Atomic and Molecular Physics
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Lecture - 30
Quantum mechanical treatment of H-like atom (Contd.)

So, we are in a position now that using the separation of variable method, we have separated r theta phi equation. So, we have 3 equation.

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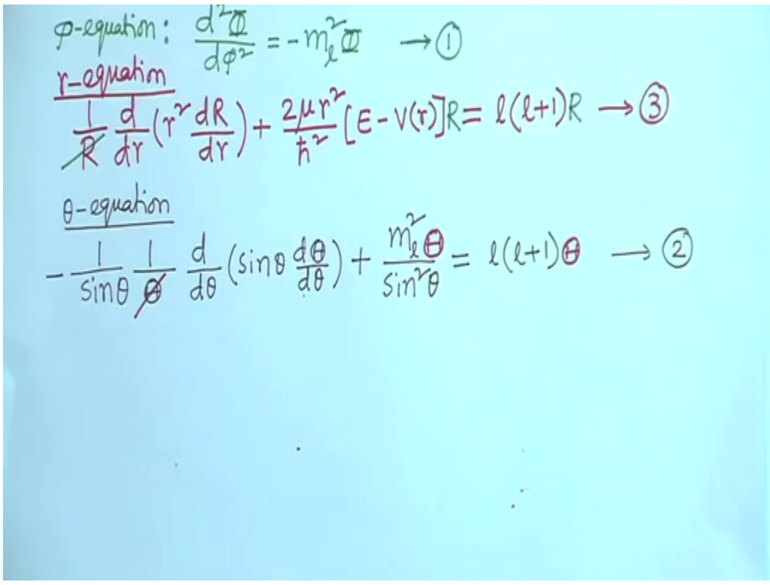

So, that is basically we are telling phi equation, and r equation, and theta equation. So, we will solve 1 after another, and find out the form of this function of r function theta function, and phi function ok. So this let us find out the solution for r equation sorry phi equation.

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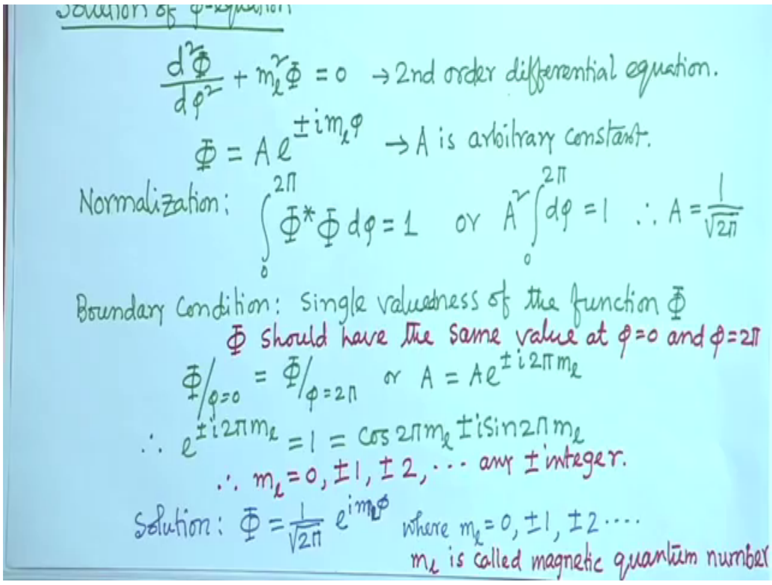

So, phi solution that equation was d 2 phi by d phi square plus m l square phi equal to 0. So, this is a second order differential equation ok, this standard equation, and if solution is generally 1 can just seeing the form of this one. So, 1 can guide phi equal to A e to power plus minus I m l phi ok. So, basically people can take the trial solution e to the power I and phi. So, then put here, and then 1 can get the form of this of this function capital phi ok. So, this basically for this equation second order differential equation this kind of equation standard equation, and form of the solution is this ok.

Here A is an arbitrary constant right. So, now, this function general function is this open, now always we normalize the function and what is the normalization, as I discuss you that to find to confine the function with in some space within some region or within some limit ok. So, generally we consider this is the probability total probability whole probability is 1 ok. So, here so, what is the limit of this phi, what is the limit of this phi. So, phi is limit is 0 to 2 pi right. So, with in 0 to 2 pi so this it will it will cover the whole region whole angle.

