Atomic and Molecular Physics
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Lecture - 29
Quantum mechanical treatment of H-like atom

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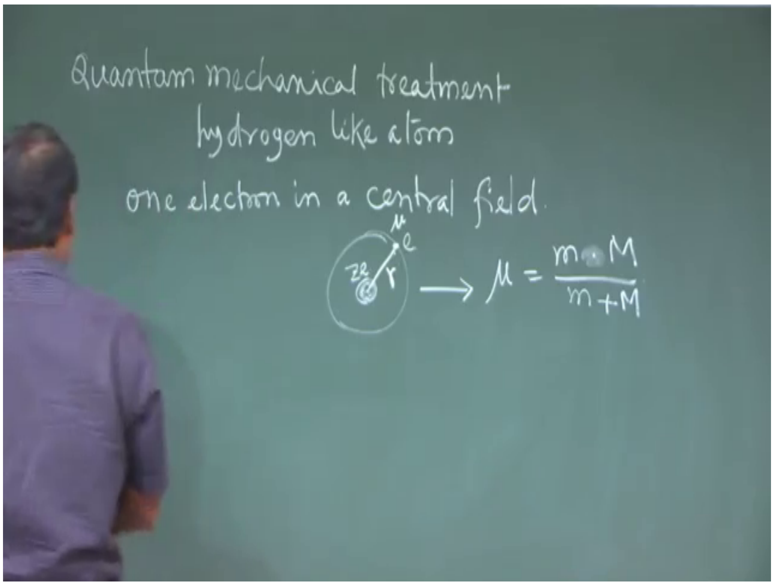

So, we will continue our discussion on Quantum mechanical treatment of hydrogen like atom ok. So, basically one electron system, one electron in a central field so, for it is basically two body problem. So, there is a nucleus and then electron ok. So, it is two body problems. So, it is reduce to one body problem considering the reduced mass mu equal to m plus m into M into m plus M.

So, mass of electron and mass of nucleus this both are finite mass. So, when it is when this reduced mass will be used. So, then it is a one body problem since this nucleus is infinitely heavy ok. So, there is no motion of that one. So, I get this electron is moving or electron is moving in the central field by the nucleus positive charge here nucleus and this mass is mu ok.

So, then now it is one body problem and is distance between these two nucleus and this electrons is r. So, so for quantum mechanical treatment already I have discussed that one has to one has to write.

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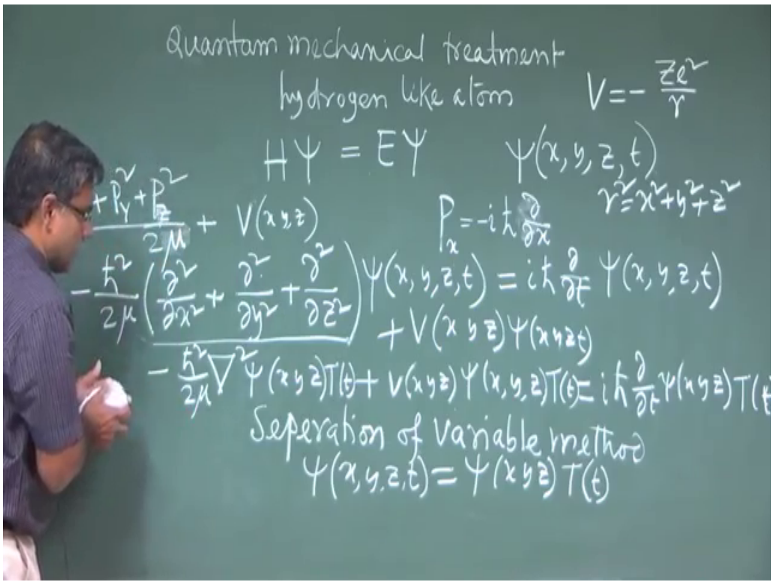

Schrodinger equation right H psi equal to E psi that is Schrodinger equation. So, psi is the wave function it is a function of x, y, z position and time and time ok. So,. So, this H is the Hamiltonian H is the Hamiltonian. So, this Hamiltonian is the energy operated basically.

