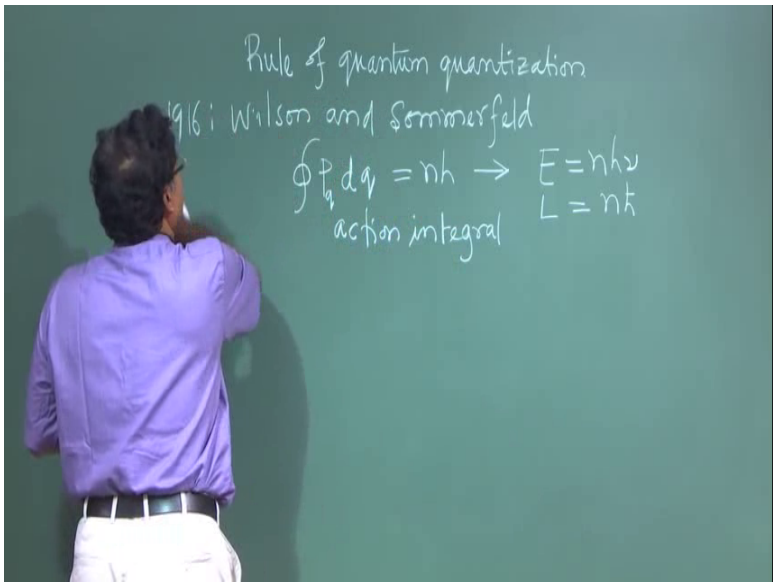
Atomic and Molecular Physics
Prof. Amal Kumar Das
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture - 12
Atomic structure of an atom

So, in last class we have discussed about the Rule of Quantum Quantization. It is actually in 1916.

(Refer Slide Time: 00:28)



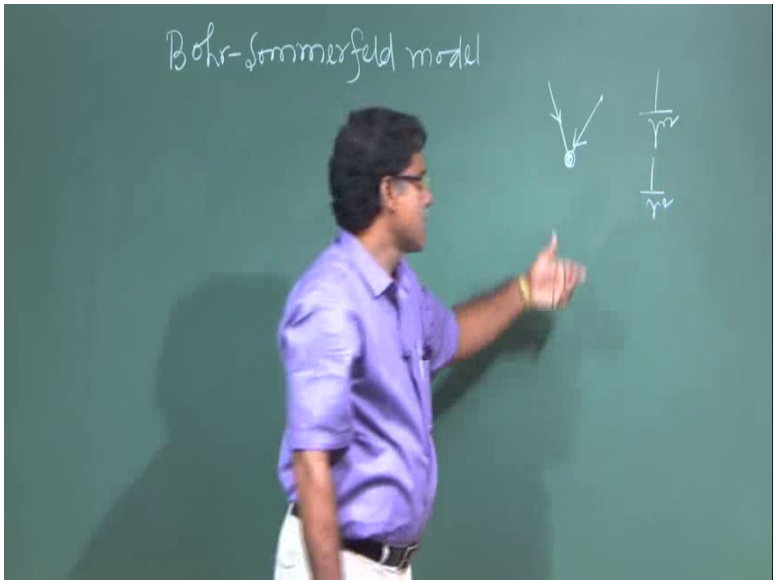
After Bohr model, Wilson and Sommerfeld. So, they try to find out that. Since Bohr model was not able to explain fine structure of hydrogen atom, fine spectral lines of a hydrogen atom. So, they realize that we need more Quantization to get more energy level. So, there will be more transition and number of lines, spectral lines will be more. So, then they set general rule for Quantization; that specific quantization rules one was the Planks Hypotheses Energy Quantization and another was the Bohr Quantization that was Angular Momentum Quantization.

So, now they set rule that for any system, any particular system, the system is described by co-ordinate. Now if co-ordinates are periodic function of time. Then there will be a quantization of that co-ordinate. So, general co-ordinate if you consider P and q. So, P for P and q; one is momentum and momentum co-ordinate and another is space co-ordinate. So, they found that this P q d q over a closed integration that will be quantized

n h. So, that was the general quantization rule, they set and from this rule I have shown you in last class that one can get the Planks Quantization E equal to n h nu as well as one can get Bohr Quantization L equal to n h cross.

So, from here, so whatever existing quantization condition was used. So, that was derived from the general quantum condition and it is called action integral also; action integral. So, so after this Sommerfeld that we call Sommerfeld Model of atomic structure. Sommerfeld model or sometimes call Bohr-Sommerfeld Model for atomic structure.

