Atomic and Molecular Physics
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Lecture - 24
Multielectron atoms (Contd.)

So, we are discussing about Multielectron atom.

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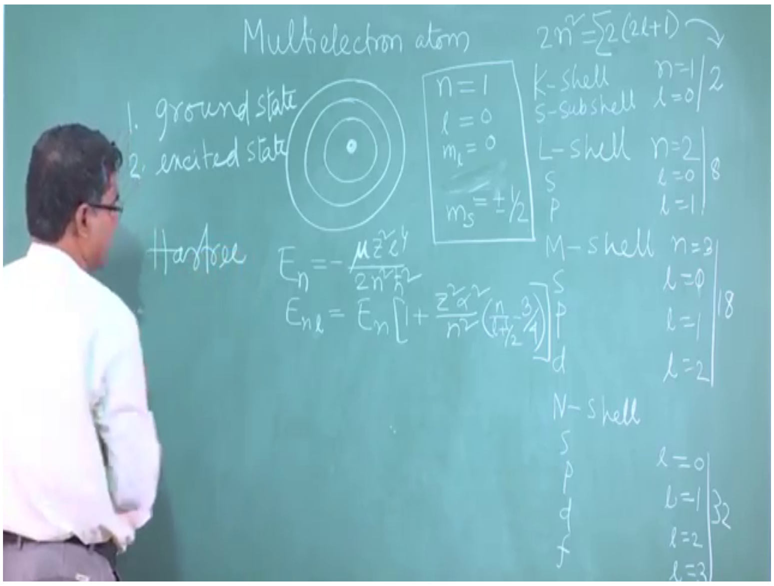

So, atomic structure we have seen that whether in that atom whether 1 electron or more electron, but the structure is same for all atoms. So; that means, this atom is having a nucleus and that nucleus proton and electron neutrons are there. And electrons are revolving in different orbit is circular and elliptical it mixed and the orbit or orbitals of atom, where electron can revolve; electron can stay. So, that are specified by quantum number; so, n equal to n is principal quantum number n equal to 1 is specifically K shell; n equal to.

So, for K shell another quantum number this l; say it for n equal to 1 it can take value 0 to 1. So, n equal to 1 say l equal to 0; l can take value 0 to n minus one ok. So, this under K shell; so, this l equal to 0; it is S subshell or S orbital's ok. So, then another could two quantum number is space quantization due to space quantization magnetic quantum number; m l it can take minus l to plus l or plus l to minus l. So, this for l equal to 0; m l will be 0 and then spin quantum number for that this S; is equal to spin of the electron.

So, so, S 1 has to one has to write for if it is for 1 electron. So, it will be half, but 2 electrons, 3 electrons, 4 electrons for; so, what will be the S? Similarly for l also that will I will I will already I have discussed. So, another quantum number M S; so, let us not write here, so, this m s equal to for single electron it is plus minus half ok. So, these 4 quantum number is used is used to used to label the energy levels; label the energy levels as well as one can say to designate to define the state of the electron ok.

So, what I want to tell that we have now it is known this for n equal to this K shell n equal to 2; this is l shell this for n equal to 2; this for n equal to 1, this l equal to 0. So, under l l shell; so, there are subshell S and P ok. So, this l equal to 0 and l equal to 1 then M shell M shell S P d; S P d. So, corresponding l equal to 1; l equal to 0, l equal to 1, l equal to 2 similarly N shell; N shell ok. So, for if S P d f; S P d f; so, this for this l equal to 0, l equal to 1, l equal to 2, l equal to 3.

So, so, now, for a particular n l value; so, here so, each shell each shell it contains how many electrons? It contains how many electrons? 2 n square electrons; it is basically 2 n square electron. So, it is equal to for each n; so, it should be equal to 2 into ah for each subshell; 2 l plus 1, for each subshell; 2 l plus 1 and then 2 is coming from this m s for particular l value it can take two value of m S.

