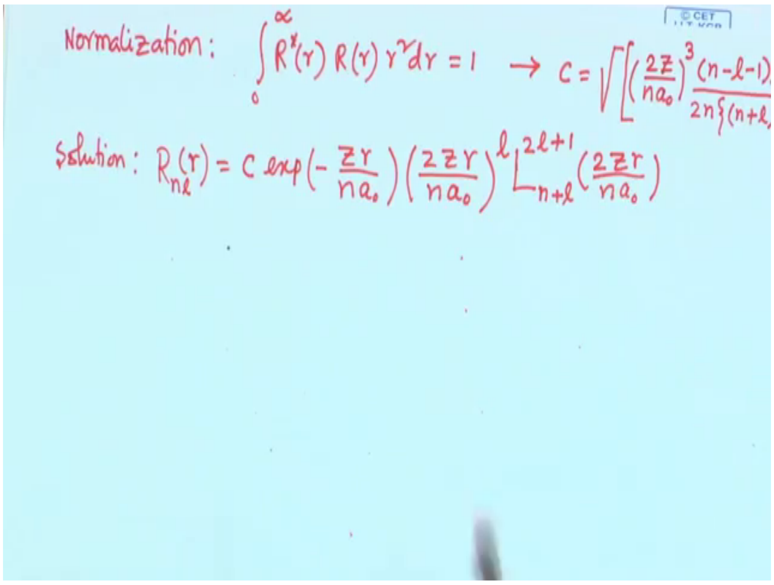

And this normalization this one has to this follow the procedure normalization procedure. So, R star r and this r square d r, why r square that I have explained. So, this elementary volume is basically r square sin theta d theta d phi these the volume elementary volume. So, from there basically this r square come. And using this normalization value one can write complete solution for radial part in terms of Laguerre associated Laguerre polynomial. So, here this polynomial just we have writing in terms of polynomial, because these are the standard polynomials we learned from mathematical physics. And what are the characteristics of this polynomial that is also from chart from table one can find out for different value of n and l, what are the what are the polynomials, what are the exact value of the polynomials for that n and l, so that one can get from the table.

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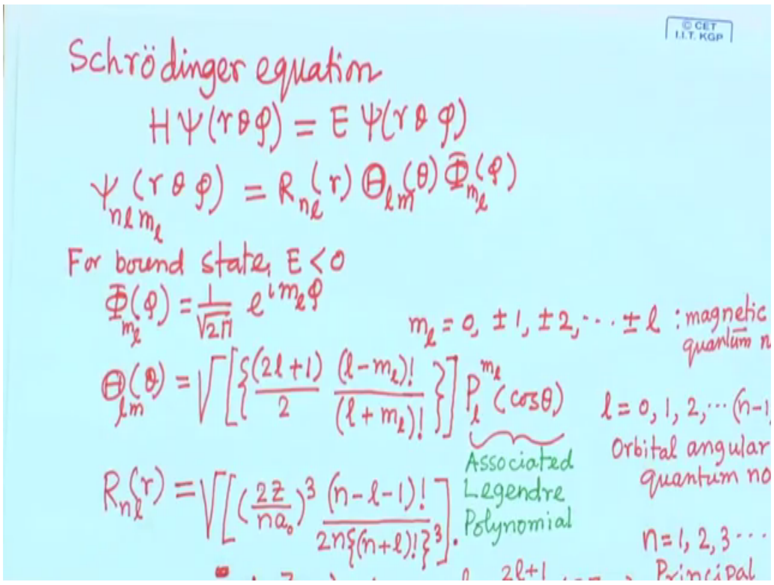

So, so finally, after solving this Schrodinger equation in spherical coordinate, so what we achieved we achieved basically energy e n equal to minus mu z square e to the power by 2 n square a square, so that was basically we achieved from the Bohr model. So, after this tedious calculation using this Schrodinger equation, we are getting same result as we got from the Bohr model in terms of basically in case of energy. So, why should we should we do this tedious calculation one reason is that in Bohr model. So, on atom basis on assumption basis there are many things we considered, but from quantum mechanics from quantum mechanical treatment that same things has come automatically in natural way. So, we have not considered we have not assumed anything. So, it has come in natural way.

