Introduction to Quantum Mechanics
Prof. Manoj Kumar Harbola
Department of Physics
Indian Institute of Technology, Kanpur

Lecture - 04
Quantum conditions and atomic structure, electron spin and Pauli exclusion principle

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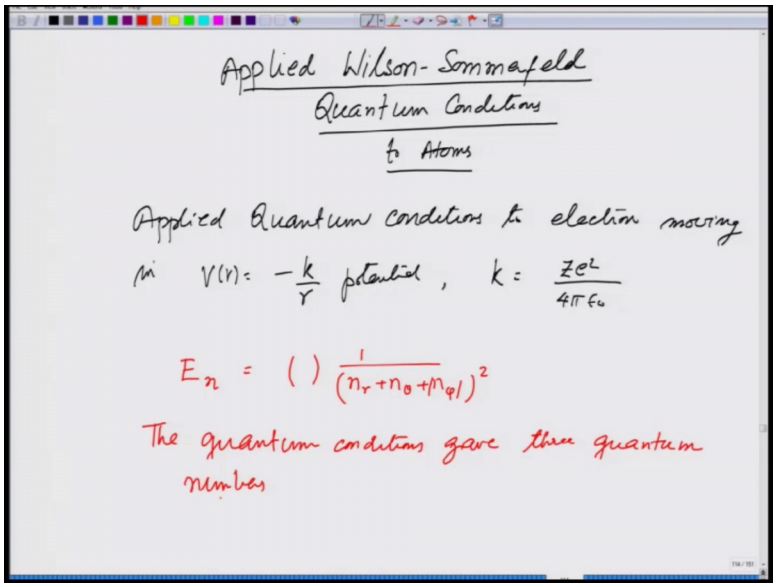

In the previous lecture what we had done was applied Wilson Sommafeld quantum conditions to atoms, or what I would say is applied quantum conditions to electron moving in V r equals minus k over r potential. And for a nucleus k was z e square over 4 pi epsilon 0. And what we obtained was that the energy for the nth level was given as whatever some constant, but important thing was there was an n r plus n theta, plus n phi modulus square. So, it gave the quantum conditions, gave 3 quantum numbers let me explain further.

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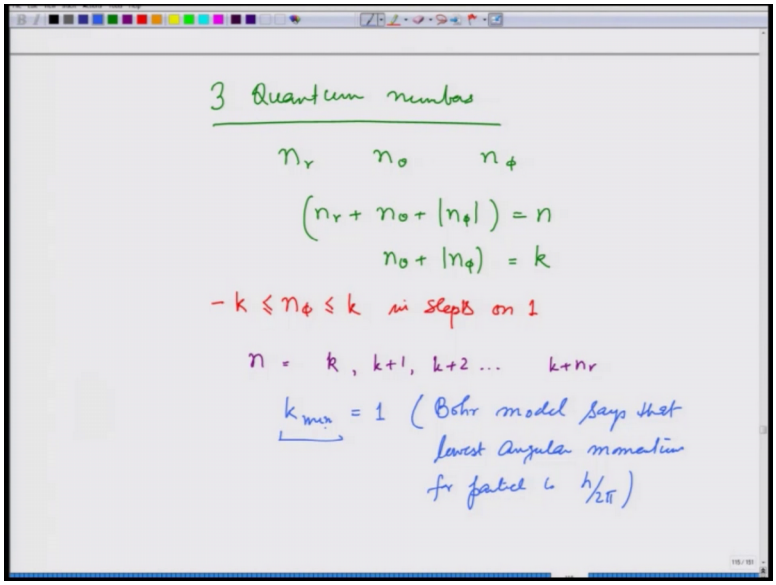

So, we have now 3 quantum numbers n r and theta and n phi, let me call this n r plus n theta plus modulus of n phi to be equal to n. N theta plus modulus of n phi equals k. Then the conditions on these numbers were that n phi varied from minus k to k in steps of 1, because the angular momentum of it is component was k times h cross and it could vary in steps of 1. Also n for a given k who took values n k, k plus 1, k plus 2 and so on k plus n r. So, let us now enumerate if I have k minimum was equal to 1, why? Because Bohr model says that lowest angular momentum for a particle is h over 2 pi. Since this k gave the angular momentum the minimum value was 1.

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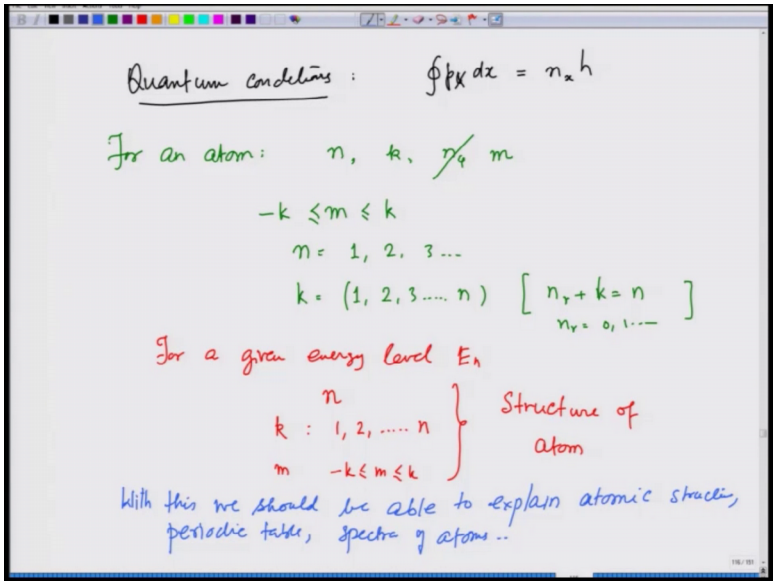