So, normalization phi star this I have already mentioned, you phi star phi d phi within this limit integration so that you will be equal to 1 ok. So, that is the so this the phi star phi d phi that is the that is the probability to find the particle within phi phi 2 plus d phi in this angle range, d phi angle range. Now if I integrate over the whole region, I integrate over the whole region. So, it should be 1. So, if you just put this phi phi equal to this and then integrate and you will find out that a that arbitrary constant is 1 by 2 pi.

So, now we have normalized way function that is phi equal to 1 by 1 by square root of 2 pi e to the power plus minus i m l phi fine. So, now also we have to get the realistic we have to get the realistic wave function which will describe our system right. So, so we have to adopt the wave function with our system real system. So, in reality that this function phi it has to be single valued function single valued function. So, boundary condition basically is coming because of this demand requirement.

So, phi has to be single valued function means at 1 place at 1 angle it should have only 1 value ok. So, now you see this phi limit is 0 to 2 pi. So, basically 0 and 2 pi angle these are same point same angle same point ok. So, phi value has to be same at this at this at this phi equal to 0 and phi equal to 2 pi ok. So, that is the boundary condition. So, phi value has whatever this at phi equal to 0 that should be equal to the phi at phi equal to 2 pi ok.

So, now this you have this phi you have this phi, it has to obey this condition boundary condition and if you put here so, you will get basically A equal to A so, a is this that you know, but for convenient just we are using A so A equal to A e to the power plus minus i 2 pi m l 2 pi m l. Now to be equal to this so, this has to be 1 e to the power this status. So, this part has to be has to be has to be basically, this part has to be this 1. So, this is nothing, but cos 2 pi m l plus minus i sin 2 pi m l ok.

So, from here so this has to be 1 so that means, this has to be 0 this has to be 0, and this has to be 1 so, cos 2 pi m l has to be 1 plus 1. So, only it is possible when m l equal to 0 plus minus 1 plus minus 2 means any positive, and negative integer value ok. So, here now we can recognize what you why we consider m l we could consider any other constant, but ultimately it nature of it could come like this. So, since we are in in Bohr theory or this earlier discussion, we know this m l, m l is constant ok, and it has some it is it has some integer value.

Now, here you see this because of the restriction, because of the boundary condition. So, this quantization quantized value has come automatically in r in our earlier discussion. So, everything was ad hoc, but here in natural way this this number this constant has come out with some specific values, and we are familiar what now what is this type of constant, it is nothing but the magnetic quantum number ok. So, this m l is called magnetic quantum number, and it is value is 0 plus minus 1 plus minus 2 and whatever I have we have seen earlier.

So, that has come from Schrodinger equation automatically. So, for phi equation so, for phi equation what is the solution phi equal to 1 by square root of 2 pi e to the power i m l phi. So, plus minus I have not taken because m l itself we are taken plus minus integer value ok. So, this is the solution of phi equation, and from here we saw the nature of the wave function. So, later on we will physic will discuss some physics from this solution. So, let us now first get solution of all 3 equations. So, this is the solution of phi equation next we will see the solution of theta equation say.

Next we will see solution of theta equation ok; so theta solution of theta equation.

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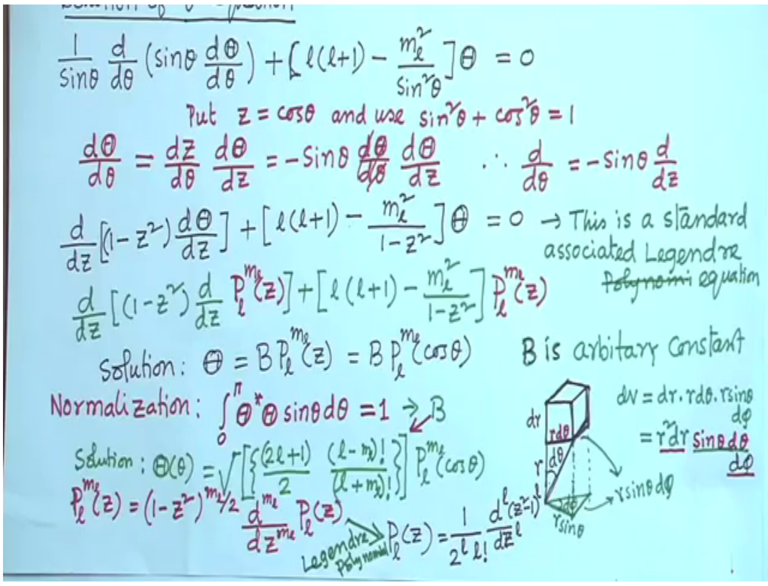