(Refer Slide Time: 04:39)

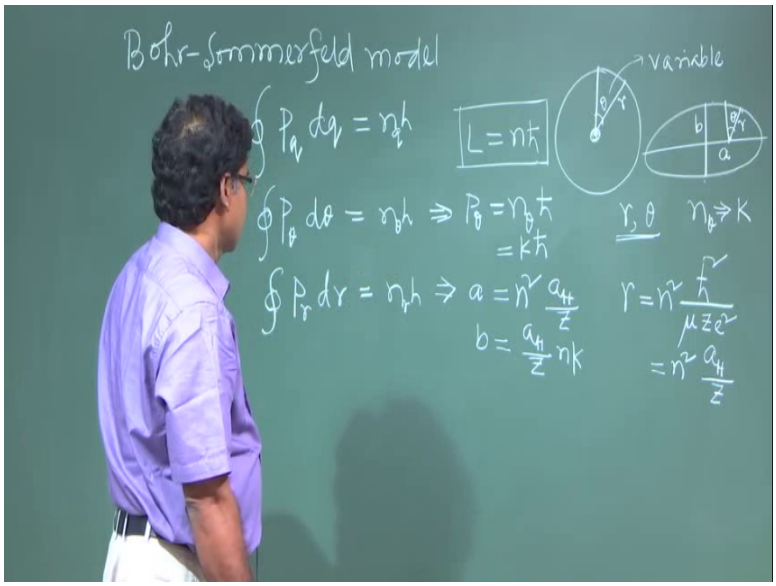


Or Sommerfeld model whatever this generally in either Sommerfeld model or Bohr-Sommerfeld model. So same thing. So, Sommerfeld point out that I think Bohr model that circular orbit was considered, but circular orbit is not the right consideration it should be elliptical. Because in any central force means when particle any particle is attack the force towards a fix point say centre.

So, then this motion of this particle it has to be elliptical. So, we know that planet motion around the sun in solar system, that is under gravitational force and that is proportional to 1 by r square, the distance between sun and planet. So, that was the gravitational force and in this case electron and nucleus here, this attractive force is proportional to also its proportional to r square.

So, because of this central force is always acting towards the centre, towards a fix point. So, because of this force planet motion, planet orbit are elliptical. So, here also it should be elliptical. So, he considered elliptical orbit for a electron rotating in a around the nucleus.

(Refer Slide Time: 07:19)



So, for circular motion so, you we use 2 coordinate r theta, but for circular motion r is constant. So, only variable is theta, only variable is theta. So, means 1 degrees of freedom. But in case of ellipse say if it is centre value, it has two focus. So, one of them can be taken as a centre. So then, we can describe the motion of the particle using 2 coordinate again r and theta.

But now, in this case this r and theta both are variable. So, we have now, 2 variable; one is angle another is radial radius radial co-ordinate. So, now, we have 2 variable r and theta and both are periodic with time. So, 2 quantization, quantum quantization should exist. So, starting using that quantum quantization rule that P q d q equal to n h.

So, now our co-ordinate is r and theta. So q, q basically r and theta. So, one rule can be P theta equal to n h and another can be P r d r equal to n h. So, generally here, I write n q. So, here I can write n theta and here I can write n r. So this, from here so, here angle varies from 0 to 2 pi.

So, you will get basically P theta equal to here, P theta is constant basically. So, d theta 0 to 2 pi, it will be 2 pi. So, divided by 2 pi, I will get n theta h cross. So, it is exactly same as the Bohr Quantization, P theta Angular momentum. So, it's a similar to L equal to n h cross; whatever Bohr quantization was used. This is basically same.

So, now from this quantization it's slightly lengthy calculation. So, I will avoid calculation, but you should try to calculate. So, this Bohr Model, Bohr-Sommerfeld Model, this calculation is quite lengthy, but it is simple. So, you should try, but I will just follow logic; logically I will try to develop. So here, in this case if I it is radial; it is coordinate is radial coordinate r.