Let me also remind you what were these quantum conditions, or as many variables are there are in the problem, these were that integral over a periodic motion p x, where x is the variable d x is equal to n x h these were the quantum conditions.

So, what do we have for an atom now? For an atom we have n, we have k, we have n phi. And let me call that n phi m, and m goes between minus k and k. And n could be anything n could be 1 2 3 and so on, and k would be equal to either 1 2 3 all the way up to n. Remember n r plus k is equal to n, and n r would be 0, 1 and so on. So, for a given n a given energy level right, that energy is fixed E n, I would have n the quantum number k would vary from 1, 2 and up to all the way up to n and m which varied from minus k to k. And this would give me structure of atom. And what we anticipate with this we should be able to explain atomic structure, periodic table and spectra of atoms and so on. So, people started investigating these, because now we had this theory that gave us different quantum numbers, different levels and what all was there all right. And let us see what are our investigation tools.

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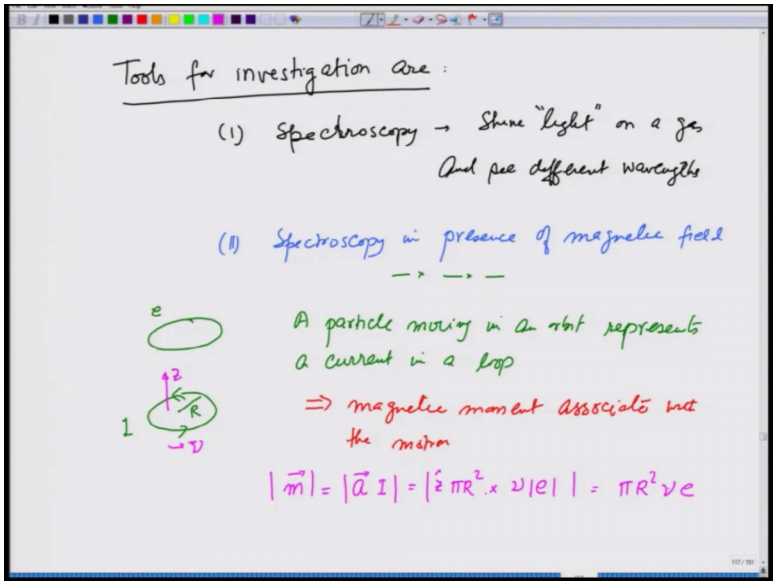

The tools for investigation are mainly spectroscopy, spectroscopy remember this is precisely what gave us the atomic structure the level structure. So, what one would do is shine light on gas and see different wavelengths. One could also do spectroscopy in presence of magnetic field what would that do? So, this is I am going to need to discuss next. You see whenever there is a particle moving in a circle a charged particle for an example an electron right. So, a particle moving in an orbit, represents a current in a loop and current in a loop, if there is a current I in a loop of radius R, this implies magnetic moment associated with the motion and just a quick calculation how much will be the magnetic moment. Magnetic moment is given by area, I am writing area as a vector times I. Area for a circular orbit will be pi R square and suppose this direction is z I will write z unit vector times I would be frequency of going around. So, the frequency of going around times the charge itself e. Right Now let me just worry about the magnitude. So, that I just like the magnitude which is equal to pi R square nu e.

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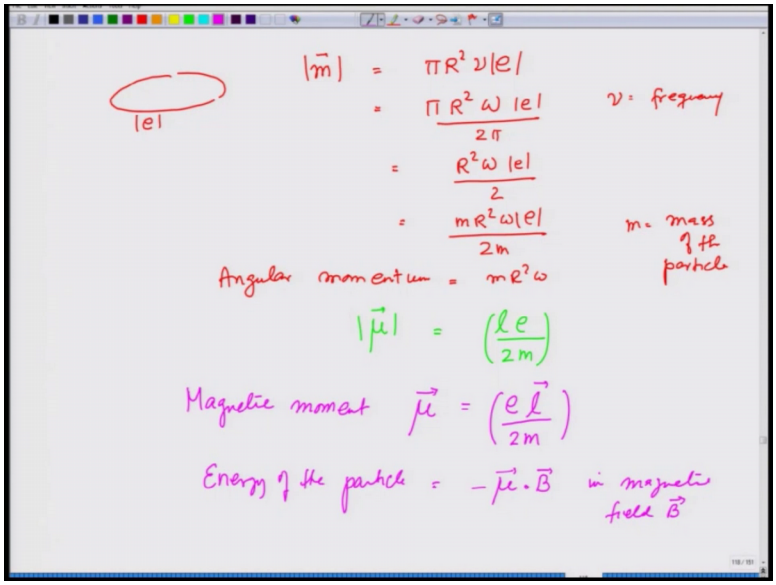

