Lesson 3: The Quantum Mechanical Model of the Atom

electron in Orbital.

Lesson Objectives :

At the end of this lesson, students will be able to:

- state Heisenberg's uncertainty principle
- describe the significance of electron probability distribution.
- explain the quantum numbers n, l, m, ms
- write all possible sets of quantum numbers of electrons in an atom.
- describe the shapes of orbitals designated by s, p and d.

Brainstorming Question

- If particles have wavelike motion, why can't we observe its motion in the macroscopic world?
- If electrons possess particle nature it should be possible to locate electrons.
- How can an electron be located?
- Is there any wave associated with a moving elephant?

Key Terms and Concepts

- Quantum mechanical model
- Quantum number
- Heisenberg principle
- Shapes of orbital

The quantum mechanical model of the atom, also known as the wave mechanical model or the Schrodinger wave equation, is the current understanding of atomic structure based on quantum mechanics

1.6 The quantum Mechanical model of the atom

The Bohr model of an electron orbiting around the nucleus, looking like a planet Around The Sun,doesn't explain properties of atoms.The planetary view of one charged particle orbiting another particle of opposite charge does not match some of the best-known laws of classical physics.Scientists have developed quantum mechanics,which presents a different view of how electrons are arranged about the nucleus in the atom.This View Depends on two central concepts the wave behavior of matter and the uncertainty principle.The combination of these two ideas leads to a mathematical description of electronic structure .

1.6.1 The Heisenberg Principle

- Werner Heisenberg (Heisenberg uncertainty principle): It is impossible to know simultaneously both the momentum(mass times velocity)and the position of a particle with certainty.
- Mathematically,

$$\Delta x \Delta p_x \geq \frac{h}{4\pi}$$

- The probability of finding the electron in a certain region in space is proportional to thesquare of the wave function, ψ2.
- The squareof the wave function, ψ2, definesthe distributionof electron density inthree- dimensional space around the nucleus (schrodinger).
- He agreed that electrons have a specific amount of energy
- Quantum the amount of energy needed to move from one energy level to another
- The electrons move in regions of probability around the nucleus calle Orbitals

1.6.2 Quantum Numbers

- The quantum mechanical description of the atom is based on the assumption that there are waves associated with both matter and radiations. The mathematical description of such wave provides information about the energy of electrons and their position.
- Erwin Schrödinger (1927),suggested that an electron or any other particle exhibiting wavelike properties can be described by a mathematical equationcalled awave function (denotedGreeklatterpsi,ψ).The equation is very complex.However, it leads to series of solutions that describe the allowed energy states of electrons.
- The square of a wave function, ψ2, gives the probability of finding an electron in a certain region of a space.The results of a quantum mechanics indicate that the electron may be visualized as being in a rapid motion within a given region of space around the nucleus.Although we cannot determine the precise position of an electron, the probability of the electron being at a definite location can be calculated.The region in which an electron is most likely found is called an orbital.the electron may occupy anywhere within an orbital at any instant in time.So, an electron can be considered as a particle that can rapidly move from place to place, behaving like an“electron cloud” whose density varies within the orbital. In quantum mechanicsburg,each electron in an atom is described by four quantum numbers
- Three of the quantum numbers specify the wave function that gives the probability of finding an electron at various place in spaces.
- The fourth one Is used to describe the spin (magnetic property) of the electrons that occupy the orbitals.

thee are 4 quantum number

- The principal quantumnumber(n)
- Theangular momentum quantum number(ℓ)

- The magnetic quantum number (mℓ),&
- the spin quantum number (ms)

The principal quantum number (n)

- describes the main energy level,or shell,an electron occupies.It maybe any positive integer,n=1,2,3,4,etc.ItdescribesThe Size And Energy Of the shell in which the orbital resides and it is analogous to the energy levels in Bohr's model.

The Angular momentum quantum number

- The Angular Momentum Quantum Number(ℓ)Designates The shape of the Atomic orbitals.within a Shell different Sublevels or Subshells are Possible,each with a characteristic Shape It takes values from 0 to n-1.Orbitals of the same n,but different ℓ are said to belong to different subshells.It is also called azimuthal quantum number. Example ,in n =4,ℓ has values of 0,1,2,and 3
- Each value of ℓ corresponds to an orbital label and an orbital shape.

