Atomic and Molecular Physics
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Lecture 23
Multi electron atoms

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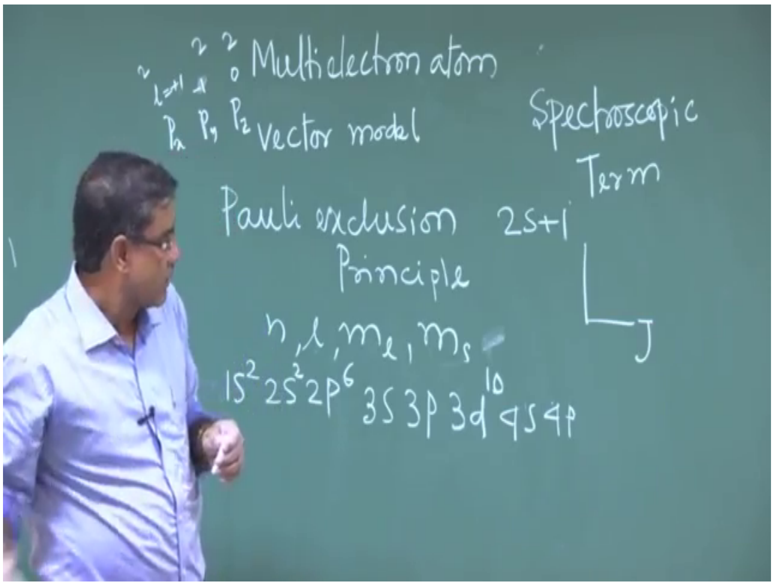

So, we started Multi electron atom, if atom is having more than 1 electron. So, actually most of the all atoms are having more than 1 electron accept hydrogen atom and other ionized atom helium plus 1 lithium plus 2 means additional atoms electrons are taken out. So, that is the single atom system that we have studied and in case of multi electron system.

So, first of of you see this important thing is that this Spectroscopic Term. What is that? That I have L that 2 s plus 1 and the J value so, that was the Spectroscopic Term which basically represent a represent the state of electron or state of the atom basically. Now, earlier I told state of the electron for single electron system, now for multi electron atom. So, I can tell that the state of the atom at which energy this item is having ah. So, this will tell this atomic states ok, means if 2 electrons are there, so, 1 electron is at a particular state, another electron is another state. Now, resultant state will be the state of the atom ok.

So, instead of filling there is that electron is at minimum energy level instead of filling that one, so, in case of multi electron atom or in general one, we can tell that atom is in a lowest energy state or excite state etcetera ok. So, this just language which here, we just modified for as a state of atom ok; so, these are basically Spectroscopic Term; whatever for single electron system we have used. So, that was represent the state of the electron basically state of the atom.

So, it since it was single electrons, either electron or atom this it was there is no there was no difference, but in case of multi electron. So, now, we are telling it is not this will represent this is basically will represent the state of the atom ok, not state of the electron. So, although we use state of the electron in single electron system so, because that both basically meaning of both was same, but actually in general, we will use this Spectroscopic Term it represent it represent the state of the atom ok. So, that it is single electron or multi electron. So, for multi electron, so, I have to know the s, now s is for total angular total spin quantum number of the of the multi electrons in the atom ok.

And l is the total angular orbital angular momentum of all electrons. Similarly, this J value ok. J value is the total angular momentum of this atom is some taking l s coupling or J coupling, one can find out the J value ok. So, I have discussed, we using the vector model using the vector model.

So, how to find out s? How to find out l? And how to find out J value ok, How to find out J value? So, so, basically to find out the J this term Spectroscopic Term, so, I have to know the distribution of electrons in the atom right, atoms of different energy states orbit or orbitals. So, how electrons are distributed in the in the atoms? Ok. So, that we have to know and this I think all of you know one has to. So, to distribute the electrons in the atom, one has to consider the Pauli exclusion Principle; Pauli exclusion Principle Right.