So, let me write this I am talking about a particle moving around charge e magnitude then the magnetic moment is equal to pi R square nu e. Which is nothing but pi R square omega e over 2 pi, nu is the frequency of going around which is R square omega e over 2. I can write this as m R square omega e over 2 m. What is m R square omega? Angular momentum is equal to m R square omega and therefore, magnitude of mu for the magnetic moment m is the mass of the particle here, is equal to l e over 2 m. In the vector form I am going to write magnetic moment of a charged particle going in an orbit is going to be equal to e of electron since the charged particle happens to be electron l over 2 m and if this is put in a magnetic field. So, the energy of the particle is going to be equal to minus mu dot B in magnetic field B all right. Let us see what are it is implications for our atomic structure.

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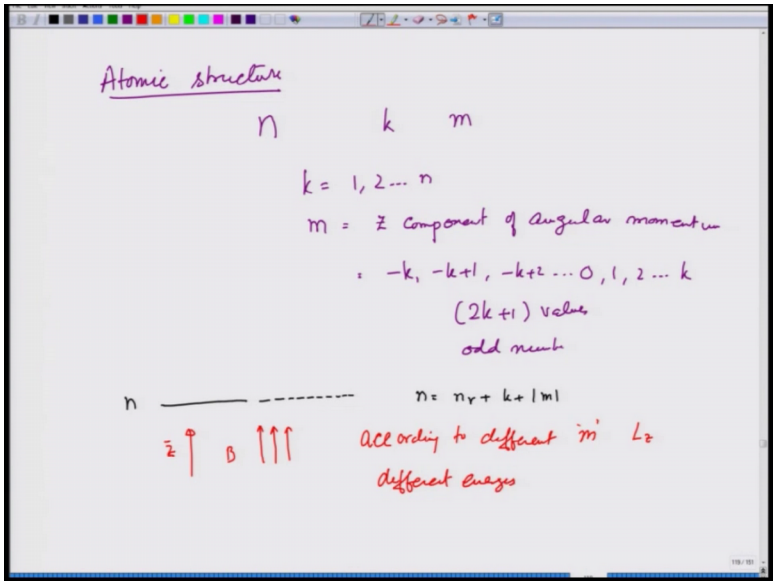

So, in the atomic structure what we had was n level k level and m level. K is 1 2 and up to n, and more important m which represents is z component of angular momentum is equal to minus k, minus k plus 1, minus k plus 2 all the way up to 0, 1, 2 all the way up to k 2 k plus 1 values. And keep in mind this will be always odd number. So, if I take an energy level here, it has in it many many energy levels. All such that n equals n r plus k plus mod m is the same right. So, this n th energy level has many energy levels. What happens now if I apply a magnetic field? So, if I apply a magnetic field B according to different m's that represent L z. So, I can take this direction in which I have applied the magnetic field to be z. I am going to have different energy levels, different energies. So, all these levels are going to split. So, let us see what happens, I take this atom. It is an energy level E n and in this now what is going to happen if I apply the magnetic field right.

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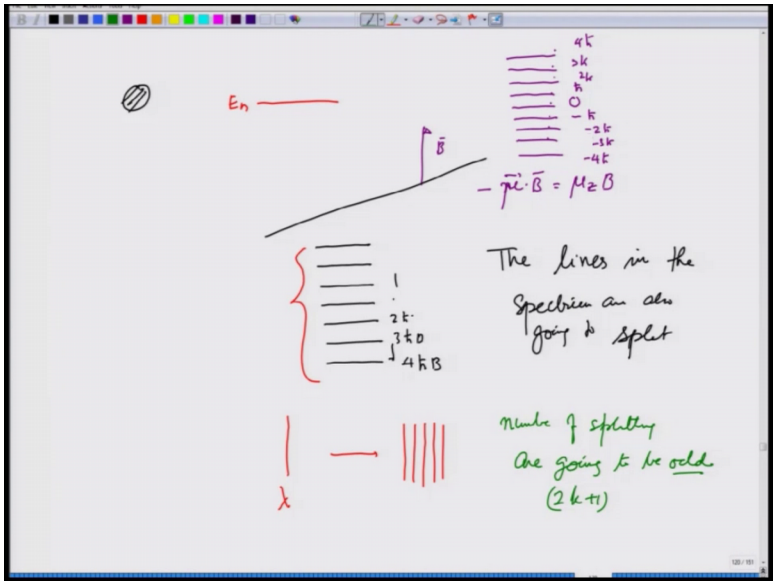

So, this is the magnetic field, I am going to have levels split for different m s. So, this could be some m value let us see how many are there 1, 2, 3, 4, 5, 6, 7, 8 let me make 9. So, there is 0, there is minus h cross, minus 2 h cross, minus 3 h cross, minus 4 h cross and h cross, 2 h cross, 3 h cross, 4 h cross. These levels have different energies. So, the energies are going to be minus mu dot B which is going to be equal to mu z times B all right. Now depending on what these values are, so negative energy value levels are going to move up and positive z component values are going to come down. So, this will be 4 h cross B for example, 3 h cross B, 2 h cross B, and so on. So, these levels are going to split and therefore, the lines in the spectrum are also going to split. So, suppose I had a line like this, which is coming a certain wavelength lambda. This is going to split into nearby lines. And what is going to the number? Number is going to be decided by how many levels are there. And this number, number of splittings are going to be odd, because this is precisely 2 k plus 1.