So, this is one. Another is so Bohr model, basically their energy expression we got fine and in this quantum mechanical treatment will got the same energy. But in quantum mechanical treatment, we are getting additional things that is the wave function ok. So, we got the wave function for the for the hydrogen like atom. So, these the additional things we got now this wave function basically contains all information about the about the hydrogen atom in this case. So, one has to now what information what are the information how to extract those information from this wave function that one has to know; and one has to interface this wave function to get different information about the about the hydrogen atom.

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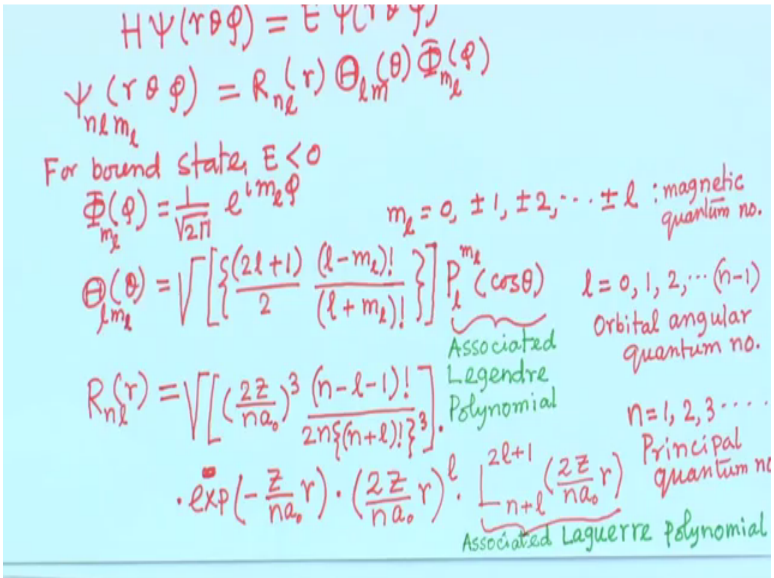

So, so basically here we have we have got wave function that is for phi dependent phi m l. So, this is e to the power i m l phi. So, this other part this the normalization part. So, if I drop this normalization part, so this is the e to the power i m l phi that is the wave function. And then theta capital theta it is the l m theta l m function of theta. So, here it is the this wave function in basically this associated Legendre polynomial where l equal to here l is involve m l is involve. So, here basically this is m l. So, this l value is 0, 1, 2, 3 up to n minus 1 and this orbital angular quantum number m l is value 0, plus minus 1, plus minus 2 up to plus minus l. So, this is the magnetic quantum number.

And then this another function R n l as function r. So, this, this, this function is basically this the (Refer Time: 13:28) part is there. So, if we forget it, drop it. So, it is basically this function is exponentially it has 1 exponential term e to the power minus z r by n a 0. And then it has r dependent r to the power l this other constant terms are there 2 z n a 0 up to the power basically l, and this then this associated Legendre polynomial

So, for details wave function, so one has to know assoc what is associated; what is the form of associated Legendre polynomial? What is the form of associated Laguerre polynomial? So, that one has to has to know from mathematical physics. And these are standard there are standard wave function polynomials one; so that from mathematical method one can get of this of this polynomials.

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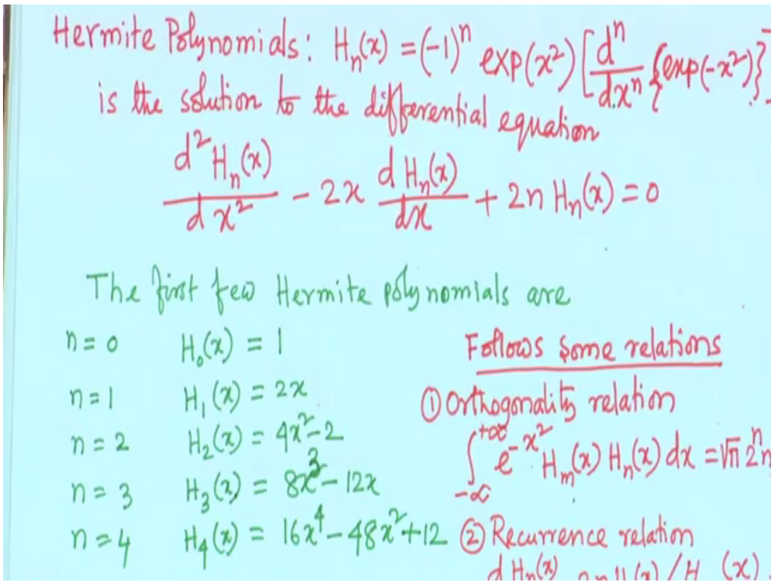