Pauli exclusion Principle what it is telling? it is telling that this no electron each electron will have distinct quantum number, each electron have so, it is defined in different ways basically. So, n, l, m l, m s ok, so, no electron can have or can have the can have the same quantum numbers n, l, m l, m s ok. So, each electron have distinct this number quantum number ok. So, they can have these three same, but this other one has to be different ok. So, no 2 electrons can have the same quantum number of this 4 of this other way quantum step of the atoms multi electron atoms has to has to have this anti symmetric wave function ok.

So, that way also people defect. So, there are different ways this Pauli exclusion Principle is explained. So, you are familiar with this one and in quantum mechanics in quantum mechanical language, one use this symmetric wave function anti symmetric wave function that way one can define. So, let us consider the; whichever we are familiar. So, let us consider that one. So, considering this one, so, electron can be distributed in the in the in the atoms and how they are distributed, so, building blocks of periodic table is build based on this distribution of electrons in atoms and this. So, any atom any atom have different different what is call this orbit or orbitals, right. So, we generally write n, say n equal to 1.

So, I have written 1, so, and then l equal to 0. So, it is s . So, 1 s means n equal to 1 and l equal to 0 ok. So, n equal to 1 and l equal to 0 s, l equal to 0 ok. So, in this case what will be the m l value? l equal to 0; m l value 0 right, so, n 1, l 0, m l 0. So, m s, s equal to half 1 electron for each 1 electron is half. So, m s can be plus half and minus half ok. So, here, so, this these 3 are same. So, this can be different plus half and minus half. So, 1 s 2, we write 1 s 2 ok. So, in this orbitals it can have maximum 2 electrons right. Similarly, 1 s 2 if it is 1 electron that is fine, 1 s 1 if it is 2 electron, then one more it can put here 1 s 2, but third one, we cannot put here because there is no option right. I cannot put third one because there is no option ok. Because n equal to plus half and n equal to minus half that is the only difference between these two left the other three quantum number are same.

So, then I have to go the hierarchy level for any cal 2 I have to go. So, then I have to go for n equal to 2 ok. So, why I need for n equal to 2 because if I have more than 2 electron, so, then where I will put? I will put the next higher energy level. So, that is n equal to 2 n equal to 2 ok. So, n equal to 2 it can have l equal to 0 and 1, n equal to 2, it can have l equal to 0 and 1. So, l equal to 0 means s and l equal to 1 means P ok. Now, n and l these are fix, here n equal to 2, l equal to 0. So, for this case again m l equal to 0 so; that means, here whatever I will put n 2, l 0, m l 0. So, that is fixed from here. So, now, only I can vary this one this one plus half and minus half. So, again only next cell it can have 2 electron s sub cell can have 2 electron ok.

And then for more electron other electron if I have. So, 4 electron so, I can accommodate them within 1 s 2, 2 s 2. Now, more than 4 electron fifth one, I have to put here fine, I can put here. Sixth one where I will put? 7th one where I will put? So, let us let us see in this case is l equal to l equal to 1 means m l equal to 12 plus 1, how much m l value? 3. 12 plus 1, l equal to 1. So, 12 plus 1 this 3, so, m l value will be m l value will be plus l to minus l means plus 1, 0 minus 1, see it will have 3 value ok, it will have 3 value. So, this p again have 3 value due to m l.

So, it tell p x, p y, p z; p x, p y, p z, ok. So now, so, there p x it is a say if it is l equal to plus 1, then p y say exactly I have to see if it is if it is 0 and it is I think this may be 0 and this minus 1 l equal to minus 1 may be s, that one has to see it depends on angle say any way. So, if I pursier this 3 value p x, p y, p z, l equal to plus 1, minus 1 and 0 ok.

So, now for n equal to 2, now l equal to 1 that is also fixed, l equal to 1. Now, m l value there are 3 value there are 3 value, now for each m l value for each m l value for each m l value say plus 1. So, I have 2 option m s is plus half or minus half ok. So, for l plus l equal to plus 1 this I have 2 option, I can put 2 electron for similarly, for other minus 1, I can put 2 electron and l equal to 0. I can put 2 electron m s plus half, minus half ok. So, here plus half, minus half, but m l varies. So, that thus this 6 electron one can put here 6 electron one can maximum; 6 electron one can put here.

