Atomic and Molecular Physics
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Lecture - 25
Multielectron atoms (Contd.)

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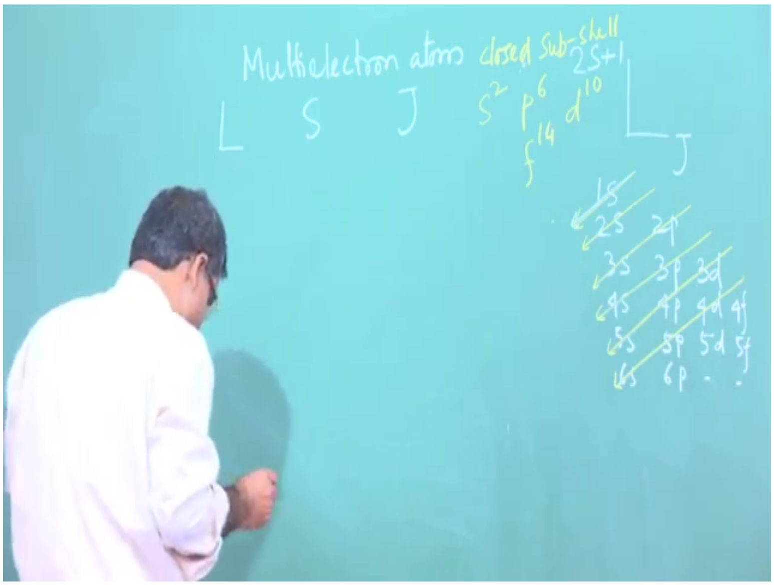

So, we will continue about Multielectron atom ok. So, so we have seen the structure of atom basically how these energy levels for electrons are available in a atom. So, apart from the discussion on single electron system means if 1 electron is put in atoms. So, it can it can be at any energy level so, but what will be the minimum energy for thus for the atom.

So, that is called ground state and that that one has to find out that we know that is for minimum smallest n and smallest l the energy of the system will be a minimum and, yeah energy level is basically we have seen this energy e n l it depends on n and l. Now, so we have enough discussion for 1 electron in atom, now if I put 1 more electron in second electron, then third electron fourth electron.

So, it will so, it define the basically different atoms helium atom, lithium atom, then beryllium, boron, carbon, neon right so, chromium, copper etcetera depending on the number of electrons in the atom. So, it is a different name of atoms. So, we are interested to find out the spectroscopic term for multielectron atom. So, to find out the spectroscopic term I need L and then S and then J ok. So, for single electron this file we have discussed, now for multielectron if I want to find out so, I have to take help of vector model.

So, so far so, already we have discussed that the what will be the resultant angular momentum, orbital angular momentum, that is for multielectron system generally we write capital L and what will be the resultant spin angular momentum so, that for multielectron atoms so, that we write by capital S and, then what will be the resultant this J means from L and S due to L S coupling we get J. So, what will be the resultant J? J also we get from the J J coupling also as I mentioned earlier.

So, but here we will consider L S coupling because, most of the atoms they shows this L S coupling, rather than J J coupling; J J coupling generally is found for heavy heavier atom means high gain value. So, that will not discuss now, but mainly we will consider L S coupling. So, so that is our aim to find out. So, as I see in general and also I have shown that electronic configuration of multi electron atom. And it is one is to for any for any number of electron, you have to distribute you have to distribute electrons in different orbital's. So, that orbital's I have I have mentioned earlier. So, this let me write here just 1 is then energy wise, this is the smallest energy 2 S 2 p, 3 S 3 p 3 d right 4 s, 4 p, 4 d, 4 f right.

So, this say 5 s, 5 p, 5 d, 5 f, 6 s, 6 p, etcetera ok. So, and how we distribute electrons so that I have mentioned I have mentioned that this just we follow the building block principle or above principles. So, this say 1 can filled up the electrons multi electrons in the in the orbital's.

So, and also we know that how many number of electrons can it can this S s orbit can take it is 2. So, this so, S 2 in general whatever the n it does not matter. So, for S 2 or S 2, then p 6 d 10 f 14 so, this is the maximum number of electron the sub shells this orbital's can accommodate. So, these are called closed shell closed sub shell is called closed sub shell say a closed sub shell closed sub shell and closed shell, it is you see when this n principle quantum number, depending on principle quantum number. This it has 2 sub shells, if this whole shell is filled with the electrons. So, then that will be called this closed shell closed shell, or closed sub shell.