The Magnetic Quantum Number(mℓ)

is also called the orbital-orientation quantum number.it has integral values between-ℓandℓ,including 0.The value of mℓ is related to the orientation of the orbital in space relative to the other orbitals in the atom.The number of possible mℓ values or orbitals for a given ℓ value is 2ℓ+1

The electron spin quantum number(ms)

refers to the spin of an electron and the orientation of the magnetic field produced by this spin.For Every set of n,ℓ,and mℓ values,ms can take the value+½or-½.Each Atomic orbital cannot accommodate more than two electrons,one with ms = +½ and another with ms = -½.

n	ℓ	Orbital Designation	m_ℓ	Numb
1	0	1*s*	0	
2	0	2*s*	0	
	1	2*p*	−1, 0, +1	
3	0	3*s*	0	
	1	3*p*	−1, 0, 1	
	2	3*d*	−2, −1, 0, 1, 2	
4	0	4*s*	0	
	1	4*p*	−1, 0, 1	
	2	4*d*	−2, −1, 0, 1, 2	
	3	4*f*	−3, −2, −1, 0, 1, 2, 3	

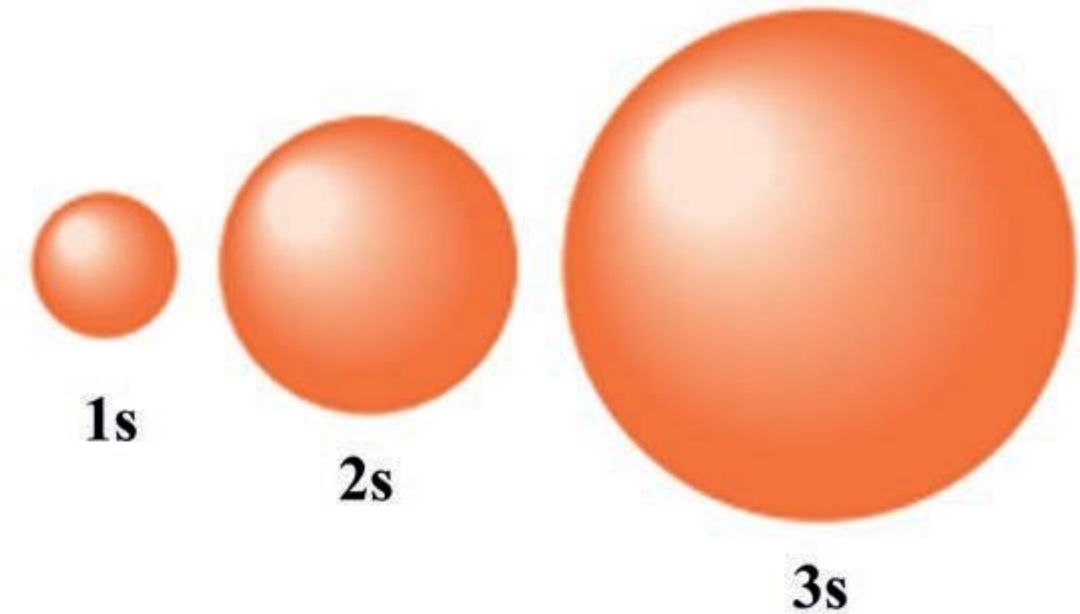
1. hat values of the angular momentum quantum number (l) and magnetic quantum number(ml)are allowed fora principal quantum number(n)of3?
2. How Many Orbitals Are Allowed for n=3?Give the name, magnetic quantum numbers, and numbers of orbitals for each sublevel with the following quantum numbers a).n =3, l =2 c.n=5, l =1 b).n =2, l =0 d.n =4, l =3
3. What is wrong with each of the following quantum number designations and/or sublevel names
   Exercise

- Give the sublevel notation for each of the following sets of quantum numbers a).n =3, l =2 b). n =4, l = 3 c).n =2, l =0 d.) n =4, l =3
- 4 Indicate whether each of the following is a permissible set of quantum numbers.Ifthesetis not permissible, state why it is not.
- a.n =3, l =1, ml =+2 b. n =4, l =3, ml=–3 c. n = 3, l = 2, ml = –2d.n =0, l =0, ml =0 e. n =3, l =3, ml=–3
- Consider The Electronic Configuration of anatomy:
- What are then, l and ml quantum numbers corresponding to the3s orbital?
- List all the possible quantum number values for anorbital in the 5fsub shell.
- In Which Specific sub shell will an electron be present if the quantum numbers n=3,l=1, and ml =–1?