So, I have put already 10 electron, now, eleventh one where I will put? So, I have to go next higher energy level 3, now 3 n equal to 3, l equal to 0, 1, 2, 3. 0, 1, 2, 3 right so; that means, s 3 s, 3, p, 3 d right. Similarly, 4 s, 4 p, 4 p, 4 d, 4 f, so, this say one can one can put and one can see that this d electron can, so, so s orbitals have maximum capacity that 2 electrons it can contain 2 electrons, p, it can contain 6 electron and d it can contain 10 electron, one can show it because d equal to this is l equal to 3. So, l equal to 0, 1, 2. So, for l equal to 2, it is d ok. So, now, when d l equal to 2, so, m l will be have 5 value 12 plus 1.

So 5, so, plus 2 to minus 2; so, 5 value and for each it will have m s plus 1 and m s minus 1 2. So, 5 into 2, so, it will be t 10 electron, f it can contain 14 electron this. So, one can one can put electrons in different orbitals ok. So, that way in multi electron system, one can arrange electrons in the in the in the atoms ok. Now, if this is the case now, if I consider helium atom, if I consider lithium atom, if I consider beryllium atom, so, I have to I have to know I have to know that it is 2 electron of course, say if simplest one, helium atom it has 2 electron it has 2 electron ; helium atom it has 2 electrons.

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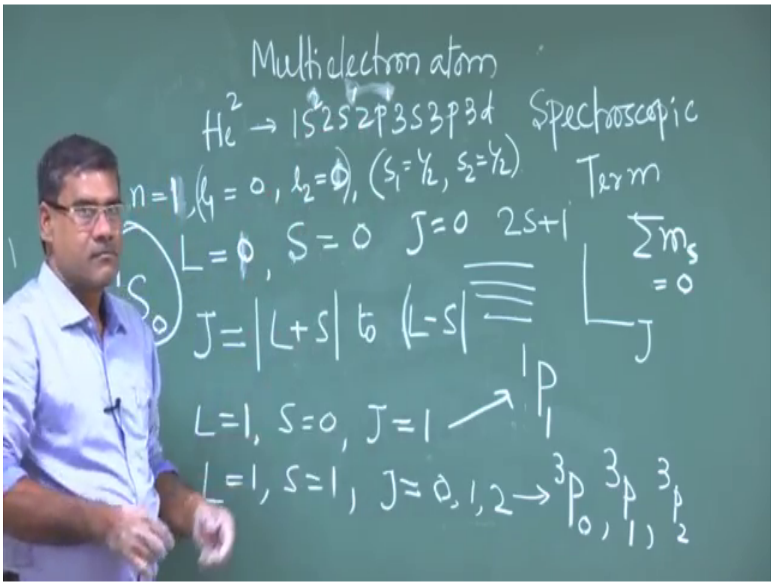

So, it has 2 electron right, but in helium atom, in helium atom or any atom this orbitals are available, 1 s, 2 s, 2 p; 1 s, 2 s, 2 p, 3 s, 3 p, 3 d. So, this orbitals are available. Now, there is no restriction of electrons 2 electrons to stay to go in any of these orbitals right. Both of both of the electrons it can be here, it can be here, but it may happen that one electron is here and another electron is here, that is also possible or one electron is here in another electron is here or both electron are here; one is here, another one is here. So, all sorts of distribution of electron is possible right. Only difference that difference what will be the difference?

Difference will be the how will express this difference. This difference, we express basically in terms of the state of the atom, we tell the state of the atom ok. Now, difference will be in terms of energy, difference will be in terms of energy and because of the different configuration of the electrons they are staying at different orbitals, the energy of the atom will be different ok. So, for each distribution of the electrons there will be one state of the atom right. So, that state of the atom is expressed by this by this Spectroscopic Term as I mentioned right.