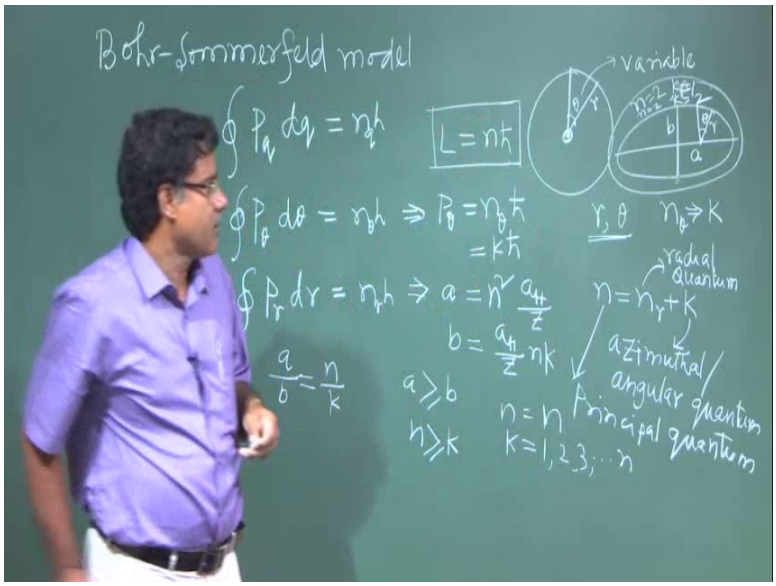
So, in case of Bohr we have seen that r equal to Bohr radius in hydrogen atom. What we have seen? We have seen n square h cross square divided by mu or m you can write; so, m Z e square. So, this I can write just n square. Here, Z equal to 1 then, it will be for hydrogen atom and Z is greater than one. So, that is hydrogen like atom. So, if Z equal to one. So, whatever h cross square by mu e square. So, that s the Bohr radius.

So, if I can if I write it h that Bohr radius h; so, divided by z. So, r is n square a H by Z from here you can write. So, here following the similarity, but here in case of Bohr there is a only r was constant for a particular orbit, but here for a particular orbit in case of ellipse, it will have major axis and it will have minor axis right. So, one is a; one is b, major axis and minor axis; a is major axis and b is minor axis. So, here this a just following the similarity.

So, a is basically it comes exactly this one, a H by Z and b comes a H by Z n. It is so, generally I will use notation from books whatever I have referred. So, generally this one in n theta; so, generally people write K h cross later on again we will change k to l small l. So, I will come later. So, here basically just we have replaced n pi to K; K also quantum number; n pi quantum number, K also quantum number. These are same just we have replace by another letter. So, it is we write n K. So, b will be this. So, after calculation one will get this a and b.

So, that I have taken here from the taking the singularity from fro Bohr radius. So, I have written so. If so, if we accept this one. So, here and what is n? N is basically that is n r n is basically n r plus n pi n theta n r plus n theta. S, now, n theta.

(Refer Slide Time: 15:18)



I am writing k. So, n r is called radial quantum number and K is called azimuthal quantum number or angular quantum number. So now, n r plus K; so, this is basically called Principle quantum number. So that is what this. In case of Bohr here; so, that whatever this n that s the principle quantum number n value is 1 2 3 4 5 integer value.

So, now here that n is basically summation of radial quantum number plus azimuthal quantum number. So, that n is this n. So, so what we are seeing here. So, if I write a by b equal to I am getting a by b equal to n by K. So, a is greater than equal to b; because in ellipse b is less than equal to a or a is greater than equal to b.

So, n is greater than equal to K; n is greater than equal to K. So, for a particular value of n so, what will be the K value? K value again, it is quantum number, it is integer. So, K value will be K value. So, n can be n is greater than equal to K. Because a is greater than equal to b. So, n value is 1 2 3 4. So, K value will be also if we start from 1. So, n value minimum value is 1.

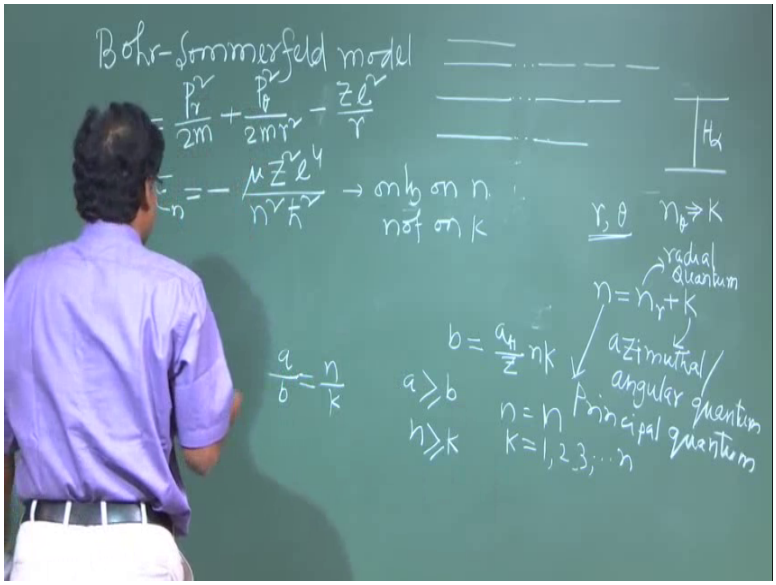
So, then for n equal to 1 K will be 1; k equal to 0 is not allowed. K equal to 0 is not allowed. Then, if K equal to 0, then, you will see K equal to 0 then, we will see b equal to 0; that means, b equal to 0 So, only a will be there. So, motion will be along the; a axis passing through the nucleus; passing through the nucleus so, that is impossible. So, that is not feasible.

