

we saw how french scientist de bruy provided a major breakthrough he provided a radical idea that matter has wave like nature another radical idea came from another from one german scientist werner heisenberg and this is what we are going to discuss now the famous heisenberg's uncertainty principle this uncertainty principle says that we cannot simultaneously

so it says that simultaneous determination we cannot simultaneously determine something and what is that simultaneous determination of exact position and exact momentum of a particle is impossible there are some key words in this statement first keyword is simultaneous we must this principle forbids simultaneous that means at the same time we cannot measure exact position and exact momentum of a particle the simultaneous determination is impossible this impossibility does not arise because of a limitation of instrument instrumentation rather this impossibility is forbidden by nature this is the fundamental nature of the particles that that we we see

so heisenberg's uncertainty principle is not an outcome of insufficient instrumentation that that means it it is not going to happen that in a future time we will get some instrument using which one can exactly locate the position and momentum of a of a particle simultaneously this is the fundamental principle of nature mathematically this is given as Δx multiplied by Δp_x which is greater than h by 4π what is this Δx x is the position of the particle p_x is the momentum of the particle along x direction this Δx or Δp_x are called uncertainty in position Δp_x is called uncertainty in momentum exact determination of position would make Δx as 0 exact determination of momentum will make $\Delta p_x = 0$.

the uncertainty is given by this Δx suppose that we have a two dimensional box within which my electron can move around if i want to locate this electron with certain amount of precision the precision let us say this is the this is my precision

so i can say that the electron is certainly present in this box but it is present between this and this this is this is the this is what is known as the uncertainty in determining the position

so we can say where it is but with with an error bar

so this is given as Δx and similarly its uncertainty in momentum and that is Δp_x the multiplication of these two uncertainties is always greater than or it can maximum minimum be equal to this constant h by 4π h is planck's constant you know and 4π is again a constant

so heisenberg's uncertainty principle said that you cannot simultaneously measure the exact position and exact momentum of a particle there has to be a certain amount of uncertainty and this uncertainty is given in this way in other words if you want to measure the position exactly you must sacrifice the accuracy in terms of momentum and if you want to exactly look measure the momentum of this particle you must sacrifice the knowledge of the exact position of this particle you can actually show that the uncertainty of an electron

so if i want to measure the uncertainty of electron

so i have Δx multiplied by Δp_x is greater than h by 4π i can rewrite as momentum momentum is i know mass into velocity and mass is if i want to measure the uncertainty of the of an electron i would get i have h the value of h i know point six two six into ten to the power minus thirty four joule second divided by four pi mass which is nine point one into ten to the power minus thirty one kilogram which is coming out to be if you see something about ah its not exact is approximately ten to the power minus four meter square per second all right we keep this in mind for uncertainty of an electron is coming out to be 10 to the power minus 4 meter square per second and then what we ah we let us write this down uncertainty principle Δx multiplied Δv_x for an

electron came out to be ten to the power minus 4 meter square per second let us find out the same $\Delta x \Delta v$ which is greater than h by $4\pi m$ but in this case let us find out when m is 100 gram an everyday object in this case the uncertainty is given as 6.

6.26×10^{-34} second four π mass which is now zero point zero point one ah kilogram is it this is ten to the power minus ah one

so this comes out of the order 10^{-33} meter square second inverse

so this is an uncertainty this is what the uncertainty in position and momentum for an electron which is 10^{-34} meter square per second this is the uncertainty in position and momentum according to ah heisenberg's uncertainty principle for an everyday object like an object which weighs 100 gram whose mass is hundred gram

so you can see the uncertainty is extremely small it's almost negligible for everyday object

so therefore uncertainty in principle is alright but it is mostly manifested or it has severe significance for microscopic particles with with very small mass but for everyday objects when the mass is mass becomes larger even in the scale of grams or milligrams the uncertainty principle can be safely ignored

so therefore the uncertainty principle the corrections that were coming out because of uncertainty principles they only apply to microscopic world the macroscopic world or the world that we see around us can be safely we can safely ignore the consequence of uncertainty principle into the macroscopic world we are now adequately equipped to discuss why force atomic model failed what is the reason that bohr's atomic model could not give out all the answers that we wanted