So, now, if 2 electrons, if this is the configuration of helium-helium 2 electrons are there, but these electrons are in this way; it is a distributed in this way. So, here immediately, I will write for first electron l 1 equal to 0 ok, n is fine; n is I do not bother n I do not bother, but one can write also n equal to in this case n equal to 2 for both electron ok. l 1 equal to 0, l 2 equal to 1 right and then see this is l and then s s 1 of course, s 1 equal to half, s 2 equal to half fine.

So, I know n l and s for this configuration. So, I have to find out resultant l; resultant l will be l 1 plus l 2 to l 1 minus l 2. So, resultant l will be of course, here it is 1, 0 plus 1 and 0 minus 1 we are taking magnitude. So, is 1 basically, so, l will be 1 and capital S, what it will be? It is plus half and minus half. So, s will be resultant s will be s 1 minus s 2 to s 1 plus s 2 magnitude. So, s 1 minus s 2 it will be 0 and s 1 plus s 2 it will be 1. So, s can be 0 or 1 ok. So, now, here I have n value it is too fine. Now, I have resultant total angular momentum orbital angular momentum is 1 and total spin angular momentum is either 0 or 1 ok, both are possible either 0 or 1. Now, here, what will be the then. .

Now, what will be this Spectroscopic Term? So, I have to find out J value, I have to find out J value. So, J value will be J value as I told this l plus l plus S to l minus S right. So, l is 1 fine, but S either 0 or 1. So, it will consider for l equal to 1 and S equal to 0 . I will get J value J value is 1 right, J value is 1 and for l equal to 1 and S equal to 1; what will be the J value? J value will be J value will be 0 to 2. So, 0, 1, 2 right because l plus S to l minus S magnitude, I will take magnitude, so, l plus S that is; obviously, 2. So, 2 then minus 1, minus 2, minus 3 up to 0 1 has to proceed. So, I will get basically this 3 value, J equal to 3 value.

So, what will be the Spectroscopic Term then? So, so the Spectroscopic Term will be l equal to all the time, it is l equal to 1 means P; this is P and for S equal to 0 means this is 1, 2 S plus 1 is 1 and J value is 1. So, this will be 1 Spectroscopic Term. So, it will represent one state of the atom and this will tell you this Spectroscopic Term will be P, P and S equal to 1 means 3 3 and then J value is 0. So, this is 1 0, this is 1 will be Spectroscopic Term, another will be P 1, another will be 3 P 2 ok. So, this 3 Spectroscopic Term, so, for these distribution of electron, so, this it will have 4 states; this atom will have 4 states and these 4 states are this ok.

And their energy, you see this here their energy this e it depends on J, how it depends on J? It will follow the same rule whatever we have found earlier. So, it will for lower J value will be, lower J value will have that J plus half N by J plus half. So, let J 1 mean it will be higher value that term, so, it will be more negative yes it will be more negative. So, this will have this time will have the lower energy, then this J value 1, then this j value 2 ok. So, that way, so, you can tell this due to this l s coupling, due to the l s coupling, the energy will be splited although their n value are same both electron n value are same, but their l value are different.

So, obvious l value are different; obviously, their energy will be different. Now in for same for now, due to this coupling due to this coupling here this considering the interaction coupling, this we are seeing that it will have 4 spectral lines ok. It will have 4 spectral lines ah. So, it can have 1 of these 4 states, it can have in 1 of these 4 states ok. So, in which state it is it will be take 1 of them. So, which state it is? So, that will be basically the because of this J value and difference of this resultant S value. So, that is decided ok.

So, now, here as I mention this Pauli exclusion Principle . So, when this electron helium case of helium if electron distribution is like that. So, these are the 4 states; possible 4 states. It will be in one of them ok. Now, if really their if their configuration is like this 1 s 2, then what is the difference with the this earlier configuration ok. So, in this case; obviously, one has to find out this l equal to 1, fine n equal to 1, l equal to l 1 equal to 0, l 2 equal to 0 right both electron are here. So, for each case yes of course, half and half. So, in this case, I will get l 1, this will be 0, this 0 n equal to 1 ok. So, resultant L will be 0 or resultant S will be 0 or 1 right 0 or 1.