One is Hermite polynomials, you know harmonic oscillator for harmonic oscillator. So, this solution comes in terms of Hermite polynomials. So, this is this is the definition. So, these the polynomial associated H n x that is equal to minus 1 to the power n exponential x square and then d n by d x to the power n exponential minus x square ok. So, this is the Hermite polynomial this basically Hermite polynomial. And this is the solution of this differential equation of this d 2 H n by d x square minus 2 x d n d H n by d x plus 2 n H n equal to 0. So, if your differential equation from comes like this, then is solution is this H n. And H n this form is like this. So, this so this is the readymade things available in mathematical physics mathematical method from there one has to pick up this solution.

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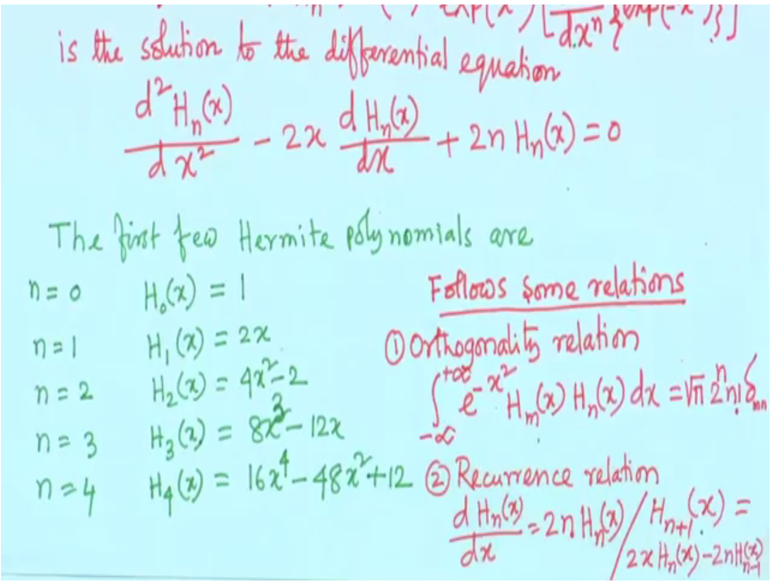

And this in as I told in table tally, you will find out this polynomials for different value of n l m l. So, in this case, it is H n is independent. So, for n equal to 1, this H and x it is 1; H 1 that is 2 x; H 2 that is 4 x square minus 2. So, these are the form of this Hermite polynomials for different value of n, so that will be available from the from the from the table in mathematical method. And these polynomial general if satisfy some relation. So, like its follows the orthogonality relation; what is orthogonality relation that is defined it follows the recurrence relation, so these are the characteristics of this of this polynomials ok.

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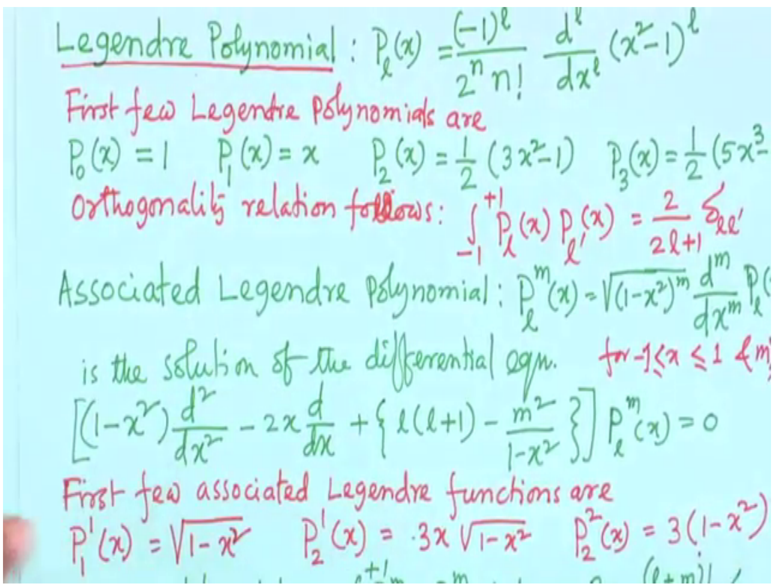