So, that is why K equal to 0 is not allowed. So, K value can take for a particular n value. So, it can take up to n value. So, if n equal to say n. So, then K value will be 1 2 3 4 up to n. So, for a particular n value, we will have how many number of K value; n number of K value we will get. So, n equal to 1.

So, it will represent a it will represent a orbit, elliptical orbit and for that n value; so, n equal to 1, n equal to say n equal to 2. So, then there will be 2 K value 1 and 2 means again that n equal to 2 whatever the another elliptical path. So, that will have sub orbit basically for different K value. So, n equal to 2, will get K equal to 1. K equal to 1; so, it will represent a orbit, sub orbit and another sub orbit will be n equal to 2 K equal to 2. Now question is, now this sub orbit or sub cell or orbitals whether they will have different energy or they will have same energy.

So, that is the question. If they are same then, we will feel again same difficulties, that number of spectral lines will not be more; whatever in case of hydrogen from Bohr model, whatever the number of spectral lines we will get from elliptical from Sommerfeld model also, number of spectral lines will be same. So, let us see this, whatever the energy whether it depends on K or not. So, so for energy again, this is a long calculation.

(Refer Slide Time: 22:28)



So, I will not do so. So if you calculate total energy of the electron in a elliptical orbit. So, then, that E will be your kinetic energy plus potential energy. So, now, kinetic energy

will have 2 parts; one is radial part and another is angular part. So, linear momentum and another is angular momentum. So, so kinetic energy will have 2 parts. So, one is P r square by 2 m.

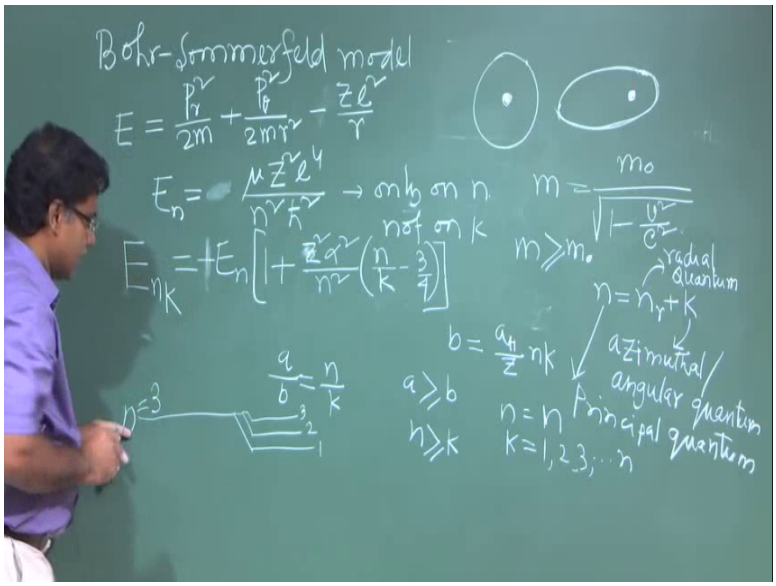
So, linear momentum another is P theta angular momentum, P theta square by 2 m r square. So, that will be the energy for angular momentum and your potential energy plus b. So, in our case we know the potential energy for nucleus and electron that is minus already we have calculated earlier minus Z e square by r; Z e square by r and starting from this energy, if you calculate as I told this calculation is slightly longer.

So, I will not calculate. So, what I will get. So, I will get this E equal to the same expression whatever we got from Bohr model m or mu m Z square e to the power 4 divided by m square h cross square. So, same energy expression whatever we got from Bohr. So, this elliptical orbit also this energy we get same. So, it depends energy depends only on n not on K. So, what does it mean?