So, this 2 is coming from here; so, for say M shell; n equal to n equal to 3. So, 3 means 18 electron; 18 electron now it has basically what has to sum over l. So, l equal to 0, l equal to 1, l equal to 2. So, for l equal to 0; so, it will be 2 electron; 2 and then l equal to 1; 6; 2. 6 8 and l equal to 2 is 10. So, 8 plus 10 is 18; so, this n equal to 3 so 18. So, one has to sum of for a each orbitals; so, so; that means, this K shell, it can take it can take 2 n square. Basically it is a it can take two electron; this can take 8 electron 2 plus 6; 8 electron this can take 18 electron.

Similarly, one can 18 and this l 3 means 6, 7; 14, 14 and 18; 32 electron ok. So, so this the atomic structure; it has shell, subshells and electrons can put in this structure. So, for 1 electron that I have discussed at n equal to; so, it can be n n equal to 2, 3, 4 and l equal to 0, 1, 2, 3 ok; so, it can go anywhere.

Now two questions; now, question is what will be the minimum energy of the of the electron or of the atom? So, that is called ground state that is called ground state ground state of atom and another is called excite state; excited state excited state. So, ground state and excite state means electron can be it at any orbitals ok. So, it will have definite state, but whether that state is ground state or excited state.

So, ah; so, rule is that or energy expressions tells that smallest smallest n and smallest l so, that will be that will be the quantum number for lowest energy. And if you go higher n and higher l of for a for a particular l; lowest l will have the minimum energy and highest l will be the higher energy. So, l is increasing energy is increasing ok; so, similarly for n also. So, that way one can; one can find out tell which one is ground state. Similarly now here one restriction we are putting that that in one shell; how many electrons can stay so, that already we have we have mentioned here, we have mentioned here and that that is based on Pauli exclusion principle.

Pauli exclusion principle is that this all each electron will have the distinct this number n, l, m, l, m s and it will not be same for 2 electrons based on that; so, this distribution of electrons in atom has come ok. And energy wise that expression energy E n has; E n equal to minus mu z square e to the power 4 by 2 n square h cross square E n l; E n l equal to E n 1 plus z square alpha square by n square this n by l plus half minus 3 by 2; 3 by 4 ok. So, this is the energy and this from here you can tell the energy of different orbitals. So, this what I emphasize; I want to emphasize here.

So, this we have found for single electron system; now if multielectrons, if more than 1 electrons if you put. So, atomic structure overall structure is same only it is energy; energy of different orbitals will be different for 1 electron whatever; for second electron we put second electron. So, its energy will change its energy will change, but the structure of the atoms remain same means it has orbitals only; only the energy separation between the between the levels or penetration of energy levels or sequence of the energy levels for 1 electron system and for two electron, three electron system. So, that sequence may be affected in some extent.

But it is it is not abrupt it follow some rule and there are reason why there will penetration of energy levels or deviation of the normal rules of energy levels following this one. So, this because of some other reasons ok; so, here we have not whatever here I have mentioned we have not considered any interaction; we have not considered any interaction like L S coupling we have not considered we have not considered yes mainly

L S coupling that is a origin is magnetic interaction that that is not consider here when will considered that one. So, then j will come ok.

So, so, this will be the one reason for the deviation of this of this regular regularity of energy level following this energy formula. And in case of in case of multielectron; so what about the consideration for this derivation; so, we have to consider something more. Because here only one electron; so, interaction between electron and the and the nucleus coulomb interaction coulomb force act on that.

Now if you put second electron then electron electron some interaction will be there repulsive force. So, that one has to consider for multi; so, starting from the single electron system, we can go for multielectron. So, we have to we have to correct this formula following some additional effect; so, immediate effect is 1 electron is there; so, there is no inter[action]- electron electron interaction; see if I put another electron ok.

So, there will be electron electron repulsive that is coulomb force also its repulsive force, so, that one has to consider. So, that is that is considered its some Hartree Hartree Hartree Hartree Hartree Fock method or Hartree method Hartree Hartree's method. So, in that method for multielectron system he considered the spherical distribution of the of the of the charge; so, he considered the average so, for single electron just detect coulomb interaction electron and nucleus ok.