So, this is the kinetic energy and potential energy kinetic energy again it has three dimensions. So, I get. So, it has three component P x, P x square P y square plus P z square by 2 m m. Now we will write by mu following mu the mass plus nu V also function of x, y, z, it can be function of T also, but in our problem hydrogen like atom problem. So, this potential is independent of time potential is independent of time. So, in quantum mechanics so, what are observable? So, we have to write in terms of in terms of operator.

So, that I have to discuss. So, p is really i h cross minus i h cross del. So, P x will be del by del x, P y, P z similarly one can write. So, here is here will get P square x square. So, basically you will get minus h cross square by 2 mu and I will get del 2 del by del x square plus. So, if you put here you will get; this expression and we have to we have to. So, this operator now it is an operator from; so this operator applied on your on your wave function and then other side also this I also operator it is i h cross del by del t E operator this i h cross del by del t then you your psi.

So, this time dependent Schrodinger equation time dependent Schrodinger equation and now here depending; so I missed here this so, one has to one has to write this side V. So, in our case this V what is V? V is basically for hydrogen like atom V is minus Z e square by r and r equal to r square equal to x square plus y square plus z square. So, V is a function of x, y, z is not function of time.

So, V is independent of time. So, says V is independent of time and this operator is basically this is called one can write del square or Laplacian operator this one. So, ultimately your equation will come minus h cross square by 2 n; 2 mu del square then psi x, y, z, t plus V V here also one has to write psi x, y, z, t ok. So, plus V here x, y, z, psi x y, z, t equal to i h cross del by del t your psi x, y, z, t psi x, y, z, t. So, since V is independent of time and this also independent of time this operator also independent time and this side. So, we can here we can apply one technic it is called separation of variable technic of separation of variable or se separation of variable method separation of variable method separation of variable method.

So, in this method this psi x, y, z, t it; so this function this function of x, y, z and t position and time. So, this can be written as a function of x, y, z position and function of time is T. So, it is the one very powerful technic separation variable method. Now, here if we apply here if we apply just replace this psi x, y, z t by this psi of position and psi of function of time.

So, then here this partial differentiation it will; it will be basically in this case it is it is depends on it is depends on psi depends x, y, z. So, this partial differentiate it will remain partial differentiation and this part here this psi x, y, z here basically it will be multiplied by T and this also one can write. So, let us simply write psi and T or let me write function of T and this also you can write this way write. Now this operator applied on this basically this T it is a it is a independent of position right it is only function of time. So, this operator will apply only on this function psi x, y, z. So, this t we can take out. So, for yes; so and here this both are there and here.

So, this operator will be applied only on this not the other one. So, now, if I divide by divide by this on both sides. So, here it will remain only this one, but by this.

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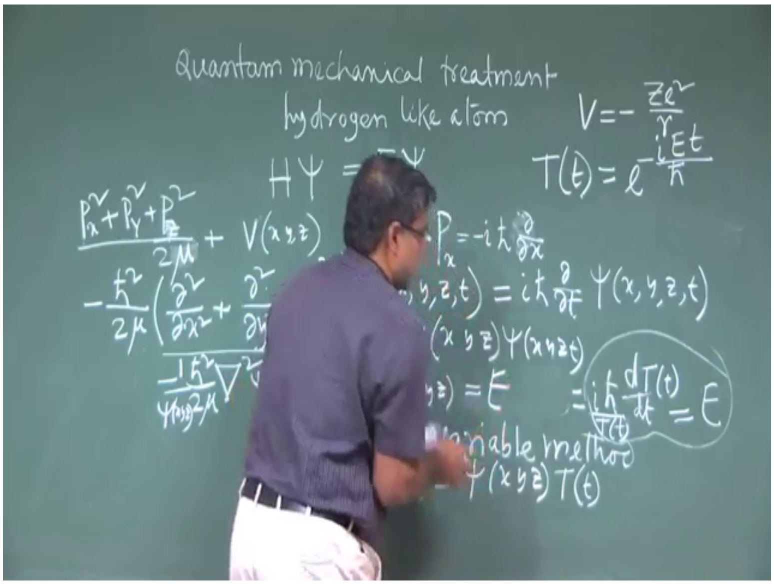

So, this and. So, here both will go divide by this and here apply on this one. So, it was it came out. So, this will go, but 1 by psi there will be 1 by psi; there will be 1 by psi ok.

So, now we can see. So, this side is only depend on time; and this side only depend on the position ok. So, this equal to this so, it is independent of position it is independent of time. So, this will be equal to this only if it is equal to some constant; if it is equal to some constant if that constant will take E E. So, from here basically what we will get we will get.