So, what is that equation? So, this equation 1 by sin theta d by d theta sin theta d theta capital theta by d theta plus l l plus 1 minus m l square by sin square theta. So, this is a is theta function is multiplied by this equal to 0. So, that is the theta equation, now it is we have to find out the solution we have to find out the solution for this equation. So, note that it is a phi equation the solution was it is quite simple.

But for theta equation and r equation, the solution is not very simple 1 has to know really mathematical physics, you have to familiar with some standard polynomial. So, from mathematical physics, or from mathematics one can learn that one. So, 1 is Legendre polynomial, and another is all Legendre function also 1 can tell, and this other 1 is Laguerre polynomial or Laguerre function, and then you know here I do not know this other kind of function is the Bessel function. So, these standards some polynomials are there functions are there ok.

So, it has so that function satisfy some differential equation, means that polynomials are the basically solutions of that differential equation ok. So, here is a this our theta equation whatever this present form. So, it is not representing any equation of known polynomials so, but here we will see that this theta equation this basically it follows the Legendre polynomial it follows the Legendre equation of Legendre function ok. So, we will now basically one should try to reformat one should try to reformat this function, this equation to the form of form of Legendre equation ok. So, that is what we will try and that is how to do that one so, 1 has to 1 has to follow these steps.

So, here so we will we will we will put z equal to cos theta ok, and use sin square theta plus cos square theta equal to 1 ok. So, now so here basically in terms of d by d theta it is there. So, we would like to write it in terms of d by d z, in that d by d z in that form. So, here just here we have d theta by d theta small theta. So, this now here this z is a function of theta. So, I can write d z by d theta and again now, now this capital theta when theta theta is replaced by z.

So, now capital this theta it will be function of z. So, 1 can write d capital theta by d z. So, basically here you can see here you can see it is basically equal to d capital theta by d theta. So, d capital theta by d theta can be written in this 2 terms ok. So, d z by d theta d z by d theta is nothing, but minus sin theta ok. So, minus sin theta, and this is there. So, so this this d by d theta this operator will be equal to minus sin theta d by d z. So, we replace d by d theta by minus sin theta d by d z. So, that is what 1 has to do first.

So, and we will use sin square theta plus cos square theta equal to 1. So, sin square so 1 minus sin square theta equal to z square or sin square theta equal to 1 minus z square. So, these things we have used, and 1 can write this one this equal to 0. So, now, it is the standard format of this called associated Legendre equation ok, this equation is standard equation associated Legendre equation ok, why associated so, this I think it is basically Legendre polynomial Legendre function is there.

So, now associated because here 2 terms will be there so these function only this l term so that is called Legendre polynomial, but when this n is associated with this function. So, it is called associated Legendre function. So, this is written P l m l is a function of z ok. So, this equation basically nothing, but this phi this phi it is it is it is since it is Legendre equation associated Legendre equation. So, this phi is basically this not phi this theta capital theta this is the function of theta function of z.

So, this equation will be satisfied when this theta will have this is equal to this this Legendre polynomials. So, Legendre polynomial is written like this P l. So, it has expression. So, it has expression that will say, but is the notation for writing this Legendre polynomial. So, solution is basically theta equal to this Legendre function as usually Legendre function, and some constant all the time we write some constant, and later on we have to normalized and find out the value of this constant; so B P l m l the function of z ok and z now you can replace z equal to cos theta. So, this B is arbitrary constant now 1 has to normalized.