so let us discuss now the reasons for the failure of bohr's model if you remember both the results that were coming out from bohr's model we had an analytical expression for r_n the radius of the orbit we also had an analytical expression for the speed of an electron in an orbit v_n

so in bohr's model we knew precisely the radius therefore we we know the location of the electron we also knew precisely the speed of the electron that is orbiting

so what bohr's model said is that it gave exact position and exact momentum because we knew the mass of the electron and if we know the ah velocity at the n th orbit

so we know exact position and exact momentum of the electron in both model and this is contrary to what heisenberg's uncertainty principle suggests heisenberg's uncertainty principle tells that you cannot simult simultaneously measure the position and momentum of a microscopic particle which is which is electron in this case since bohr did not know about heisenberg's uncertainty principle by the time when he was devising this atomic model

so therefore heisenberg's uncertainty principle is not satisfied in bohr's atomic model and that is the key reason as to why bohr's atomic model could not explain all the results we have we can now ah go on to discuss a new branch of theory which would take into account the knowledge that we get from heisenberg's uncertainty principle the de brois hypothesis and this is what we are going to do next it is now time for us to take a stock of the things that we have learned

so far ah

so far as the structure of atom is concerned we have travelled a long way we started from the hypothesis of john dalton which said that atoms are the tiniest indivisible particle dalton did not provide any other any more clarity towards the structure of atom

so they were simply assumed to be hard spheres from there we went to the work

of jesus thompson the famous plum pudding model where now in addition to the atom there are like positive charges negative charges were also discussed in plum boarding model it was suggested that atom consists of a uniformly distributed positive charge within which the electrons are embedded plum and plump pudding model did an improved job compared to a dalton's atomic theory however it was far from the truth then we came out came up with the idea of brother ford who found the who established the existence of nucleus employment pudding model the positive charge was uniformly distributed that constituted the space of the atom but now rather force improved atomic model suggested that the positive charge as well as most of the mass the entire mass of the atom are concentrated in its very small place small space in the in in an atom and he called it as the core or we what we call ah it is nucleus and the electrons they move around the nucleus but rather force atomic model ah could not satisfactorily explain why the atom should be stable because from maxwell's theory it was understood that the moving electron should undergo a spiral motion and should collapse under on the nucleus and therefore the atom should never be stable we again encountered one more improvement on the story that was the work of nils bohr whose provided the bohr's atomic model where he said that electrons so again the nucleus are at the center the electrons move around the nucleus but they move around the nucleus in fixed paths called orbits are or they are also called stationary states they have fixed energies

so that gave is as yet another improved version of the atomic structure however none of these four models are daltons atomic theory uh plum pudding model rather force model or nil sports model none of them could give us the complete complete picture of art well this was the growth in the story of atomic the structure of atom simultaneously other things were happening in science for example it was proved by max planck and einstein that light which we believed to be a wave also has particle like nature without that the black body radiation the photoelectric effect experiments could not be explained

so now light has both wave like nature as well as particle like nature then there was the hypothesis of deep roy who suggested that even matter has wave like nature

so now light is both wave and particle now the matter that we normally think of as particles are also behaving like wave as well as particle in addition to that there was heisenberg's uncertainty principle which suggested that you cannot simultaneously determine the position and momentum of a microscopic particle all these new things actually were very puzzling we did not know how to take them the scientists took a stock of the situation they realized that the newtonian mechanics served a great deal of purposes using newtonian mechanics newton's equation of motion we could not only discuss or talk about the trajectory of everyday objects but we also could explain the planetary motion but when it came to the microscopic world the electrons the proton sub atomic particles newton's equation of motion or newtonian theory failed and it failed miserably at that point there was unanimous agreement that we needed a new theory a new set of ground rules that will explain the very complicated and very exciting things that were happening at the microscopic world and this is where the birth of quantum mechanics took place to begin with ah in the year 1926 and 1927 two great scientists one austrian another german the austrian scientist erin schrodinger and the german scientist werner heisenberg roughly at the same time 1926 1927 around that time they put forwarded two different versions of quantum mechanics two different formulations of quantum mechanics and later on it was shown that actually both the versions were equally valid they are essentially one and the same that's where the birth of formal birth of quantum mechanics took place and since then quantum mechanics has moved quite a lot in today's