Now if put second electron say instead of this; so, we will have two interaction; coulomb interaction electron nucleus and electron electron; so, Hartree he considered this overall this potential spherical potential considering this nucleus and the surrounding electrons keeping one electron. So, what would be the effect of other electrons.

So, nuclear nucleus have nuclear that coulomb interaction that is there; apart from that if more than one electrons so, due to other electron what will be the effect on this electron? So, that was consider as spherical that is a average spherical potential was considered ok; so, so that effect will be introduced here ok. So, because of this kind of additional interaction; so, what I told that this that arrangement of the energy levels following these energy expression; so, in some cases it will deviate ok. So, that that one has to consider for multielectron system.

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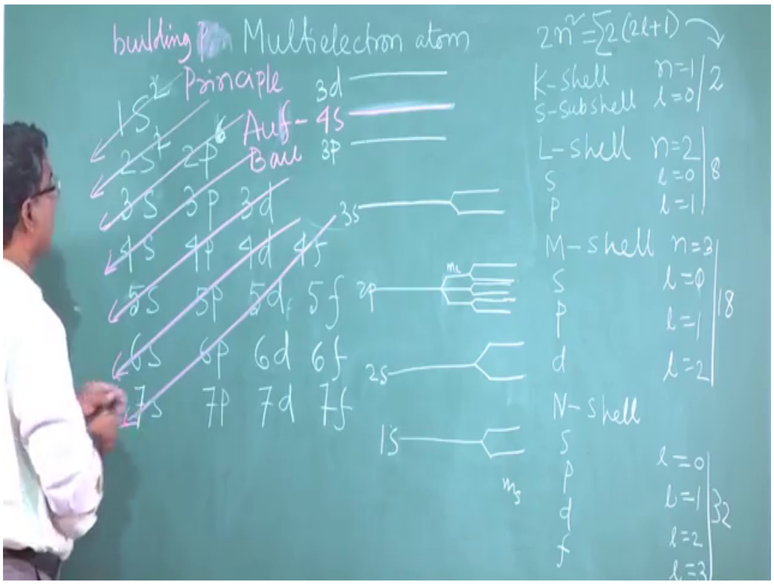

So, so ; so, I have atomic structure, I have many shell subshells now if I put 1 electron that is fine. So, this hydrogen atom 1 electron; so, so 1 electron; so, I have basically. So, let me let me first see how many orbitals we have ok. So, for n equal to 1 I have 1 S orbitals, n equal to 2. So, I have 2 S, then 2 P, then n equal to 3. So, I have 3 S, 3 P, 3 d n equal to 4; I have orbital 4 S, 4 P, 4 d. Then n equal to 5; I have orbitals 5 S, 5 P, 5 d, 5 f. So, I think 4 S, 4 P, 4 d, 4 f also is there 4 f similarly 6 S, 6 P, 6 d, 6 f 7 S, 7 P, 7 d, 7 f etcetera ok.

So, if we are not going f g h I; we are not going because we do not need that many shells subshells or orbitals to put electrons; in case of whatever available known atoms are there. So, these are the available orbital's orbitals; so, I can put electron at any places ok; if I want to put 1 electron and at ground state minimum energy. So, I have to put here 1 electron 1 electron I have to put here. So, if I take second electron in case of helium helium; so, for minimum energy for ground state. So, I can put one more here ok; so, basically 2 electron, I can put. Now third electron I cannot put here as for Pauli exclusion principle; this maximum 2 electron I can put.

So, I have to go for next one; so, that will be the ground state for for lithium; so, this is 2. So, this for lithium 1 S; 2; 2 S 1; so for beryllium; so, 4 electrons; so, I can put here 2 ok. So, this way if then beryllium. then boron one more electron here then carbon; so, I can put 2 electron then 3, 4, 5; so, up to 6 electron I can put here ok. So, that is the configure electron- configuration of neon 10 electron; neon 10 electron 2; 2; 4 and 6 10 for neon 10 electron.