So, similarly, so we have Legendre polynomials. So, definition of the Legendre polynomials, so these the basically P l x, this is the this is the form of this Legendre polynomials. And corresponding few Legendre polynomials having different value of l. So, P 0 l equal to 0. So, this P 0 is 1, P 1 is x, P 2 is half 3 x square minus 1. So, these are the form of polynomials Legendre polynomials for different value of l. Similarly, it follows the orthogonality relation.

So, these are the here just I am showing these are the standard, it is available in mathematical method. And you will get this all characteristics and different term or different value of saying this case l. In case of associated Legendre polynomial, it is in terms of Legendre polynomials. So, P l m x this is a square root of 1 minus x square to the power m d m by d x to the power m P l x. So, this is the Legendre polynomials. So, then this is the associated Legendre polynomial. So, already P l x we know, P l x we know. And this is the associated Legendre polynomial, these the solution of this kind of differential equation ok.

So, when we are solving the hydrogen equation, so Schrodinger equation. So, in that case always we try to take the take the equation in the standard form in the standard differential form. So, that it solution is readily available. So, so in case of radial part, so this Laguerre polynomial in case of in case of theta for so that is the regional polynomial ok.

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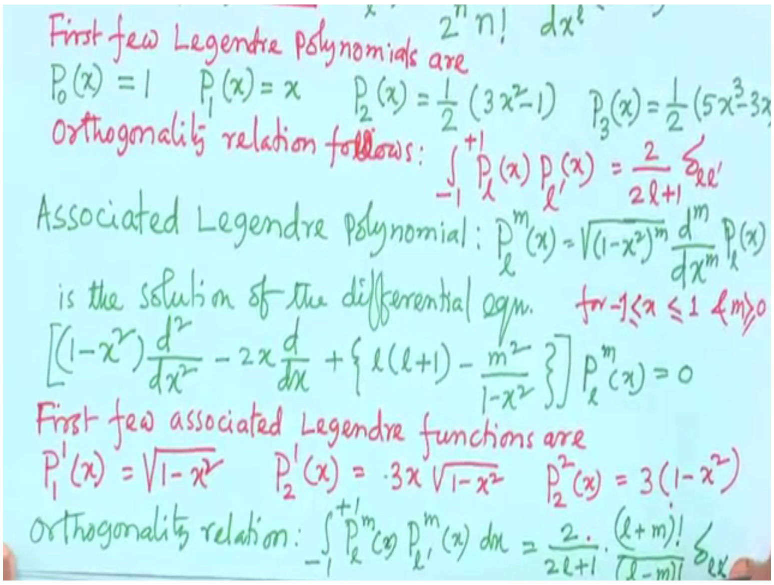

So, these here just from table I have written what is the value of P l equal to 1, and m l equal to 1. So, what will be the value, so that is the square root of 1 minus x square P 2 1 function of x, it is the 3 x square root of 1 minus x square. So, these are the few associated Legendre function for different value of value of l and m l. And it also follows the this orthogonality relations, this Legendre polynomial also satisfy the orthogonality relation ok.