So, this had has importance. So, this distribution follows the Pauli Exclusion Principle spine. Now as I told the; I am interested to find out the find out the spectroscopic term for multielectron atom. So, this would be say I have to find out capital L capital S and capital J.

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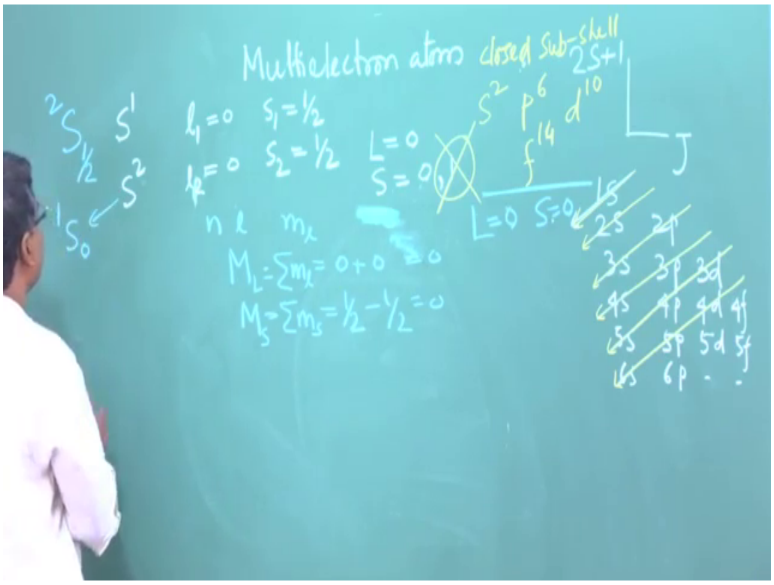

So, let us so for 1 electron that already I have seen it S orbit say if S orbit 1 electron, say immediately I will write it is what is the n equal to 1 2 3 whatever that we are not considering.

So, just if so, S means l equal to 0. So, l 1 let me write l 1 equal to 0 and, this 1 electron is there. So, S 1 is half right S 1 is half and this fine. So, it is it is spectroscopic term for 1 electron it will be basically this l is 0 means it will be it will be a spectroscopic term, it will be for this case S equal to 1 spectroscopic term here, I can write I will write here. So, S and then S is half. So, it is 2 and, then j will be l 1 plus S 1 or l 1 minus S 1 so, here it is take only positive values. so, it is half.

So, so this will be the for S electron 1 electron. So, that will be the spectroscopic term. Now if you take 2 electron if you take 2 electron S so, it is put in S orbital's. So, now, I have 2 electron so, l 1 equal to so basically l 1 equal to 0 S equal to half therefore, 1 electron it is here. So, now for additional electron so, this L 2 is 0 S 2 for second electron, it is half ok. Now 2 electrons are there it has angular momentum, orbital angular momentum l 1 and l 2 both are 0.

So, using the vector model what will be the resultant L, what will be the resultant L that is say capital L, it will be 0 definitely ok, l 1 plus l 2 to l 1 minus L 2 that is the vector summation of a orbital angular momentum. And now I have I have spin S 1 half and S 2 half now what will be the resultant S. So, resultant S will be resultant S will be S 1 plus S 2 to S 1 minus S 2. So, it will be basically S 1 plus S 2 magnitude this 1 S 1 minus S 2 magnitude is 0.

So, basically it will be 0 and 1 ok. So, it will be 0 and 1 and, now here we have to see whether, if I take this S equal to 0 and 1 whether it satisfy the Pauli Exclusion Principle. So, Pauli Exclusion Principle as I told earlier that n l n l n l m l and m S so, that has to be the set has to be different from the different for each electron. So, so here l equal to 0 total l equal to 0. So, l 1 l 2 is this both are 0. So, m l; obviously, is 0 m l for this m l so, generally we write sum over m l equal to what is there m l 1 plus m l 0. So, both are 0.

So, they are; obviously, for 2 electron 0 plus 0 ok; that means, m l 1 is 0 and m l m l 2 also 0. So, now n is same l is same for both electron and m l also same for both electron ok. So, S m S has to be different for these 2 electrons m S has to be different. So, there is no choice that m S has to be m S has to be m S has to be for this case so, here I can think. So, m S yeah or sum over m S if we right so, if it is half, then other one has to be minus half. So, summation of m S will be 0 this also 0.