So, this way we can we can put electron one after another and for ground state so, I have to find out the minimum energy level from I have to fill the energy level of minimum energy ok; so, this way one can proof fulfill ok. So, now, here rules are there to get the minimum energy as I told these sequence of the energy level is slightly different for multielectron system for multielectron system.

So, if I if I scale; so, it is a; so, this for one is if this is the basically if I; I think I should draw here if it is say it is 1 S ok. So, I should write 1 S here; so, 1 S and 1 S have again it has two level for m s plus half and m s minus half ok. And then for second energy level is 2 S; so, I can put 2 S, 2 S; 2 S again it has two level plus half minus half. Then I will have energy level 2 P; 2 P; again 2 P have 3, 2 P will have actually 2 P.

Now 2 P have 3 m l; 3 m l; so, I will get basically let me short it. So, 1, 2, 3 this m l plus 1, 0 minus 1; so, this for m l depending on m l and this basically for m s and now for m l here again each one will be splitted into two each one will be splitted into two (Refer Time: 25:02) m s. So, it has 1, 2, 3, 4, 5, 6; it can care can take 6, this can take 2, this can take 2 maximum electron. So, this is 2 P and then I will come to 3 S; I will come to 3 S, 2 P then 3 S ok.

Then I will go to 3 S, 3 S; so, 3 S have basically 2 and then I will come to 3 P; I will come to 3 P, 3 P, 3 P and then I will come to 3 d ok. So, this way I can arrange the energy level; now here next I will 3 d now now 4 S. So; now this 4 S where this 4 S will be? So, next.; so, 4 S is supposed to be here n is higher, but it is not the case 4 S is generally its below the 3 d say; it is the 4 d.

So, I should I should use this one you see this will be the 4 S. So, this 4 S energy of this 4 S that is lower than the 3 d level three d level now it is deviating right from normal sequence as per this energy expression. So, this because in multi electron system because as I told this some other interaction its will be present because of that this deviation. So, what will be the sequence of the energy levels? So, that that is one can follow this building of principle; building of principle, building of principle. So, it is called also Auf-Bau; Auf-Bau principle Auf-Bau principle.

So, Auf-Bau; Auf-Bau principle all 6 called Auf-Bau principle. So, it is telling if you just follow this arrow ok; so, if you; so, these are the sequence for the lower energy level to higher energy level. So, 1 S, 1 S then 2 S; then 2 P, then 3 S then, 3 P then 4 S and then 3 d, after that in 3 d, after that 4 P after that 4 P ok; so, that way one can go ahead. So, so, this is the one can follow this building principle Auf-Bau Auf-Bau principle. So, following this one; one can put the electrons for ground state one can put the electrons for ground state.

So, ah; so, now, either this energy level following the energy level, one can put multielectrons in an atom ok. And now it is easy if I just follow this building principle Auf-Bau principle. So, this principle based on some experimental results, but it comes from the theory as I as I told that one has to consider other effect rather than whatever for single electron system whatever you have considered if you consider the other effect.

So, then this type of irregularity in in energy levels comes means one can explain the irregularity of this energy level arrangement. So, if so, now, if I know this sequence; so, for any number of electron for any number of electron one can one can find out the configuration.