So, then this I can write from partial differentiation to ordinary differentiation. So, from this part from this part you can show you can show that that function T it is basically e to the power minus I h cross is there minus I i E t by h cross this function will come like this some constant will be there. So, after normalization you can you can get this value of this constant.

So, now these parts also again it is independent of time. So, this equal to this equal to this equal to E right; so this equal to E so now this part is independent of time. So, it is called time independent Schrodinger equation time independent Schrodinger equation ok. So, corresponding wave function is psi in a function of x, y, z. So, that is why; in last class I started from here. So, and try to solve it. So, actually this complete wave function is this one it has to for it.

So, separation variable method on can show that it has two part one is position term and as well as time part. So, so your actually wave function will be this into it if we consider the time also this i E t by h cross.

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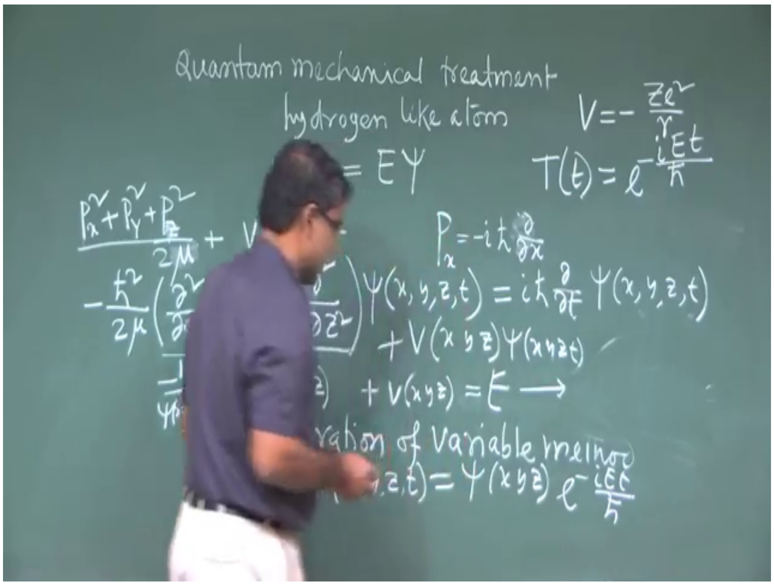

So, generally we are interested to study the stationary states of the of the of the of the system with time what is happening. So, that that we are not interested now at least we want to find out the stationary states of the system or stationary energy of the system. So, that is why mainly we deal with this with this time independent following equation right.

So, again what we have seen that this potential this as spherically symmetric potential spherically symmetric potential. So, this V actually can write V is a function of r and since this potential is spherically symmetric.

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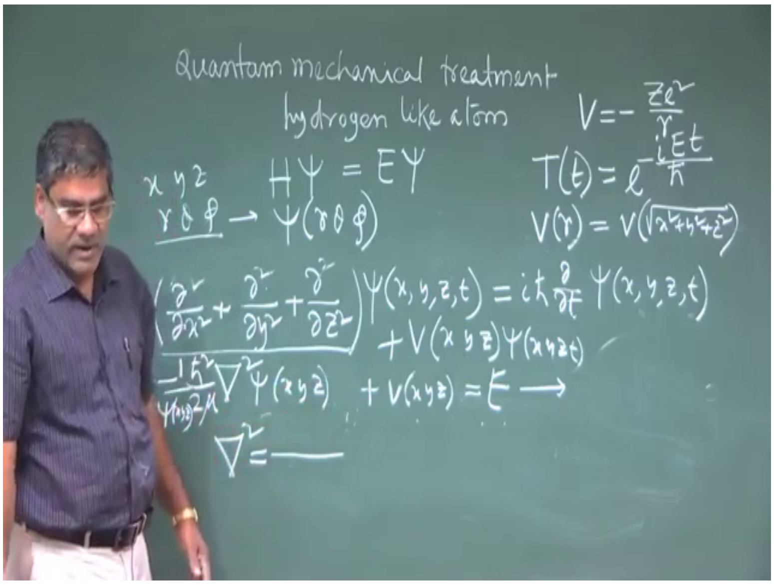

So, instead of x, y, z Cartesian coordinate; if we consider the spherical polar coordinate r theta phi r theta phi ok, then it will be g to solve this equation; using the separation of variable method because V r. So, this function V square root of x square plus y square plus z square.