scenario quantum mechanics plays a very important role in advance physics advanced chemistry i will talk about uh quantum mechanics the applications of quantum mechanics in chemistry i myself i am a practice i am a quantum chemist ah by by profession we normally in the field of chemistry use the principle of quantum mechanics to solve the atomic and molecular structures and we also derive chemical properties chemical reactivity of different molecules we can predict or we can calculate the feasibility of chemical reactions by using the principles of quantum mechanics and this branch of chemistry which uses quantum mechanics the principles of quantum mechanics to solve chemistry related problems are called quantum chemistry quantum mechanics being a new theory required a set of new rules or new postulates that to be formulated we will first go through two basic postulates of quantum mechanics on the basis of which we can carry on our discussion further there are more than two postulates of quantum mechanics but ah for our discussion the first two will be sufficient the first postulate of quantum mechanics tells that there exists something which is called wave function this wave function is denoted by let the greek letter psi either in capital or in ah small ok in the small case or in capital case quantum mechanics tells us that there exists this for every quantum mechanical system there exists this wave function which is denoted as psi that contains all the information that we need to have everything that we need to know about a system is present in this wave function this wave function can be a simple function let us say it can be as simple as a function like x or x^2 or $\sin x$ or e^x or e^{-x} it can be real or it can be complex it can be $e^{i\theta}$ or $e^{-i\theta}$ or it can be a plus i b or it can be combination of one or many of these functions it can be as simple as this this wave function or it can be extremely complex that i even cannot begin to start writing if i have a system where there is one electron the wave function will contain all the information about this single electron its position its momentum and

so on

so its energy and

so on

so forth if i have let us say hundred or thousand number of electrons then also this wave function will contain all the information about the entire system which now consists of hundred or thousand electrons

so therefore you can imagine if i have ten to the power three number of electrons then this wave function will contain the information about the position of each of these electrons

so this wave function can become very complex or it can also be very simple

so we do not know or we didn't we need not define the wave function at the moment

so what for our discussion it is sufficient to appreciate the fact that for every quantum mechanical system by that i mean it could be an atom or it could be a molecule ah it could be a cluster it does not matter for every quantum mechanical system there exists a wave function what physical picture ah does this wave function give actually none the wave function may not does not have any physical meaning this wave function does not have ah it has got no physical meaning because it does not have to be it does not have to carry a physical meaning this is a complex mathematical construct a mathematical function that contains all the information it does it does not have any physical meaning however max bond the german physicist ah suggested that although the wave function itself does not have a physical meaning what has a physical meaning is this ψ^2 this has got a physical meaning and what is the physical meaning of this ψ^2 this is nothing but the probability of finding a particle in our case it will be an electron at a given point in space

so the wave function itself does not have any meaning however this mod square of this wave function ψ^2 has got a physical meaning and it means that what is the probability of finding an electron at any given point in this in in in space

so if an electron which is going around the atom if i know the wave function i know ψ^2 and therefore i know at any point around the nucleus what is the chances that i can find this electron that i am interested in now since it since it signifies a probability therefore it cannot be negative it is always a positive ah quantity

so let us see a few example this ψ^2 actually has a special meaning for example if my wave function is x then ψ^2 is easy it is x^2 if my wave function is e^{-x} then ψ^2 is e^{-2x} however please note when my wave function is a complex this ψ^2 has this meaning actually ψ^2 should be written like this ψ^* which is actually the complex conjugate of ψ multiplied by ψ as long as your function is real like x^2 $\sin x$ e^{-x} it does not matter we do not have to write in this format but if your function is complex like this $a + ib$ then i must find out the complex conjugate of $a + ib$

so which is $a - ib$ and $a + ib$ and this gives me $a^2 + b^2$ remember this definition is necessary because max bond suggested that ψ^2 has a physical meaning and this physical meaning is that it is the probability of finding an electron at a given point in space