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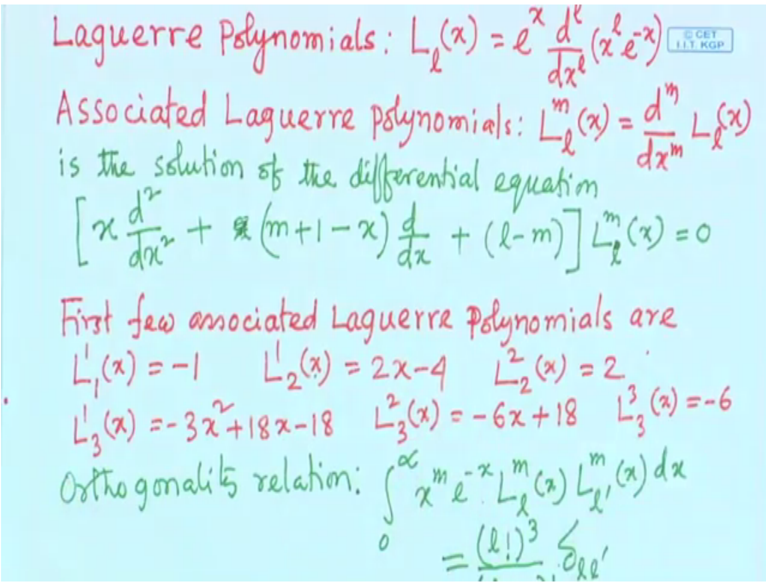

Similarly, this another important polynomial that is Laguerre polynomial, Laguerre polynomials. So, this Laguerre polynomial is form is this e to the power x d l by d x to the power l of x to the power l e to the power minus x. So, this is the form of Laguerre polynomial. So, associated Laguerre polynomial is basically in terms of Laguerre polynomial, so d m by d x to the power m of Laguerre polynomial L x. So, this is the this is basically this polynomial is the solution of this differential equation of this form. So, in case of radials, so we tried hard to get the equation in this form then because we know this if we convert the equation in this form then we have a readymade solution, so that is associated Laguerre polynomial the solution.

And first few associated Laguerre for the polynomials, so that is available, and we can get from the table. So, like L equal to 1, and m l equal to 1, so that is equal to minus 1. L 2 1 that is 2 x minus 4; similarly, L 2 means L equal to 2 and m equal to 2, so in this case, so it is 2. So, these are the different polynomials for first few values of L m, m l. So, these are the here just standard things. So, we have to use them and we should get we should find out the solution for a particular physical system. So, in case of harmonic oscillator, so solution in terms of Hermite polynomial; in case of hydrogen like atom, the solutions are in terms of Legendre polynomial, Laguerre polynomial or there associated form.

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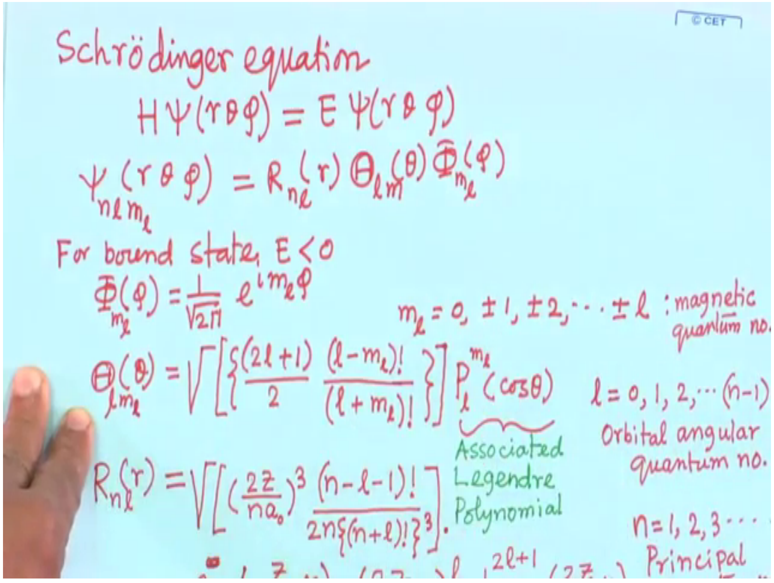

So, now as I showed you that we have, we have complete solution in our hand, we have complete solution in our hand. So, this is the Schrodinger equation. And for that Schrodinger equation putting all boundary condition, we got the we got the physical form of this of this wave function, so that is that psi independents are n l and m l. And it has three words. And this r, theta and phi; and their form of this 3 for this 3 wave functions of phi, theta and r, so that is we have written here. So, these solution is in our hand.