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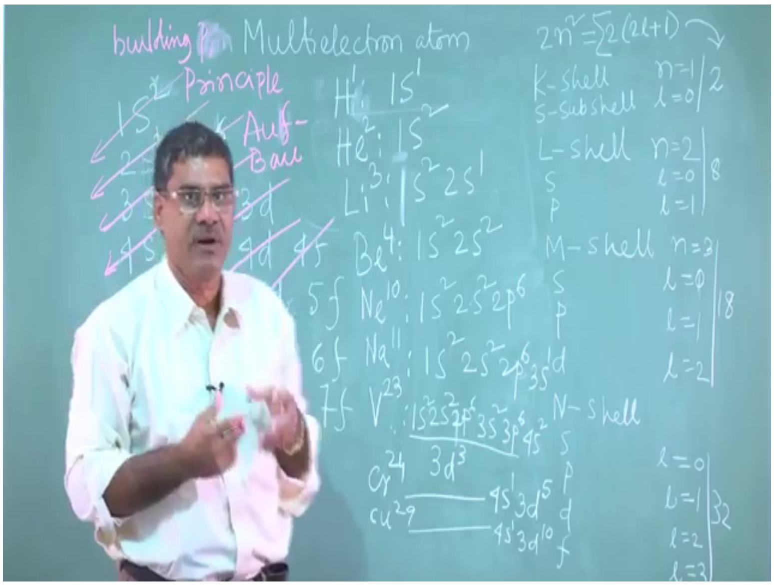

So, for for hydrogen for hydrogen 1 electron; so, its arrangement is like this ok; helium helium 2 electron say it is 1 S; 2, for lithium 3 electron say it is it is 1 S, 2; 2 S 1 for beryllium 4 electron ok; so, 1 S 2; 2 S 2 ok.

So, similarly if you go for neon is 10 electron ; so, one can 1 S 2, 2 S 2, 2 P 6 then if you consider say sodium sodium 11. So, 1 S 2; 2 S 2; 1 P 6, 3 S 1; 3 S 1; then if you go for vanadium; vanadium it is 23; it is 23 ok. Now it will come 1 S 2, 2 S 2, 2 P 6, 2 P 6; so, it is neon configuration neon configuration.

And then this 10 electron then I have to come 2 P 6, 2 P 6 then 3 S 2, 3 S 2 then I will come 3 P 6, 3 P 6; 18 18; 3 P 6, then 4 S 2, then 4 S 2, 4 S 2, 4 S 2. So, then it is I think 10; 10; 20 and then 3 d, then 3 d, then it will come 3 d 1 S 2; 2 S 2; 2 P 6; 3 S 2, 3 P 6, 3 d 10 consider 3 d. So, its 4 S 2 and then rest of this its 3 d ok; so, 3 d; 3.

Now, for chromium next one chromium 24 apart from this; up to this now 4 S its configuration is 4 S 1 and 3 d 5; instead of 4 S 2, 3 d 4; we write 3 4 S 1, 3 d 5. So, here is for when the subshell is or orbitals it is the; it is when it is half filled or full filled ok. So, it is telling that is a reason as I will tell you the reason. So, here what we consider this for if 4 S 2 and 3 d 4; as per the rule it should be like this, but it breaks here it consider that this half filled or full filled subshells are more stable electron configuration why it becomes more stable; I will I will tell you later on what is the explanation of that.

So, here instead 4 S 2 and 3 d 4; 4 S 1 and 3 d 5 is more stable; so, it is considered. So, whenever this half filled of a subshell outer shell is possible. So, one has to consider that one and similarly for I think here chromium then manganese 25, iron 26, cobalt 27, nickel 28, nickel 28 and then copper 29. In case of copper in case of copper 29; so, here again you can see this here 24; 5 more electron I have to put.

So, in principle it should be 4 S 2 and 3 d 9, but since 1 electron given there. So, this it will be 4 S 1, 3 d 10. So, fulfilled one the subshell; so, here it will be 4 S 1 and 3 d 10 ok. So, fulfilled or half filled are more stable; so, its explanation mainly stress this 4 S and three d energy difference are not much ok, they are very close and that is why this type of if energy difference is very high. So, it is a this type of exchange was not possible.

Since they are very close this type of exchange configuration its considered and experiment will gives more stable configuration. So, so, this way one can find out the electron configuration of the multielectron. So why I need so; this electronic configuration? I need because I want to find out the spectroscopic term for multielectron atom, spectroscopic term for multielectron atom. So, I think; I will I will continue next class let me stop here.

Thank you.