So, this significant of the summation so, whatever summation we will get. So, to get to get m l summation of m l equal to 0 so, l has to be 0; right to get summation of M S. So, resultant m S basically capital M S; so, this generally we can write capital M S and this we can write capital M L ok. So, capital M L for resultant 1. So, so M L will be 0 so; that means, l is 0 if l is 0. So, M L will be 0 capital M L for resultant 1.

So, similarly here only this 1 choice is possible, I cannot take this half and this other 1 plus half ok. So, then all for both electrons set of this quantum number will be same that is not allowed. So, in this case restriction is if it is 1 then other one has to be minus 1 minus half, if it is half other one has to be minus half. So, this total m S is 0; that means, resulted S. So, S S is 0 if S is 0, then only I will get capital M S resultant M is 0. So, S equal to 1 that is not that we cannot take that we cannot accept in this case we cannot accept.

So, but S equal to 1 that will be allowed, if any other out of this 3 if 1 is different like S 2 2 S electron in S so, I have 1 s, 2 S I have 1 s, 2 S if 1 electron is here and another electron is here; that means, their n are different n are different. So, if n are different, so, this can be same m S can be plus half both can be plus half. So, summation of m S that will be 1 capital M S will be 1 resultant 1. So, capital M S is 1 if S is 1, then only we will get m S is 1 ok.

So, although it is S electron although it is S electron, but when this electron or in same orbit ok, they are same here n value are same, then only S equal to 0 is allowed S is not equal to 0. So, we will get S equal to we will get S equal to 0 and that is not allowed ok. So, from here only they I have mentioned this S 2 when n l value are same of 2 electron or other 3 electron 4 electron whatever n l same. So, those electrons are called equivalent electron.

And if n l n l either n or l or both are different for 2 electrons or more than 2 electrons. So, then this t that electrons will be called the non equivalent electron so, for nonequivalent electron it is S equal to 0 and S equal to 1 both are both are allowed because, they will not violate the Pauli Exclusion principle. So, so for non equivalent electrons there is no problem in straightforward whatever this following the vector model whatever L and S we will get. So, that all are allowed and corresponding this spectroscopic term we can write we can find out.

But when electrons are equivalent electrons, then it is it is slightly tricky to find out the allowed states allowed spectroscopic term, as we have seen here ok. So, here what we are seeing here these are; obviously, equivalent electron. So, for this case L equal to 0 and S equal to 0. So, so this 1 state will be 1 S and J will be; obviously, 0. So, this is the 1 S 0 state or spectroscopic term. So, here you see this S 2 is a closed sub shell. So, for closed sub shell what I am getting, I am getting resultant L is 0 and resultant, S is 0 and you can show for any other closed sub shell the same result. So, for all closed sub shells. So, L resultant L will be 0 and S will be 0 ok. So, 1 I have shown here, so, for P 6 also the same d 10 as well as for f 14. So, this resultant L and S.

So, neon it has 10 electron; it has 10 electron so, 1 S 2, 2 S 2, 2 p 6. So, for neon it is closed shell for helium S 2 it can be helium 1 S 2. So, helium is or helium is closed shell closed sub shell for neon it is closed shell. So, if sub shells are 0 L S 0 so, for closed shell it will be; obviously, 0 because yeah if you take vector sum of these all sub shells. So, it will be 0.

So, so this one observation is that these for closed sub shells or closed shell the total angular momentum and spin angular momentum, orbital angular momentum and, spin angular momentum these are 0 ok. Now so, then now we will see for p electron for p electron let us so, I will I will erase this for p electron.

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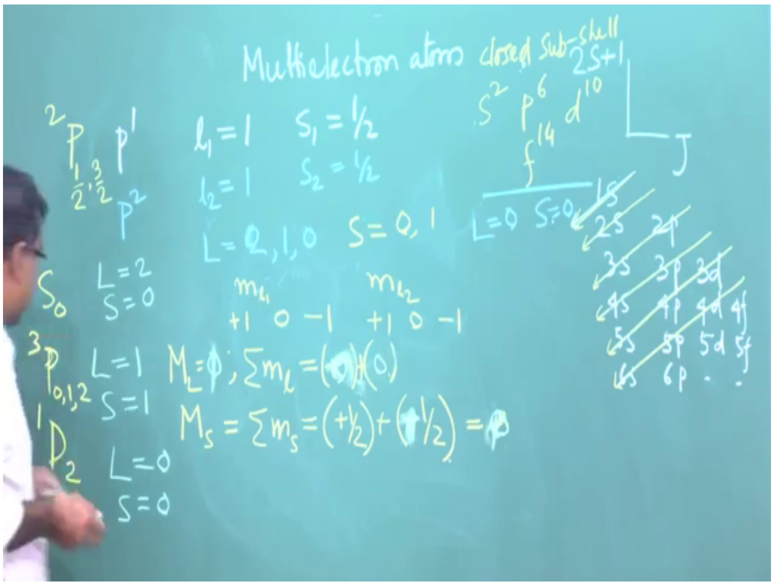