So, now, here we have to be careful. We have to be careful because whether it follows whether it obey the Pauli exclusion principle or not, that we have to check. Earlier case, we did not bother because in earlier case we did not bother because their l value was different, n value was to earlier case earlier distribution n value was to right earlier case was here and here. So, n value was same, but l value was different ok. So, n, l, m l, m s; so, whether m l and m s are same or different that does not matter. Already Pauli exclusion Principle is satisfied because their l are different. So, we did not bother about the value of m l and m s ok.

But in this case, in this case n equal to 1 and l equal to also for both case it is 0. So, n and l are same, n and l are same. So, one has to consider about m l and m s. So, one of them has to be different. Now, m l; l if l equal to 0, l equal to 0, m l is 0, m l 1 equal to 0, m l 2 equal to 0 right. So, m l value also same right. So, m s value has to be different, m s value has to be different, here it is telling resultant value. So, L total L equal to 0 that is fine, now total S it can be 0 or 1 right. So, here I have to consider which m s are allowed. So, m s m s 1 if it is plus half, m s 2 it cannot be plus half, it has to be minus half right. Then only it will be different because our n is 1, l 1, l 2 both are l is both are 0 m l also in both cases are 0 right m s so, m s 1; if it is plus half then other in other case it has to be minus half so; that means, total; that means, total sum of m s sum of s m s s 1 and m s 2 it has to be 0. In one case, if it is plus half in another case it is minus half ok. So, m s has to be 0.

So, when you will get m s have is total m s is 0. So, when total S will be 0 ok, total S it can be it can be 1 also, total S it can be 1 also then in this case m s value will be plus 1 0 minus 1 ok. So, this 1 is telling m l value will be if depending of the so, this S equal to 1. It is basically, it is it will tell that this 2 this maximum this s m s value will get that will be basically for parallel configuration for parallel configuration or both are anti-parallel configuration ok. If 1 is up and 1 is down, so, then m s value has to be 0 and corresponding if it is s equal to 0. So, m s; obviously, it will be m s; obviously, it will be total m s will be 0 means individual m s if it is 1 another has to be minus 1 ok.

So, in this case, this 1 is this will not be allowed as per Pauli exclusion Principle. So, in this case, your total J will be 0 ok. So, your state your state l equal to 0, so, your state will be your state will be our spectroscopic term will be S then 0 means 1 and J it is 0. So, this will be the Spectroscopic Term. This will be the only one possible state, only one possible state of the of the of the helium of the helium and it is basically it is a one can see or show that this the minimum energy when electron is like this, this is the minimum energy and this called when this is that Spectroscopic Term then this is called the down state of the of the of the helium ok. Now, here important things I showed you when this is the configuration and another configuration of 2 electron this, so, here that this 1, we tell this non-equivalent electron ok.

We tell this non-equivalent when this is the configuration either so, it is definition is if n l of a of 2 electrons n l of 2 electrons, if they are different than this electron is called they are called Non-Equivalent electron. If for 2 electrons if n and l are same, then it is called equivalent electron ok. So, when this is the configuration 2 electrons here n and l n equal to 1, l equal to 0 for both cases, so, this electron 2 electron is called Equivalent electron and when this is the configuration instead of this 1, when this is the configuration here n equal to 2, but l equal to 0 and 1; so, n l different for this 2 electrons ok. So, they are called Non-Equivalent electron ok.

So, for non-equivalent electron, it is easy to find out the Spectroscopic Term or state of the multi electron atom, it is without considering the Pauli exclusion without thinking about the violation of the Pauli exclusion Principle, what can write the states easily, but for equivalent electron one has to one has to think when you are going to find out the resultant J ah. So, one has to think about the resultant l and s to safe to protect or to satisfy the Pauli Exclusion Principle. So, for this of 2 important aspect equivalent electron or non-equivalent electron for multi electron atom to find out the Spectroscopic Term of the states ok; so, I will stop here.

Thank you.