so since it is it signifies a probability therefore it must be always a real number it must be it must always be a positive carry a positive value all right we saw the first postulate of quantum mechanics which says that there exist something called wave function which contains all the information that's nice because wave function contains all the information that's that's very good but you would ask me ques this question that how will i get this wave function sorry how would i get some information that i want to know about the system starting from this wave function that is given by the second postulate this is what we are going to discuss next the second postulate says that it talks about how we can get how to get information from this wave function the wave function contains everything all the information but how will i get this wave for information from this wave function this is what we are going to discuss next now quantum mechanics has the following recipe for this it says that for every observable for every observable that you want to see or you want to know ah you you can think of doing an experiment and getting a result out of it for every observable there exists an operator

so it defines with the second postulate it defines that there exist an operator for every observable what is an operator an operator can be as simple as like this and this is an addition operator it can be a subtraction operator it can be a square root operator it can be a square operator it can even be a differential operator or it can be an integration or it can be a logarithmic function

so these are different operators you know that if i apply this operator let us say ah this operator is square root if i apply this operator on a function now it is nine then i know it will give me a different val it it will give me a result that is three if i use this operator on again the same nine i will get a different value at eighty one if i use let us say this operator on a function a^x i will get a

so an operator is something it is a its a rule that applies to a function now what second postulate of quantum mechanics tells is that every observable corresponds to an operator what observables can we have let us say we want to know about the position of the particle position of the electron all right so there must be an operator for that

so we normally signify an operator as as a hat with a hat on top of it
so position operator i call it x operator i may want to know about the momentum of my electron right

so i have got a momentum operator i may want to know about the energy of the system all right the energy is associated with an operator which is called hamiltonian it is named after ah british scientist hamilton this is called hamiltonian it is h with a with a hat on top of it

so you do not have to worry about ah the form of this operator this operator or this operator ah in latter class you would actually get to know how to construct an operator but for the moment for the time being it is sufficient if we appreciate that there exist an operator for every observable that we may want to know if we want to know about energy there is hamiltonian operator if you want to know about momentum there is momentum operator and

so on

so forth all right

so i have now defined i got to know something about this wave function psi i got to know that there exists an operator but how do i get this information

so for what i said is that for energy there is an operator hamiltonian but how would i get that this is what ah is will be done next let us say i want to know about the energy of my system

so quantum mechanics tells that there exists this wave function psi there exists this operator h

so wave function contains all the information operator asks the question operator now this time since i am trying to get energy i am using hamiltonian operator using this hamiltonian operator i will ask the question to this wave function which is the citadel of all the information and when i ask the question to this wave function using my hamiltonian operator the answer that i will get will be energy

so this is the wave function which contains all the information this is the operator that i am interested in to get get and get an idea about that particular observable in this case i am interested in getting energy

so i apply this operator on this function i get the result

so this is the place for my result and in this case this is the energy this is my wave function and this is the hamiltonian operator hamiltonian hamiltonian operator and this equation that you see here $\hat{H} \psi = E \psi$ is a very simple equation to write but one of the most difficult equations to solve and this equation is called as schrodinger equation you see that there is there are two dots on top of o this is called o uml out and it is pronounced as if it is oe

so s-c-h-r-o-e story lingard this this equation was given by the austrian physicist schroedinger and this equation is schrodinger equation now to to be able to get the energy of my atom i would solve this schrodinger equation which is $\hat{H} \psi = E \psi$ what is known what do i know i actually know only the hamiltonian here because hamiltonian is the energy operator if i am asking a question i know the ingredient ingredients of the question but what i do not know is the answer

so i do not know wave function

so here unknowns are our wave function psi and energy and known to solve this equation known is the hamiltonian the operator i know the operator and what i want to know is what is the wave function and what is the corresponding energy let us see

so this this is there are several tricks to solve this equation we will not talk about any tricks as to how to solve this equation we saw that we have to solve schrodinger equation which is $\hat{H} \psi = E \psi$ to get idea or to get information about the about any quantum mechanical system if we are interested in solving hydrogen atom

so we must construct the hamiltonian of a hamiltonian operator corresponding to hydrogen atom and then solve schrodinger equation and that the solution will give us wave function ψ and the corresponding energies E now we will discuss about what solutions we get when we solve the schrodinger equation of hydrogen atom next we are discussing the results from the solution of schrodinger equation we are not going to discuss how to solve them but we will use the results and discuss what we can learn about this when you solve this this is the schrodinger equation $\hat{H}\psi = E\psi$ first outcome of it is that we get a series of wave functions