Now, normalization here theta this it can change the angle from it is a angle with the z axis right, angle with the z axis. So, it can it can change the angle from 0 to pi with z axis 0 to pi it can so, angle is theta with z axis. So, it can 0 angle and then at a pi angle. This limit is 0 to pi theta star theta. Now sin theta d theta equal to 1.

So, here we have not taken d theta we have not taken the d theta right sin theta d theta we have taken why, why we have taken this, because you see this we take always elementary volume. In Cartesian coordinator elementary volume V d v equal d x d y d z right, in spherical coordinate that elementary volume d v is basically if you write. So, r will be extended r to r plus d r means it is a extended d r, then angle change by d theta. So, it is theta is there angle theta. So, this is r so now you change by angle d theta. So, this change will be this arm of this say cube it will be r d theta ok, and this other angle is with x axis.

So, we take the projection and this on x y plane. So, this projection that is that distance r sin theta. So, r sin theta from the angle phi with the x axis. Now then you are taking d phi angle if you just change d phi angle. So, this change arm the small change that is elementary change it will take r sin theta d phi ok. Now you have d r 1 side another side r d theta, and then third side is r sin theta d phi ok. So, that will give this elementary volume in spherical coordinate, so d r, r d theta r sin theta d phi. So, here I have explained. So, this is d r change r change to d r small elementary this length d r, and then d theta change. So, it will it is r so it is r theta, and then projection I have taken here. So, of r; so this r sin theta angle make with this x axis this d phi ok.

So, so this will be this elementary change due to this d phi will be r sin theta d phi ok. So, as if this this 1. So, this elementary volume is this. Now this we have written this r's here from here you can see 1 part is r square d r r dependent another part sin theta d theta theta dependent, and another is d phi ok.

So, when we will normalize r part so, here there we will take r square d r for theta sin theta d theta and for phi d phi. So, earlier we have seen only I took phi star phi d phi ok, but here theta star theta sin theta d theta, we are taking sin theta d theta we are taking. So, that is the reason in normalization why I have taken sin theta d theta. So, this has to be 1 within this angle particle has to be there ok.

So, this so this from this normalization, 1 can find out easy as you would know that this phi is not in same 2 form it has Legendre polynomial. So, Legendre polynomial associated legendry polynomial from pebbles from different value of l and m l 1 can 1 can get the expression ok, this that function form on the function, and 1 has to use the (Refer Time: 21:35). So, calculation are lengthy so, we are not going to do that, we are not going to do that, because we are interested to discuss the physics, but we need mathematics sub course, but since it is tedious calculation we will try to avoid that calculation, but we will write the result as it is available, but only discussing the step how what are the steps and how to find out ok.

So, here if I normalize so, then this B value this normalize this B value which comes really this this was square root of here, third bracket I have given in second bracket 2 l plus 1 by 2 into l minus m l this m l, and yes and this 1 is yes, and l plus m l. So, here yes so this is the B part basically, this the B part and P l m l whatever here it is there cos theta so that is there. So, this B part is this, and then this function this function form are there. So, explicitly we will use when will discuss physics yes. So, now this P l so, this is associated legendry polynomial.

So, there is a Legendre polynomial. So, and it is relate with this associated 1. So, this how they are related. So, this P l m l z this equal to basically 1 minus z square m l by 2 d m l by d z m l P l z. So, this P l z P l as a function of z this I this is the call the Legendre polynomial ok. When it is another term m l is comes. So, then it becomes it is call the associated Legendre polynomial, now Legendre polynomial and associated Legendre polynomial. So, they are related like this ok.

So, so details form will in generally we will not discuss, but will discuss techniques some particular value of m l l, we will discuss some physics out of that 1 ok, and this P and this Legendre form of this Legendre function is here, it is a 1 by 2 to the power l factorial l d l by d z l z square minus 1 ok. So, this is the Legendre polynomial ok. So, this the solution of the basically solution of the theta equation it is looks very complicated, but do not bother this calculation only one has to know how it is calculated, but 1 if 1 sit and systematically calculate 1 will get the result.

So, for next I will I will show you the solution of r equation, solution of r equation this is also very lengthy calculation.