So, P electron is a P 1 in whatever it can be 2 2 or 3 or 4 whatever does not matter. So, P P electron say l 1 electron l 1. So, I do not bother if it is 1 S to 2 S to and then 2 p 1, because 1 S 2 already L S 0 I will not consider 2 S 2 also it is it is L and S 0 so, I will not consider so, only P electron, if any P electron.

So, so for lithium for lithium 1 S 2, 2 S 1 so, 1 S 2 there is a L S 0. So, 2 S 1 so only is the 1 electron ok. So, I have to find out this L and S for that. So, it is like single electron ok, it is like single electron like hydrogen atom. So, that is why lithium in case of sodium ok, then potassium all alkali atom, you will see that except the outer electron this rest for rest of the electron L and S are 0 L and S are 0 ok.

So, that is why it is the whatever L S and J will get that is basically for the 1 electron. So, that is why I have mentioned you earlier that this spectra whatever we see, for alkali atom there they are very similar to the hydrogen atom ok. So, for P 1 electron so, here are basically I am showing how to calculate the resultant angular momentum, either orbital or spin and then resultant 1.

So, so if you if we can calculate so for particular atom more can easily find out. So, for P 1 electron l 1, l 1 is 1 and 1 electron. So, S 1 is; obviously, half ok. So, resultant it is 1 electron. So, it is state will be a state will be spectroscopic terms. So, that will be P is half it will be 2 and, l s J J will be half and 3 by 2, half and 3 by 2, half and 3 by 2 see basically 2 spectroscopic term 1 is 2 P half another is 2 P 3 by 2 ok.

So, for P electron 1 electron this is the state, then if P equal to 2. So, 2 electrons are there now already for 1 electron l 1 this S 1 this. So, I will write l 2 another electron 1 and S 2 equal to half ok. So, here what we will get I have to find out the resultant l and resultant s. So, resultant l it will be resultant L will be from l 1, l 2 l 1 plus l 2 to l 1 minus l 2. So, L 1 plus L 2 is basically 2 and, then l 1 plus l 2 minus 1, l 1 plus l 2 minus 2 up to l 1 minus l 2 we have to process.

So, you get 2 1 and 0 ok, 2 1 and 0 l 1 minus l 2 is 0. So, I will get 3 l value, I will get 3 l value and S value I will get S value I will get, say S value I will get 0 and 1 0 and 1. Now here as I told since these electrons are equivalent electron I have to check, whether all values are allowed or all combination of L and S allowed or not ok.

So that we have to check how to check. So, this L equal to 2 L equal to 2 so, for L equal to 2 what will be the m l value what will be the m l value, m l value for individual for individual so, I have to find out so, I have 2 electron. So, for 2 electron m l m l 1, it will have 3 value is 1 so, plus 1 0 minus 1 that is why m l 1 and m l 2 m l 2. So, it can I have also either plus 1, or 0 or minus 1 plus 1 0 or minus 1. So, that is m l value for individual electrons.

So, now n and l are same now 2 electrons so, there are the so this first electron I can put at any 1, I can put at any 1. So, I have to look I have to I have to look at it. So, to get L equal to 2 so, for L equal to 2 for L equal to 2, what will be the m l value capital M L value capital, M L value will be capital M L value, capital M L value will be basically plus 2 to minus 2 plus 2 plus 1 0 etcetera up to minus 2 ok.

So, so maximum M L value can be plus 2 and that is only when this L is 2 so, but plus 1 M L value plus 1, it can be it can be from L equal to 2 it can be from L equal to 1 ok, or 0 it can be from L equal to 2, it can be from L equal to 1, it can be from L equal to 0. So, that I cannot distinguish from which L it is coming. So, that is why for L and M, for L and S L, M L value which first we take the highest 1 ok. So, here M L value highest is plus 2. So, then taking plus 2 how M L 1 and M L 2 are this which value we have to choose that way we proceed.