Now, if we use this Cartesian coordinate. So, it will be very hard to separate the variables. So, instead of that if we consider this spherical polar coordinate; so then r theta phi. So, this is only function of r it is independent of theta and phi, because spherically symmetric.

So, this potential nature of potential is telling us that one should consider spherical polar coordinate; then one can apply separation of variable method and solve this Schrodinger equation. So, that is the motivation for considering this r theta phi and I have shown you already that that psi. Now is this r theta phi time independent Schrodinger equation r theta phi and then h in polar coordinate we have to write.

So, that will be that is V r V r is this and this part this is the del square. So, that del square in polar coordinate spherical polar coordinate what is the del square Laplacian? What is the Laplacian; that I have written in last class using spherical polar coordinate how to do that? So, that I was trying to explain you. Now, since it has lengthy equation and calculation also lengthy; so I will show you. So, in you see this; now in spherical polar coordinate. So, this Schrodinger equation is this right.

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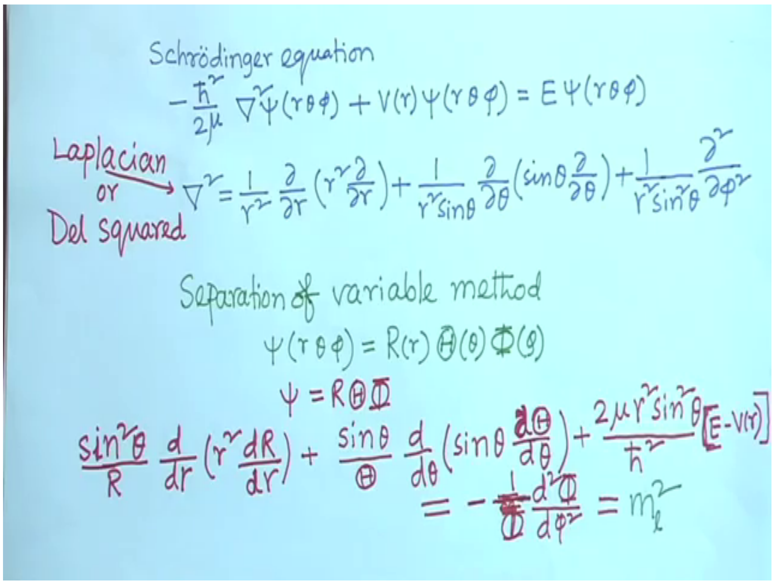

So, now where del square Laplacian or del squared is 1 by r square del by del r r square del by del r and then 1 by r square sin theta del by del theta sin theta del by del theta plus 1 by r square sin square theta del square by del phi square So, this I how it is come that I have shown you.

Now here we use separation of variable method as I discuss there in board. So, psi is a function of r theta phi ok. So, now, we have consider three function R it is function up only small r distance, capital theta is a function of theta, small theta angle and capital phi is function of as azimuthal angle phi right. So, for simplicity just we will not write this part psi we can write psi equal to r theta phi ok. So, as if this psi is a function of r function of theta phi. So, this can be written in terms of functions of only one parameter like function of R function of theta function of phi ok.

Now, if you if you for. So, this is the equation. So, here we replace this del square by this term and then psi we replaced psi r theta phi replaced by r theta phi and then what we will get I think then we will. So, here you what will get minus h cross square by 2 mu square. So, that I have I have divided by this minus h cross square by 2 mu. So, it has come. So, this part we will not be this part will not have this term, but this V V and E that part will have this mu square 2 mu square by h cross square. So, it is there.

And then I have taken in one side ok and also I have divided by, because here for 1 by r square sin square theta. So, then I multiplied to it with r square sin square theta ok. So, if

I multiplied with r square sin square theta. So, here basically 1 by r square will go. So, sin square theta will be there divided by r as I as I showed you how to how to do that divide by r, then d by d r r square d R by d r plus sin theta by theta d d theta sin theta d d theta by d theta plus this 2 mu r square sin square theta by h cross square E minus V r.