so actually we do not get one value of ψ we get a series of like quite quite a lot it depends on how we did the calculations but it forms the so called complete set of wave functions there are many wave functions available

so we get a series of wave functions and we call them orbitals or even equivalently atomic orbitals these orbitals are different from orbits that we saw in bohr's atomic model orbits were fixed path around which the electron was going around in bohr's atomic model orbitals are the solution or the wave functions obtained from solving schrodinger equations and these are also called atomic orbitals and these orbitals actually give us the address of electrons as you know according to bond max bonds hypothesis $|\psi|^2$ square of the wave functions represent the probability density of finding the electron at any point

so therefore wave function therefore contains the information code and run code address of electron how to find the electron or where to find the electron in addition to this we also get a series of energies each energy corresponds to one value of wave function

so as i said i have a series of wave function and each wave function corresponds to one value of energy

so therefore i have got a discrete series of energies and these energies are actually they form a discrete set

so they have certain values like 0 5 10 15 like this or some other it can be a real number i am just trying to say that it is not that 0 1 2 3 4 5 everything is present it could be 0 5 10 15 or 0 or 10 16 29 it doesn't matter but these are discrete values this is not a continuous continuum value continuous values

so i get what i get i do not i cannot say that energy in if i this is the result that i am getting these are the energies then i cannot say that i have energy 1 because i do not i only have 0 10 16 29

so this they form a discrete set right now first we will discuss about the orbitals and then will come up come to talk about the energies the first topic of our discussion is is a the atomic orbitals that we get from solving schrodinger's equation let us talk about a orbitals these orbitals which are also the wave functions they tell us about the size shape or orientation as i said orbital is the address of electron

so this is the the orbitals actually tell us how is electrons house what is its shape what is this orientation

so we will talk about a orbitals and then we will see where do a in which kind of place the electron leaves all right to since i said there are

so many orbitals which are coming out from the solution of schrodinger equation so we must be able to identify uniquely an orbital from its size shape and orientation

so the next target is unique identification of identification of an orbital how do i do that to be able to uniquely identify an orbital i require four sets of information these are called quantum numbers first is called principal quantum

number second azimuthal quantum number quantum number third is magnetic quantum number and fourth is spin quantum number ah principal quantum number is often ah signified with n azimuthal quantum number is given as l magnetic quantum number m spin quantum number m_s these are the four quantum numbers that we require to uniquely identify an orbital we will now discuss about each quantum number and what kind of information does it give ah about the orbital this is what we will discuss next first is our principal quantum number principle quantum number which is which is given by the letter n it tells us about the size of the orbital its like how big the house of electron is this is the size of the orbital whether it is a big ah orbital or it is a smaller battle the house is big or small this is what it gives us and to a large extent it also decides this principal control number also decides the energy of the orbital but we will come to that in a moments time the orbit the values of this quantum numbers n are can be 1 2 3 4 any integer value it can go on when a larger n we have if if the quantum number n is a large number it simply indicates that the electron this orbital of this electron is is very large that means what does that mean if this is the nucleus and we know that electron is ah going around the nucleus if n is large that means the distance between the electron and the nucleus is very large that means the orbit the pl house of this electron when it is it it occupies the principal control number n it is also large and it is found far far away from the nucleus

so n equals one means the electron is closer to nucleus n equals 2 it is like little further n equals 3 it is further further further n equals 4 and 5 and so 6 it goes on like that

so n equals 1 2 3 4 5 these are different values there there are also have a ah different name we also call them signify them as shell when n equals 1 we call that as k shell when n is 2 we call it l shell when n is three we call it m shell n shell and

so on

so forth

so this is about the principle quantum number ah n which talks about the size of the orbital which also translates to the energy of the orbital and it tells that if the principal quantum number n is large that means the electron is found further from the nucleus the next quantum number is azimuthal quantum number it is also called orbital quantum number and given the letter l if principal quantum number talked about the size of the orbital ah azimuthal quantum number talks about the shape of the orbital

so we saw the how big was the size of the house of electron now with orbital angular momentum we will see that what is the shape of the ah house of the electron or the shape of the orbit this orbital quantum number or azimuthal contour number l can be from zero which can be 0 1 2 any number up to the value of n actually the value of principal quantum number n determines the value of l if n is 1 that is the k shell if the principal quantum number n is 1 then we have got only one possible value

so the possible values of of l are ah determined by n but it actually please excuse me it goes from 0 to n minus 1.