So, here for M L value 2 for M L value 2 so, that will come basically from sum over of m l ok. So, sum over of m l is to get to it has to be plus 1 m l 1 plus 1 and m l 2 also plus 1 ok. This is one, this is another and then take there add them, then you will get m l value basically 2. So, what does it mean so, for m l 2 already I have assigned the electron, this 2 electron this m l value this value is plus 1 plus 1.

So, now m l are same equivalent electron; now m l also m l also same, m l 1 and m l 2 for this 2 electron also same. So, now m S has to be different m S 1 if it is plus half m S 2 it has to be minus half. So, I have no choice for m S so, sum over m S is so 1 if it is plus 1 plus half then other has to be minus half ok. So, it has to be 0 so, m S is 0 means S will be 0 S will be 0 from S equal to 1 also 1 can get, S equal to 1 also 1 can get ok. So, this image value as if total so, but here we are considering the individual m S 1 and m S 2 and finding out the summation of m S.

So, this basically that that capital m S it is 0 so, S is 0; so, when L is 2 so; that means, for this M L equal to 2. So, L has to be 2. So, L has to be 2 so, for this case, one case I got L equal to 2, then S equal to 0 ok. So, then second 1 I can choose L equal to 1. So, when L equal to 1 L equal to 1 so, maximum M L L equal to 1 maximum M L will be plus 1, or M L will be plus 1 0 minus 1. So, maximum M L is plus 1.

So, it is plus 1 is plus 1 is 1. So, some of our m l to get 1 to get 1 so, for 2 electron if 1 is plus 1 another has to be 0. So, another has to be 0 because, three value are there available plus 1 0 and minus 1. So, if 1 is plus 1 then another has to be 0 ok, then only will get M L equal to 1. And this M L equal to 1 it comes from L equal to so, it tells that maximum value M L is 1. So, it is L value will be 1.

So, in this case so these two are different, these two are different m l are different so, m S can be same. So, m S can be same there is no it can be different also there is no problem, but it can be same ok. So, in this case m S capital m S is 1. So, it is S has to be 1. So, in this case another we are getting L equal to 1, we are getting S equal to 1 ok. Then next L equal to 0, when L equal to 0 when L equal to 0. So, M L is 0 M L is 0 and now S can be either 0 or 1 that we have to check.

So, this so M L 0 means this either both are 0, either both are 0 or 1 is plus 1 and another is minus 1 ok. So, if it is plus 1 and then minus 1 there is no problem ok. So, they are different, but I have to see whether both are same it is that combination is coming in the picture or not yes, if both are 0 m l 1 is 0 and the same is m l 2 is 0. So, both are same m l are same. So, these has to be different m S 1 and m S 2 has to be different, see in this case m S is 0 total m S is 0.

So, I will get next 1 next 1 L equal to 0 S has to be 0 ok. So, yes so these are the these are the allowed value which would be the Pauli Exclusion principle. So, for P S 2 sorry for P 2 the 2 electron what will be the state what will be the spectroscopic term. So, L 2 L 1 and L 0 all are allowed. So, L 2 means it is so let us state L equal to 0. So, it will be it will be S, then L equal to 1, P and then L equal to D ok.

And in this case L equal to 2 and S L equal to 0 so, S are 0. So, in case of S so, S and D it will be S equal to 0. So, 2 S plus 1 that will be 1 and corresponding J 1 can write in principle, if you know L S. So, here L S both are 0. So, it will be 0 and D in case of D S is 0. So, L J will be 2 J will be 2, basically L plus S and P is L 1 S 1. So, J will be J will be L plus S 2 L minus S. So, 2 1 0 so it is a 0 P 0 1 2 and, this multiplicity 2 S plus 1 S is 1 is 3 ok.

So, here these are the actually 1, these here 3 terms are there and these. So, 5 terms are like spectroscopic terms are allowed for this and, here you see the meaning of multiplicity so, 2 S plus 1 we really tell is a is the multiplicity; multiplicity factor. So, here you see this is only 1 term right. So, here it is 3 multiplicity 3 means it has 3 terms you know, P 0, P 1, P 2 here it is 1 ok. So, it is only one term all the J value is there here J value is J value is there. So, it is one so, but other cases for in case of S you tell it is 2, but since only in S orbit only multiplicity we tell 2, but it has only one term, but in general except that 1 in general. So, this tells the multiplicity it tells the how many terms are there ok. So, yeah so there is a these for P 2 we have found; these are the terms ok. So, let me stop here, I will continue next class.

Thank you.