So, because this side here this minus sign was there. So, that is why we took this in other side so and this term here 1 by phi d 2 phi by d phi square. So, then I have taken the other side. So, from here just from here one can write this see it is just one has to just put and find out it is easy to find out and I explain also what are the steps? So, now, we can see left hand side is left hand side is independent of phi it depends on only r and theta and right hand side is only if the function of phi it is independent of r and theta.

So, now it is you see this part equal to this other part so, but they are this side depends on two variables the other side depends on the one variable. So, these are basically technic of separation of variable method. So, this is only valid if this equal to a constant. So, we have chosen one constant you can take any constant a, b, c etcetera, but for convenient for convenient we have taken m suffix l m l square. So, later on you will you will understand why we have chosen this one, but these are just for convenience we are choosing this is a one constant m l square one can write lambda or beta or alpha just simply, but for convenience we have written this one.

So, now this equal to this one equation I will get and this left hand side equal to m l square. So, this will be another equation. So, from here I can basically write.

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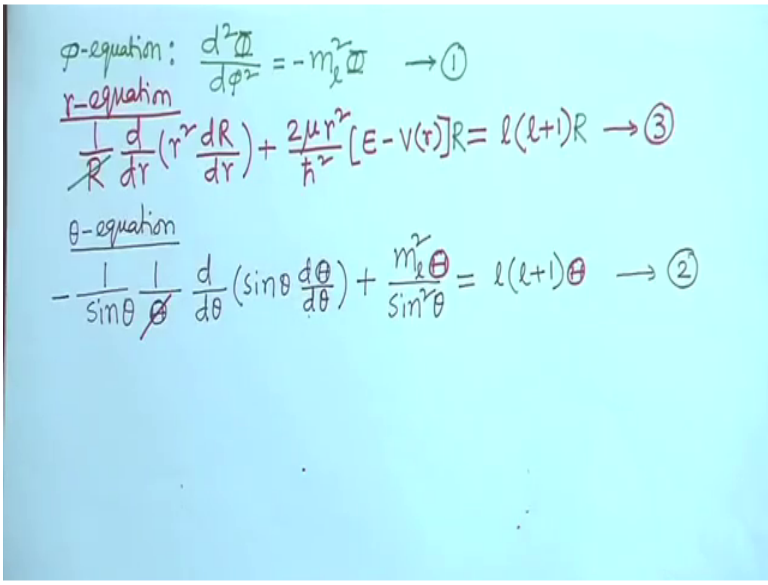

I can basically write theta phi equation right phi equation d 2 phi by d phi square equal to minus m l square pi ok, and this another part another part was the function of r and theta ok; so there also. So, this other part let me just quickly tell you. So, now, now this part left hand side equal to m l square now again we should try to separate this r and theta.

So, for that for that what we have to do. So, if I divide by. So, this part should be independent of theta. So, I have to divide by sin square theta. So, this side will be m l square by sin square theta right sin square theta. So, what I will get 1 by r d d r r square d d r d R by d r. So, this here sin square theta divides by 1 by sin theta; so this all this part will be only theta dependent and other side if I divide by sin square theta.

So, sin square theta will goes this part will be will depend on the on the r only not theta. So, I will get truth on depends on the r and own term here it will defined on the depend on the theta, but other side also because sin square divide by sin square theta. So, this part also will be dependent on the theta. So, now, I can separate these two. So, this plus this in one side and other side will be this plus this there by sin square theta.

So, now separation variable separation is done equal to I have to consider some constant. So, that constant we have taken l l plus 1 again for convenient only we have taken that constant l l plus 1. So, so just we are able to separate this three variable and we got three equation

One is phi equation this right second is r equation as I as I explained. So, this will be the r equation, because constant we have taken l l plus 1 for separating r and theta constant we have taken l l plus 1. So, this is the r equation and this the phi equation as I told this was theta theta for one term another term m l square by sin square theta ok. So, that will be again; so this constant l l plus 1 ok.

So, now Schrodinger equation of theta phi of theta phi is spherical coordinate. We have considered and we are able to separate the variable we are able to separate the variables and we got three equation phi equation r equation and theta equation. Now our task is to solve each equation and we will get phi as a function of theta will get capital R R is the function of r small r. And, we will get capital theta function of angle small theta and then our solution will be psi r theta phi equal to R function of r theta function of theta capital theta function of small theta and capital phi function of small phi ok.

So, in next class we will try to solve them and find out the wave function.

Thank you, I stop here.