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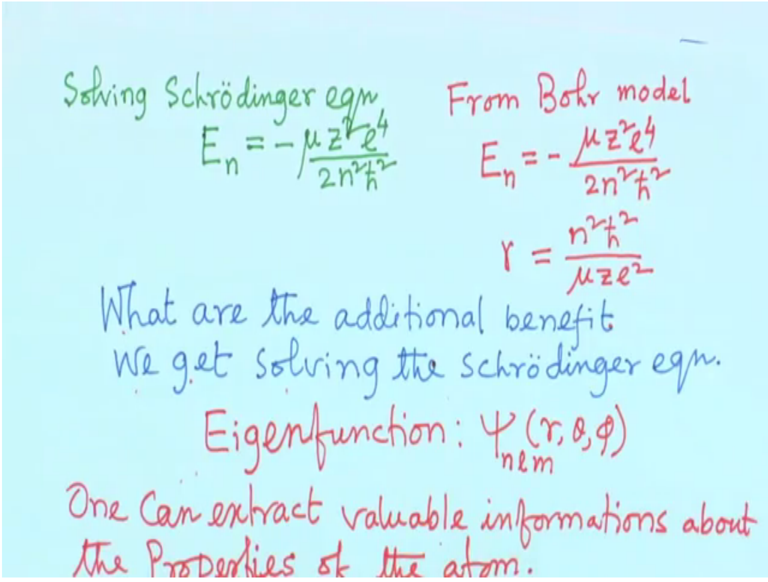

Now, as I as I told you, as I told you that solving this Schrodinger equation, we got this the energy expression, but from Bohr model the energy expression we got that is this. And also radius of orbit from Bohr model, we got this r equal to n square h cross square by mu z e square. So, but so for this what will be the r, what will be the whether any equivalent parameter is available for from the Schrodinger solution in case of Bohr orbit, so that answer we cannot give right now for that we have to we have to go further.

So, so far from Schrodinger equation we got the we got the energy expression which is same as the as the expression got from the Bohr model. Bohr model what will be the radius of the orbits that expression is available, but this whether similar information get from the Schrodinger equation, Schrodinger solution for this one electron system, or hydrogen like atom, so that we have to wait.

And basically in next I am going to detail about this. So, here as I already told what are the additional benefits we get solving the Schrodinger equation. So, that is additional benefit as I mentioned that is basically showing here that is eigen wave function wave function. Now, eigen wave function when this type of equation we write this type of equation we write H psi here is if we psi now I we have write form psi n l m l. So, psi n l m l equal to we can write E n psi n l m l. So, in this form we write. So, this we tell this Schrodinger that is the eigen equation and then psi n l m that will be eigen function and E n energy that will be the eigen value of this equation.

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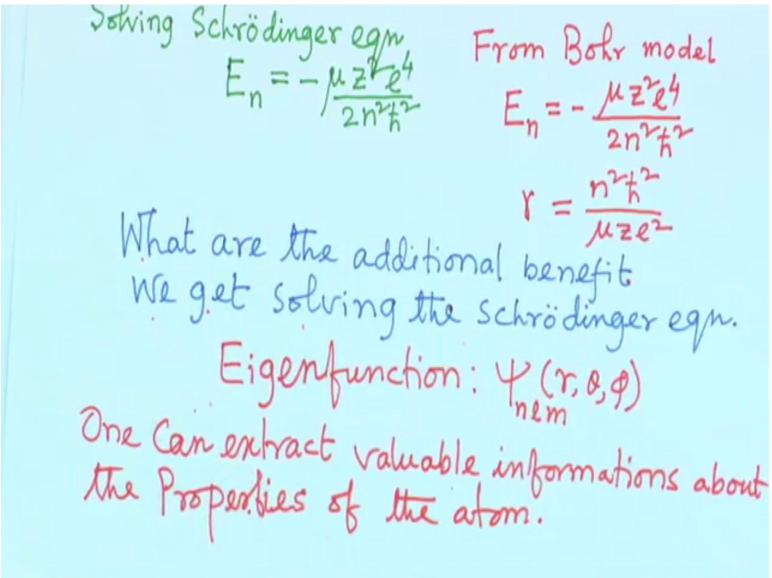

So, so solving the Schrodinger equation we got the additional thing that is eigen function and that eigen function is psi n l m. Now, as I mentioned one has to extract valuable information about the properties of the atom from this eigen function. And how to do that, so that I will discussing next class. So, I will stop here.

So, thank you for your kind attention.