So, I am doing all this is to tell you how things progress and these are once we have this in our mind, learning what happens later when we solve the Schrödinger equation becomes very easy, but these are things that can be checked experimentally.

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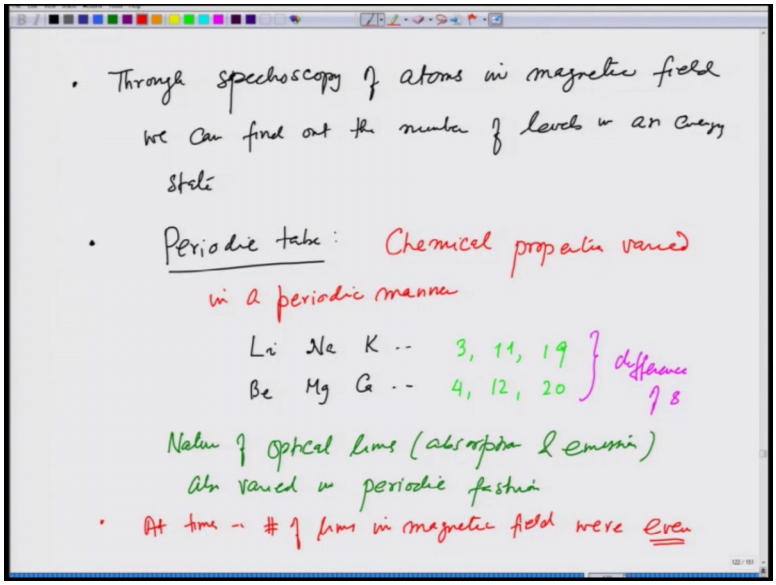

And when we develop the full quantum mechanics I should be able to explain all this through proper theory. So, that is fact number one. So, through spectroscopy of atoms in magnetic field, we can find out a number of levels in an energy level, in an energy state. That is one experimental thing. The other experiment thing that existed was periodic table. And what once it was chemical properties varied in a periodic manner. And in this case what happened was Li lithium, sodium, potassium and so on they showed similar properties, beryllium Mg and calcium and so on, they showed similar properties. The atomic numbers for these were 3, 11 and 19, for these were 4, 12 and 20. The difference of 8 periodically the property change, not only that the spectroscopic the nature of optical lines; that means, absorption and emission also varied in periodic fashion. And also saw that at times the number of lines in magnetic field number of lines split magnetic field were even. These are contradicting whatever we have learnt right. And then there was a famous experiment stern Gerlach, Gerlach experiment.

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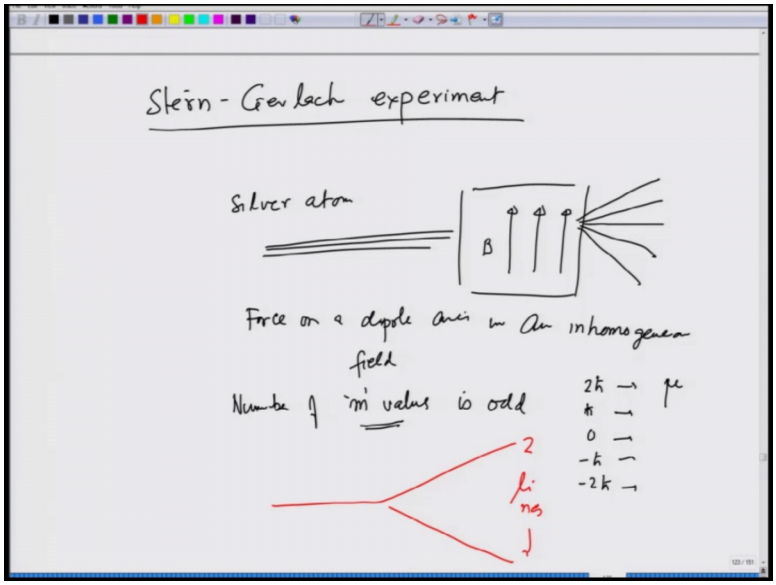

In which they took silver atoms, their beam and they passed it through an inhomogeneous b, inhomogeneous magnetic field. Why they made it in homogeneous? Because the force on a dipole arises in an inhomogeneous field.

So, if number of m values that is z component of angular momentum is odd what they would expect to see is that the number of lines here should be odd, right? Because if I put something in a magnetic field the levels split according to the m values and these values differ it could be 2 h cross, h cross, 0 minus h cross, minus 2 h cross, and the corresponding magnetic moment is also different and therefore, forces would be different. So, I would see odd number of lines. What they got instead was they got 2 lines, 2 lines, when the atoms came out. So, this was also at odds with whatever we had learnt. So, combining all these experimental, combining all these experimental evidences what was concluded and people also gave you know spectroscopic notation to things that hydrogen had a structure of 1 s.