So, this, whatever I told this about (Refer Time: 25:02) or all beta sub cells, they will have the; for a particular n value whatever the orbitals or sub cells their energy will be same. So, their energy will be same. So, in model language, in quantum mechanics language is called states are degenerate; states are degenerate.

So, so that means, whatever the energy levels from Bohr model, now energy levels are more. Energy levels are more; this it is 1 level. So, here basically 2 level; but with same energy here n equal to 3, it will be 3 energy level, but with same energy. So, so for a hydrogen atom H alpha line as I told, it is composed of 5 lines, after this Bohr modification of this orbit considering the elliptical orbit that also did not help to explain the fine structure of this hydrogen atom. So, then Sommerfeld itself, he pointed out that when so, there is a difference between, difference in motion of electron in a circular orbit and elliptical orbit.

(Refer Slide Time: 27:25)



Since circular orbit basically; so, distance between the electron and the nucleus it's all the time it is same. All the time it is same, but in case of ellipse, so, here is the nucleus and this is the electron. So, distance between the nucleus and the electron it's varies with time; it varies with time. So, at the some point it is very close to the nucleus, at some point it is very far away from the nucleus. So, its velocity will change; its velocity is not constant, here it is constant, but velocity will change with time depending on the distance between these 2.

And when it is very close to the nucleus, so, its velocity will be very high, it may be comparable to the is close to the light velocity. So, if velocity is high then whatever so far, we have considered that is electron we have considered as a as a non relativistic particle. But if velocity is high then, non relativistic consideration is no longer valid. So, one has to consider the relativistic concept or as a relativistic particle we have to treat electron.

So, then he introduced that is relativistic energy; consider relativistic energy of the electron and there basically in relativistic in relativity, there you know this mass; it changes with the velocity. What is the relation n equal to n 0 by square root of 1 minus V square by C square. So, this m 0 is the (Refer Time: 30:04) mass and m is relativistic mass; it is higher than the always it is higher than the m 0. It depends on the velocity V, velocity is pretty high. If velocity is V equal to it's when it is at rest b equal to 0.

So, this n equal to n 0, when v is comparable to the c. So, then it's you see b equal to see it will be infinity m 0 by 0, it's mass will be infinity. But it cannot, these velocity cannot be equal to c, but it can be close to the c. So, so all the time now m is greater than equal to m 0 right. So, its mass will increase. So, mass will increase.

So, because of change of mass when it is rotating in a elliptical orbit its mass is changing its mass is changing. So, so considering this electron it's relativistic motion in a orbit then, he recalculate it Bohr-Sommerfeld we calculated, this energy of the system and he found that now it depends on. So, again this we are avoiding the calculation. So, it is lengthy calculation. So, he found that now energy depends on K and this expression is E n K equal to so, I am writing minus E n; that means, it is negative value.

Now if n is this n is this. If when takeout negative here; so, I can put negative here. So, it will help me to explain. So, now, n is basically this. So, I have introduced negative sign here. So, this will be equal to 1 plus I think Z square alpha square divided by n square n by K minus 3 by 4. So, that will be the expression considering the relativistic mass or relativistic concept.

So, so now, we can see the energy depends on K. So for a particular value of n, so this when K is higher; because for a particular n, K value will be 1 2 3 4 5. So, for K equal to 1, whatever this value I will get K equal to 2; this value will be half. So, K is higher this value will be lower. So that means, this value will be lower. So, 1 plus this, it will this value will be lower.

So, so n is multiplied with that on minus sign. So, lower means. So, it will be more negative. So, K is higher. K is higher, it will be less negative. Because this is smaller; K is higher this value is lower. So, overall this value will be lower. So, negative value will be is lower; means it will be less negative and K value is smaller. So, this value will be higher. So, this value will be higher. So, it will be negative it will be more negative.

So, your energy level, say whatever n value; now for K value so, lower K say 1 then, 2 then, 3. So, it will be it will be lower. So, always these values non negative, always non negative, because something is added with 1. So, but for lower K value, it will be this. It will be more lower and K is increasing. So, it will be less negative so. But all the time E n K is value is always lower than the E n value.

So, now, energy levels are splitted. So, if this is I have taken say n equal to 3. So, now, it is split into 3 lines. So, now, free energy level each level will be splitted accordingly and we will get more transition. So, now, it can explain the fine structure of the, fine structure of the hydrogen atom. So, I will continue in next class.

Thank you.