- Which Of The Quantum numbers relates to the electron only?Which Relate(s)to the orbital?

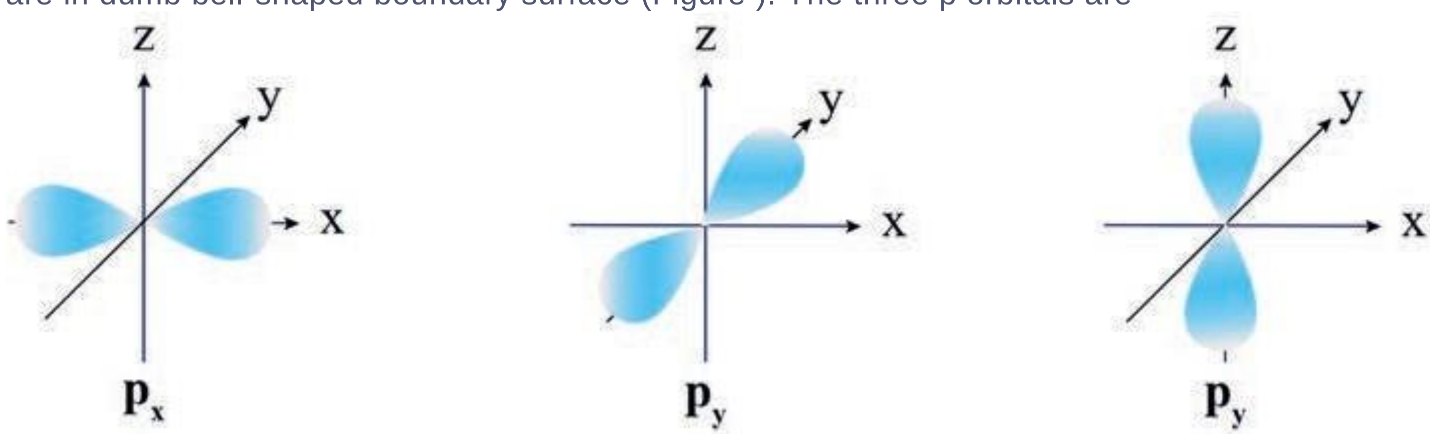
1.6.3 Shapes of Atomic Orbitals

- The three-dimensional aspects of the orientation of the atomic orbitals are usuallrepresented by drawing a boundary surface diagram that encloses the highest
- probability (about 90%) of the total electron density in an orbital.