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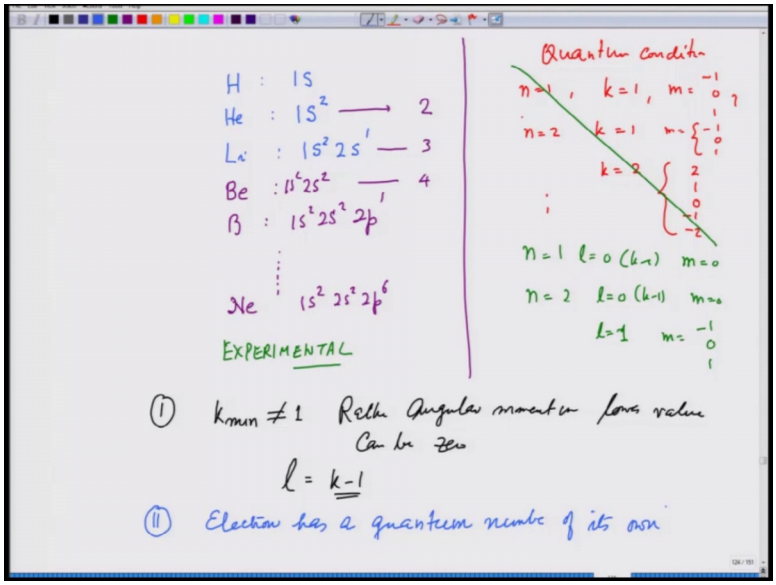

Helium, where n first level goes the first number shows n value. 1 is 2 electrons, lithium had 1 s 2, 2 s 1 structure; that means, there was n equals 1 n equals 2 were filled and the nature was s where s was given a name to certain spectroscopic, way the certain way the spectrum was analyzed.

Beryllium was 2 s, 1 s 2, 2 s 2. Boron was 1 s 2, 2 s 2, 2 p 1 right. These are all being investigated and so on. The number of electrons in this level are 2; number of electrons in this is 3 and 4. Similarly when one reached neon one could see from the spectroscopic and these periodic table evidences that this was had a structure of 2 s 2, 2 p 6. So, there were certain number that could be filled right. There was a periodicity of 8, now if you look at the corresponding quantum conditions, what they gave you for n equals 1 was k equal to 1. And therefore, m equal to minus 1 0 and 1 for n equals 2 they gave you k equals 1 and k equals 2, this was m equals minus 1 0 1 and m equals 2 1 0 minus 1 minus 2 I will reverse the order and so on. So, what one is seeing here is that in the first n equals 1 there are 3 levels. So, if each level has one electron there should be 3 electrons. And for k equals 2 there should be 5 electrons.

This is contradiction to what was observed experimentally. So, let me write this left hand side is experimental. All right, so, first conclusion that was drawn is k minimum is not

equal to 1, rather angular momentum lowest value can be 0. So, if I call this angular momentum quantum number l, it should be actually k minus 1. So, that I am now going to change right here and show it in green instead of this I am going to have n equals 1 and l equals 0, which is k minus 1 and corresponding m value would be 0. N equals 2 would have l equals 0 and l equals to 1 this is k minus 1. M value 0 m value minus 1 0 and 1 and so on. So, lowest angular momentum could be 1 and number 2 more important. Electron has a quantum number of it is own; that means, it is intrinsic to it is intrinsic to it and it does not depend on where the electron is moving.

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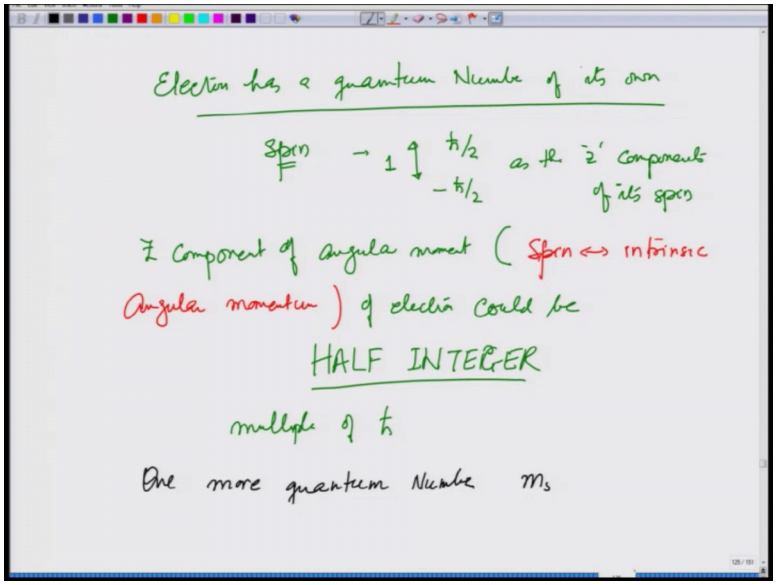

So, this is called electron has a quantum number of it is own. And it is value is called the spin and it could have value h cross By 2 and minus h cross By 2 as the z components of spin right. This difference again notice is by one integer; however, what it said was that z component of angular momentum which I will call spin. Let me write this in different colour spin, or intrinsic momentum of electron could be half integer multiple of h cross. Remember what Bhor had said Bhor had said the minimum value of angular momentum should be h cross and then it varied as you know the other integers.