so i will take this example if n is one then how many uh what are the possible values of l

so l can be only one value that is one minus one zero if n is two what are the possible values of l l can be 0 or it can be 1 because it can go up to 0 to n minus 1 and since n is 2 therefore l can be 0 or 1.

if n is 3 l can be 0 or 1 or 2 and

so on and

so forth

so the values of l can be from 0 to n minus 1

so therefore for a given principle quantum number n how many l values are possible that is the the number of possible l values is given by n because you have always have 0 and then until n minus 1 .

so therefore the number of possible l values is is n

so in this case number of l values is 1 in this case number of l values is 2 in this case number of l values are 3 there and these values are 0 1 or 2 .

we saw that the orbital quantum number l is determined by the principal quantum number

so principal quantum number is fixed and then principal quantum number decides what are the allowed values of this orbital quantum number or azimuthal quantum number and it goes from 0 till n minus 1 .

now we see that here l value is 0 here again l a value is 0 when n is 2 again here also when n is 3 there is a possibility of l value of zero simultaneously you can see that when n is two we have one possibility of l equals one and here in when n is three then also we have a an orbital where l value is one is there a similarity between the 0 value of l when n is 1 or n is 2 or n is 3 the answer is yes because orbitals as i said they determine the shape of the sorry the orbital quantum number determines the shape of the orbital this is what we would ah discuss now when l is 0 we saw that l can be 0 or can be 1 or can be 2 or any other number when l is 0 the shape of the orbital is sphere is just a sphere right and we see we identify this with a shorthand notation as ah small case s when l is one the shape of this orbital when the azimuthal quantum number l is one the shape of this orbital ah appears to be ah like a dumbbell

so dumbbell you would ah perhaps know ah that it has got two lobes

so this is what ah the shape of the p orbital sorry the orbital that has l equals one look like

so it has got two lobes on two sides and we signify that with small case p l equals two it ah slide it has got two ah dumbbells

so you can have ah one dumbbell like this and another dumbbell like this

so these are the general ah shapes of the orbitals and we call this when l is two we call these orbitals as d r d

so when l is zero the orbital is spherical in shape called s when l is one the orbital is dumbbell in shape we call p when l is two it has it has got two dumbbells and we call ah we see we the shorthand notation for this is d now ah let us go back to the previous exercise that we are doing but that we saw that when n is one l is zero

so how can we identify this orbital we can say that ok n is one and l is zero

so we can identify this orbital as in the following way

so we say that ok this is the value of n and then we use the shorthand notation of the orbit orbital shape when l is 0 we call it as s

so we call this orbital as $1s$ when n is two l and l is zero

so we see that n is two

so we first write it two and then we write the shape of the orbital we call it two s for n is three and l is zero we write this orbital as three s similarly when n is two and l is one we call that we give the value of n here two and then we check what do we call when l is one up we call it p

so we will call this orbital as two p that means its principle quantum number is two its azimuthal quantum number is one that is why we are calling it p and similarly when n is three and l is one we call this as three p principle quantum number is three azimuthal quantum number is ah one and when principal quantum number is three and azimuthal control is three ah two we say the orbital as

three which is the principal quantum number and when l is two this is called as d

so we can go on ah this way

so you would need to know actually ah what happens l equals three it has got very complicated shape i cannot ah draw them ah we call them f and it goes on for the s p d f g and

so on

so forth

so this way we saw that the principal quantum number talked about the size of the orbital azimuthal quantum number talked about the shape of the orbital whether it is spherical dumbbell double dumbbell or complex

so if n was called as shell this l values they represented what we will call as sub shell

so n is shell l is subshell n can be one one two three four five l goes from zero to one two three four until n minus one we saw the two principal quantum numbers we discussed about them the principal and azimuthal quantum number and we will continue continue our discussion on the quantum numbers in our next class when we will talk about the other quantum numbers and what are the features they will bring into the structure of atom thank you you