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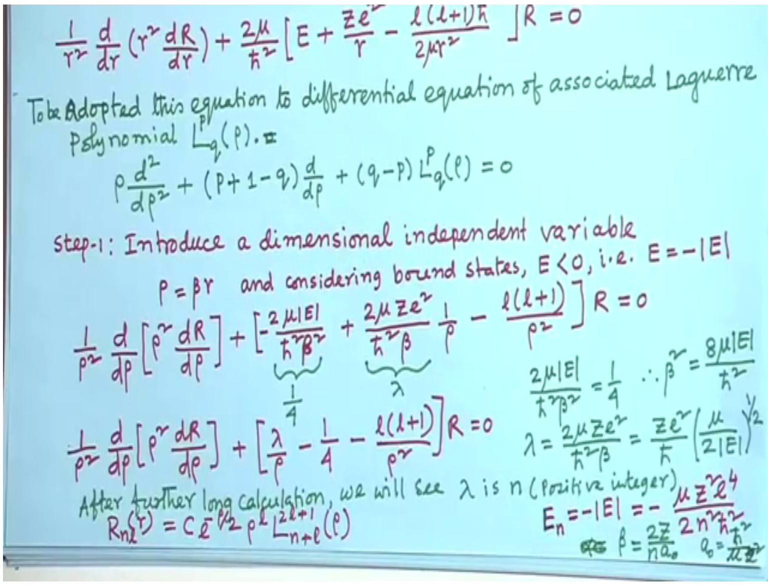

But in this case this equation is 1 by r square d by d r r square d R by d r plus 2 mu h cross square e plus z e square by r minus l l plus 1 h cross square divided by 2 mu r square r function of this is the function R capital R equal to 0 ok. So, this equation I have we have seen earlier.

So, now we have to solve this 1 again here this is not the standard equation this is not standard equation, but 1 can take it 1 can adopt it to a standard equation. So, this that standard equation differential equation of it is it is a 1 can convert to the associated Laguerre polynomial ok, associated Laguerre polynomial. So, this associated Laguerre poly polynomial this it is generally we write L q P function of say rho ok, and that that differential form.

So, it satisfy the differential equation like this rho d 2 by d rho square plus P plus 1 minus q d by d rho plus q minus P this l q P function of rho ok. So, this the form of the Laguerre associated Laguerre polynomial ok. So, now this equation is 1 can see it is it is quite close to that. So, 1 has to convert this equation or reformat this equation adopt this equation to this Laguerre polynomial Laguerre differential equation differential equation, and then then will get we can write the solution of solution is this Laguerre polynomial associated Laguerre polynomial.

So, for that is the so for that there are few steps, and the steps again it is again very lengthy calculation. So, I will not do all. So, here my aim is to show you how naturally this quantum number has come up whatever the was considered in in in our earlier discussion, that n principle quantum number, l azimuthal quantum number angular quantum number right orbital quantum number. and this m l magnetic quantum number ok. So, this was considered on ad hoc basis. Now that same things how it come out from this from this quantum. So, from this Schrodinger equation in natural way.

So, that that I would like to just emphasize that part just avoiding details calculation. So, in already I have we have we have seen how what is m l, how it has come. So, that has come basically from the from the phi equation from phi equation, and the restriction of this, restriction was it has to confine within 0 to 2 pi angle, and from single valued function from because of that. So, value has to be same at phi equal to 0 and phi equal to 2 pi ok. So, whenever this restriction put, and this natural way this parameter comes which quantize form ok.

So, similarly here so to get to adopt this equation towards the associated Legendre equation differential form of this associated Legendre polynomial. So, for that few steps 1 has to introduce. So, first we have to introduce this a dimensional independent variable here r have dimension ok. So, so this rho is basically here this dimension independent variable rho. So, here this equation we will try to make it dimension independent in terms of dimension independent variable ok. For that so, let us here just we consider that rho equal to beta beta is some constant beta some constant we do not know what it is.

And also we consider here e r there in this equation, we consider here that E is less than 0. So, E can be less than 0 it can be greater than 0. So, when E is less than the 0, then we tell it is bound state bound state, when E is greater than 0. So, it is not bound state unbound state continuous state ok. So, we are interested for bound state for this for the for our system ok. So, that is why here we will consider that E is less than 0; that means, E I can write minus minus mod of E ok.