However to explain atomic structure and all that we had to admit and this is based on experimental evidence, that spin the intrinsic angular momentum of an electron would

have the value of half integer multiple of h cross, and the difference would still be 1. So now, we have one more quantum number; let us call it m s, s for a spin.

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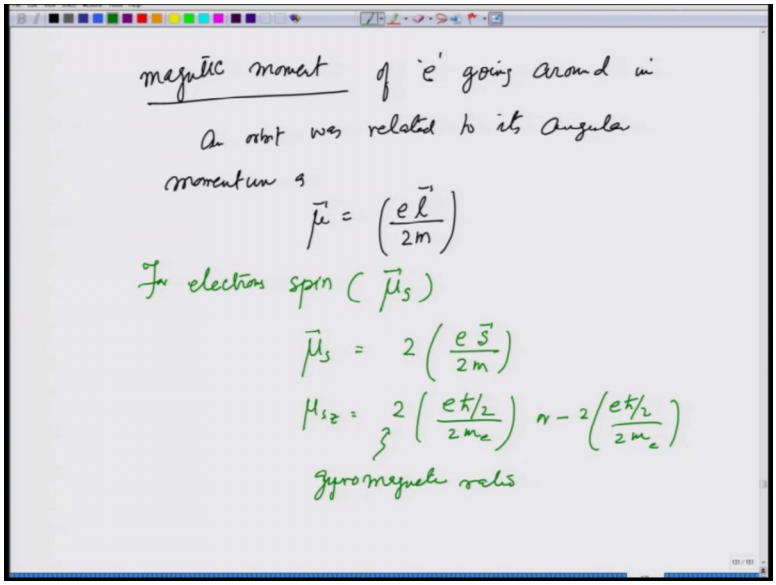

I also point out that we saw earlier that the magnetic moment of electron going around in an orbit was related to it is angular momentum as mu equals e l over 2 m. What was found in the case of electron; however, for electrons spin and the related the magnetic moment mu s. What was found experimentally to explain the spreading of lines and all that, that in this case mu s was 2 times e spin divided by 2 m. And therefore, mu spin z was 2 times e h cross by 2 over 2 m or minus 2 e h cross over 2, 2 m electron.

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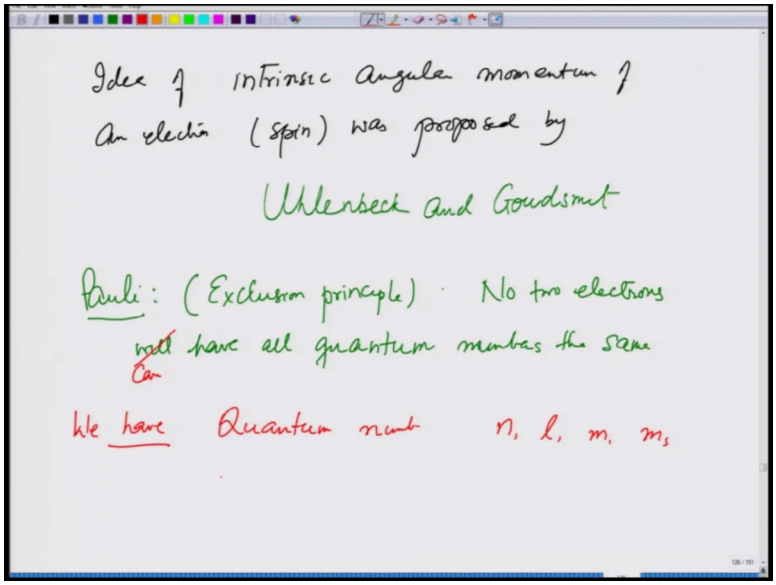

So, this was called the gyro magnetic ratio which is one for orbital angular momentum and 2 for a spin angular momentum. The idea of intrinsic angular momentum of an electron is called the spin was proposed by Uhlenbeck and Goudsmit. And then to understand the structure of atom next all he came with his exclusion principle, which said no 2 electrons will have all quantum numbers the same. Instead of will have I should actually now have can have. So, this becomes the fundamental principle. So now, let us see what apart we have. We have quantum numbers n, l, m and m s.

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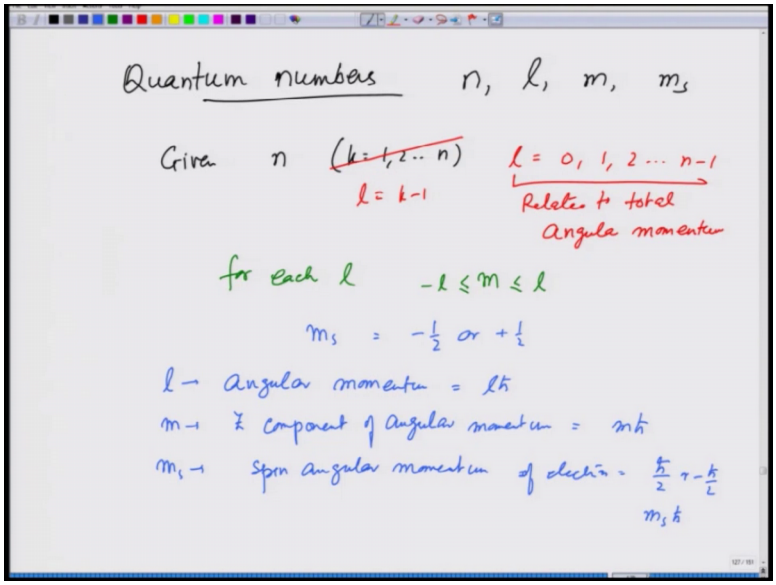

Now, for a given n and say for, So we have quantum numbers n l m and m s, for a given n, remember what were the k values k values were 1 2 and up to n, but we are no more interested in k. Instead what we have is l which is equal to k minus 1.

So, l values will be 0, 1, 2 upto n minus 1 and this is related to total angular momentum. And for each l for each l, I will have m values which are from minus l to l right. And then I have the 4th quantum number m s which could be minus half or plus half, let us see what does it mean. So, l means the angular momentum is l h cross as the magnitude m means z component momentum is m h cross, and m s implied spin angular momentum of electron which is h cross By 2 or minus h cross By 2, in short m s h cross. And when I add that not all quantum numbers can be the same, it explains the periodicity the rule of 8 and all that. And the spectroscopy is there is one more circuit point for the splitting of levels in magnetic field which I will explain in a minute.

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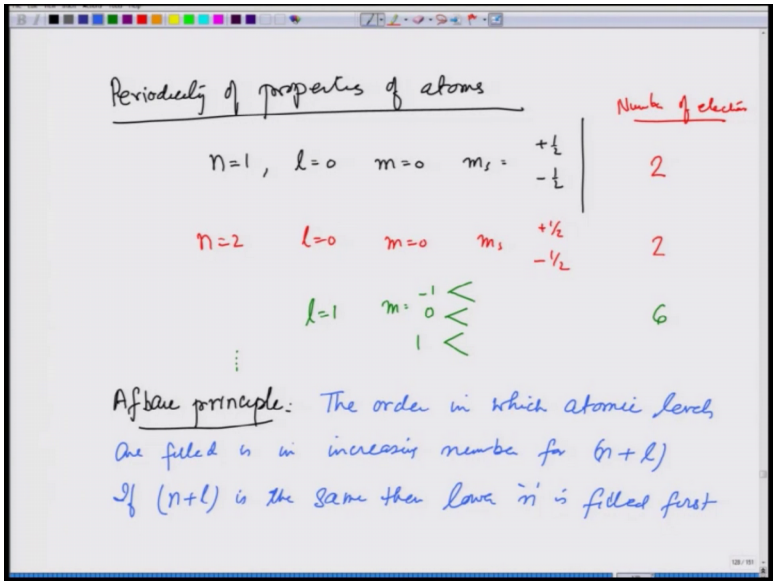

But let us see now for the periodicity of properties of atoms. So, let us see n equals 1, l maximum could be 0 m could be 0 and m s could be plus a half or minus a half.

So, maximum number of electrons let us write on the right number of electrons in this level could be 2 right. So, one for each quantum number. Let us see now n equals 2, l will be 0, m would be 0. So, m s would be plus a half minus a half number of electrons would be 2, I would also have in this, l equals 1. So, m equals minus 1, 0, 1 for each 2 levels of m s. So, number of electrons 6 and so on. So, one could see the periodicity or how the different levels are built, and one also observed the way periodicity was built and came up with something called the afbau principle, which said that the order in which atomic levels are filled is in increasing number for n plus l. And if n plus l is the same then lower n is filled first right.

So, let us let us see that. So that means, n equals 1, l equals 0 will be filled first, n equals 2, l equals 0.

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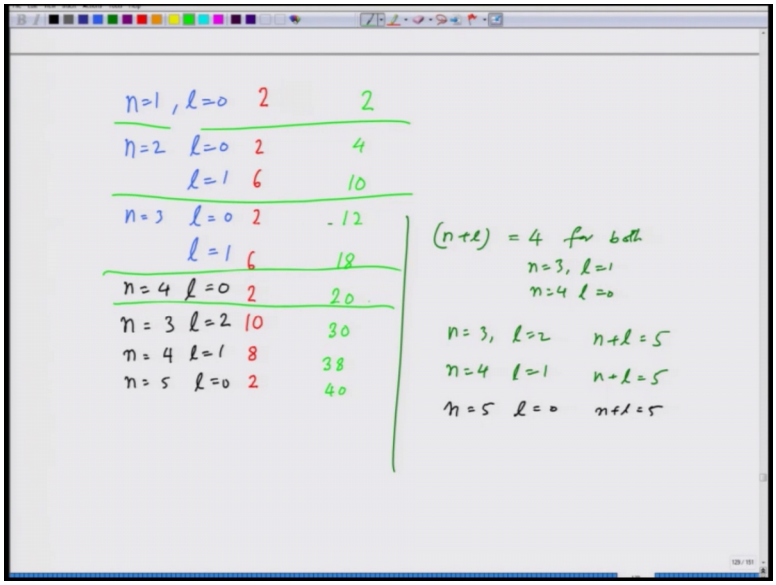