So, considering this 1 if you just put this rho equal to beta r in this equation ok, and E equal to minus mod E ok. So, immediately from there, it is 1 can write this one ok, just introduce this 1 divide multiply with some parameter adjust them, and you will get this the straight forward ok. Now from here from here basically in this form you see again as I told our aim is to go towards this, this this this equation similar to this form ok.

So, in this form. So, here this is constant basically right, beta is involve beta is involve nature of beta we do not know ok, but m as I told this rho is independent dimension. So, I i i i i expect that beta should be this dimension of beta should be inverse of length ok. So, later on we will see it is correct. So, this and then so this we are taking this equal to 1 by 4, again this is for convenient. So, I can take this terms beta will be such that. So, this value will be 1 by 4 and here this term we have taken another constant lambda ok.

So, then if you take this one so, we can write this we can write this equation like, and so this from here; so this equal to 1 by 4. So, beta square u will be this 8 mu E 8 mu E 8 mu E by h cross square and lambda equal to this so, this I can write beta value here, I got I will put beta value ok. So, z square by h cross z z square by h cross because yes; so beta we loss square root of this one square root of this one. So, here mu I think 2 E. So, beta this 1 by beta basically know 1 by beta. So, h cross will go up so, square root of this this h square.

So, here h cross square was there. So, 1 h cross will go so this, so here basically anyway. So, it is not difficult one lambda equal to z square by h cross mu by 2 E to the power half ok. Interestingly you can see, you can see that that if I take lambda equal to n lambda equal to n, then immediately from here you can you can see that this this E. So, I have written E n lambda equal to n. So, lambda is I have written E n E n equal to basically minus E mod E equal to minus this sign, and here you can see this mu here square of this 1 n lambda, then I will make square n square ok. So, this n square lambda square n square equal to this z square e to the power 4 by h cross square and this mu by 2 mod E.

So, now E will be equal to just this minus mu z square E to the power 4 by 2 n square h cross square ok. So, here lambda is whatever a constant is nothing, but n this the yes after long further long calculation, one can show one can show that lambda is n, and it can have only positive and positive integer, and it is the principle quantum number ok, and it has relation with the with the l it has relation with the l because, this I have taken lambda this nothing, but l n and that l is here. So, from this equation this quantize quantization of l, and quantization of n will get in natural way will get, and already we got the energy value ok, whatever energy we got from Bohr theory exact this energy we got ok.

And that is why from Schrodinger equation that energy of the system ok, it is the quantized and it depends on only principle quantum number it does not depend on l and m l although in this Schrodinger equation, when we are solving this m l l n all has come, but energy depends only on. So, the same result as from Bohr theory. So, on Bohr theory on ad hoc basis we got the result, but here we are getting in natural way here we are getting in natural way and, but there are some long calculation if you do thus calculation, in details you can you can find out.

But here briefly I have calculated and I and I I try to show you, that that how from where this in natural way how this m l is coming out n is coming out l is coming out ok. So, here we really need to do further calculation, but there I will avoid it and finally, if you calculate proceed. So, you will get this form of this function r. So, r is equal to some constant C right, E to the power minus rho by 2 rho to the power l, and then this as stately general polynomial ok. So, this the form this will be the form of psi n l.

So, let us accept this one without further long calculation. So, this is my solution and I got the energy level, and I got also this principle quantum number, and from when we will do this long calculation, then one can see this l is the magnetic quantum number sorry orbital quantum number ok, and it can value take value 0 1 to up to n minus 1. So, that part I could not show you for that 1 has to do more calculation.

But let us accept it and it will come in natural way, but we are more interested to discuss physics, considering this wave function energy already from Bohr theory whatever we got. So, that same energy we got, but additional things from this quantum mechanism solving the Schrodinger equation what we are getting, that is basically the we are getting wave function form of wave function for our system, and if we know the form of wave function of a system, you can you can you can you can know many things ok, you can know many things about the system.

So, next we will see this is; what is the importance of the wave function, and how it helps to describe the system ok. So, I will stop here in next class, we will discuss physics considering this wave function.

Thank you.