And then l equals 1, will be filled. Or n equals 3, I will have l equals 0 being filled, l equals 1 being filled and now I have a competition with n equals 4 l equals 0 because n plus l is equal to 4 for both. N equals 3, l equals 1 and n equals 4 l equals 0; however, now the lower end will be filled first. So, first you will fill n equal's 3 l equals 1. Now how about n equals 3? L equals 2? N plus l is 5, but n equals 4 n equals 1 n plus l is again 5 right. So, let us see now we are going to now first fill n equals 4 l equals 0 level. And after that I am going to fill n equals 3 l equals 2 level. And then n equals, now I have also n equals 5 l equals 0 n plus l is 5. But first I am going to fill for all these lowest n. So, n equals 4 l equals 1, and then n equals 5 l equals 0.

This is the order in which I will let us see the number of electrons 2, 2, 6, 2, 6, 2 this is l equals 2. So, this is going to be 10. L equals 1 again is going to be 8. L equals 0 again is going to be 2, let us see the total number of electrons. Let me now erase this and see what the total number of electrons is. If I fill only up to n equals 1 l equals 0, I have 2, 4, 10, 12, 18, 20, 30, 38, 40 and so on, these are the shell fillings. And this is where the periodicity starts coming in; these are the shell feelings, all right and so on.

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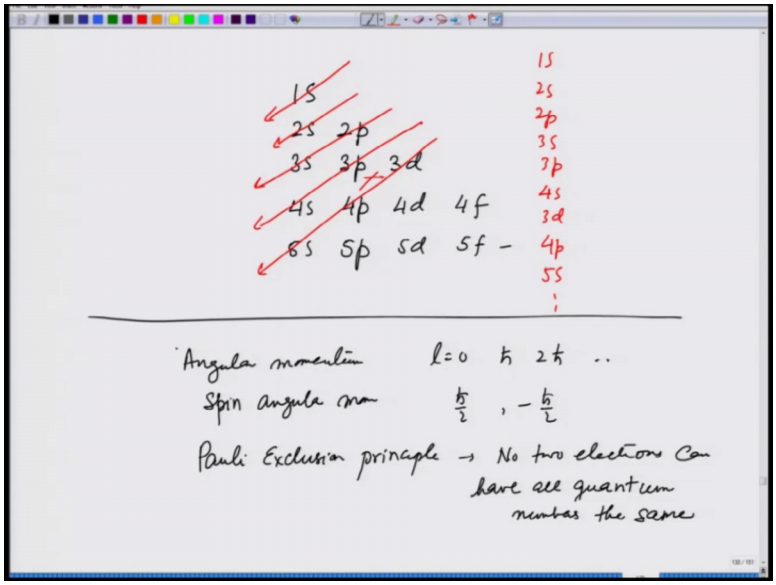

So, this is how the atomic structure was explained. Now the above principle at times is also written like this, you write the levels 1 s, 2 s, 2 p, 3 s, 3 p, 3 d, 4 s, 4 p, 4 d, 4 f, 5 s, 5 p, 5 d, 5 f and so on. And then you fill them according to this arrow.

So, you start with 1 s, then you fill 2 s, then you fill 2 p. And after 2 p you fill 3 s, 3 p, and after 3 p you cannot go to 3 d. You cannot go this way; you have to go to 4 s. And then you come to 3 d, 4 p, 5 s and so on. So, this is known as the afbau principle, it is followed by maximum a large number of atoms in the periodic table, and this is how the levels are filled. So, to conclude this what we have learnt in this lecture is that angular momentum of electron in an atom could have values l equals 0, h cross, 2 h cross and so on. And then we all have also learned that there is spin angular momentum, which is h cross by 2 and minus h cross by 2. And by the way this 2 values of spin angular momentum are what gave rise to the split of the beam of silver atoms and Stern Gerlach experiments into 2.

And then we have the Pauli Exclusion Principle, that no 2 electrons can have all numbers the same. And with this I conclude this lecture. I have given you the piece of history mix with what we know today, that this history is discussed because it is important to know how idea is developed. And all these things you can see that sometimes when we are describing angular momentum we are saying k equals h cross then suddenly we are

saying with experimental evidence, there should be not k h cross, but k minus 1 h cross right.

Then the idea of spin angular momentum also came to explain certain properties Pauli exclusion principle was introduced to explain the periodicity, and the filling of atomic shell structure.

All these things should be preserved these are experimental facts, which were explained using these principles which are being stated. All that should be preserved and should come out automatically from a complete theory, which we will see later when we develop the quantum mechanics that it does come out.