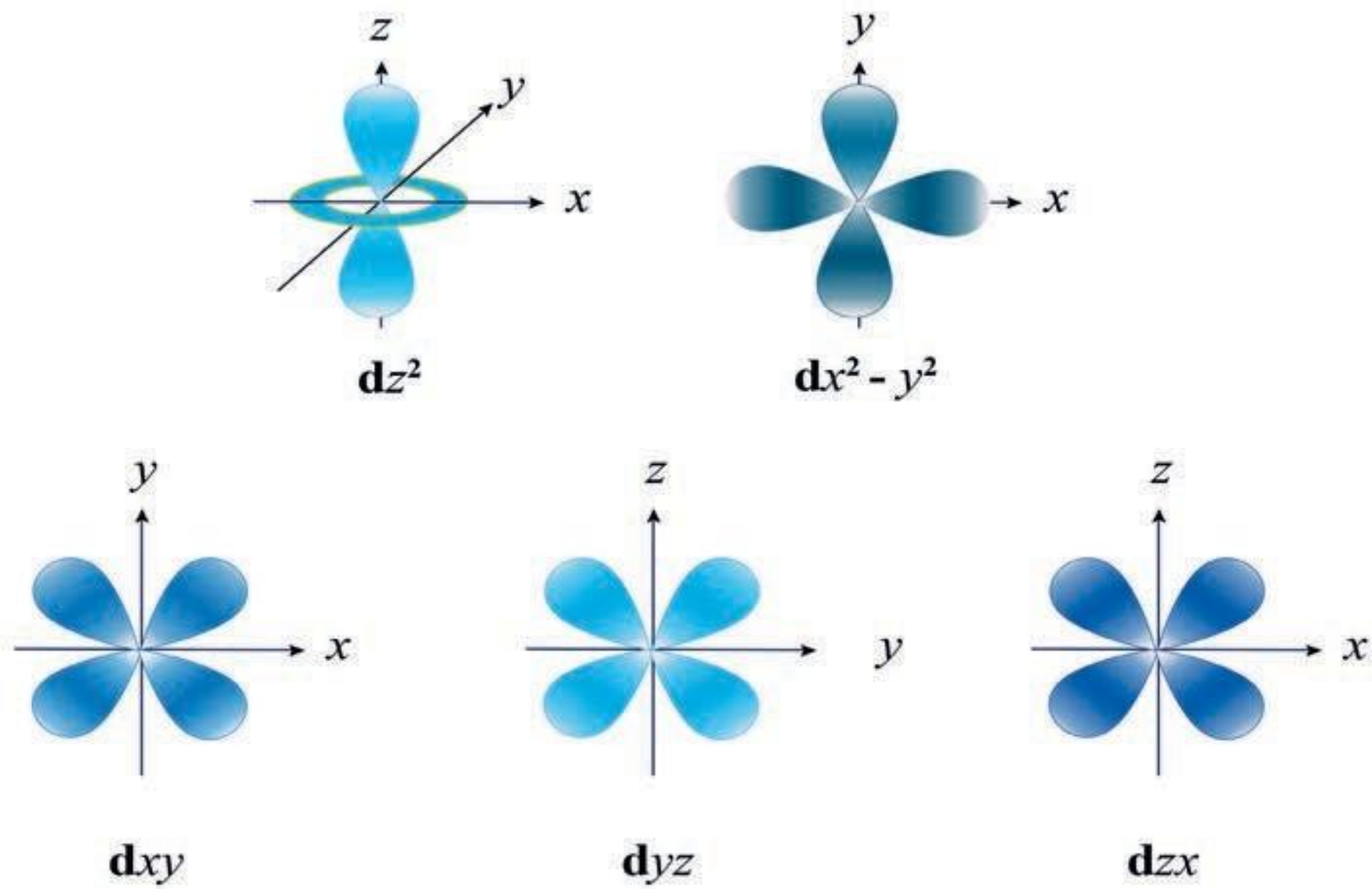
- Figure shows that the region of the greatest probability of finding an s electron
- is in a spherically symmetrical space whose origin is the atomic nucleus.
- The 1s-orbital is the smallest, the 2s orbital is larger than 1s and so on. Regardless of their principal quantum numbers, all s orbitals are spherical.

  P. orbitals
- The p orbitals of any principal quantum number are arranged along three mutually
- perpendicular axes, x, y, and z, so that the region of the highest electron density
- are in dumb bell-shaped boundary surface (Figure). The three p orbitals are



- designated as px, py and pz

- The three p – orbitals have Two lobes of each p orbital lie along a line with the nucleus at their center. Forinstance, the three 2p orbitals are classified as 2px, 2py and 2pz and in 2px the lobs on the X- axis and the other has the same thing
  Higher principal energy levels (n > 3)
  d-Orbitals
- have five d orbitals in addition to, one s orbital,
- three 3p orbitals. The special orientations of d orbitals are much more complex in
- shape than p orbitals. Figure shows the different distribution of the five d



- atomic orbitals: The five d orbital
  You have to different the shape. Example the electron density in dxy are between X and Y and on X-Axis

Lesson 3: Summary

The quantum mechanical model

Describes atoms using principles of quantum mechanics rather than classical physics

- Electrons are described by wave functions (Ψ) that determine their probabilities of being found in various regions around the nucleus.
- Electrons occupy discrete energy levels or shells (n = 1, 2, 3, …).
- Orbitals, described by quantum numbers, are regions where electrons are likely to be found.
- Provides a framework for understanding electron configurations, periodic properties, and chemical bonding.

Heisenberg Uncertainty Principle

- States a fundamental limit in quantum mechanics regarding the precision with which certain pairs of physical properties of a particle can be known simultaneously

Key Points:

- It is impossible to simultaneously determine the exact position (Δx) and momentum (Δp) of a particle with arbitrary precision.
- Impacts our understanding of the wave-particle duality and the limitations of measurement in quantum systems.

Quantum Numbers:

- Quantum numbers are used to describe the unique quantum state of each electron in an atom.

Quantum Numbers:

- **Principal Quantum Number (n)**: Determines the energy level or shell of the electron.
- **Angular Momentum Quantum Number (l)**: Specifies the shape of the orbital.
- **Magnetic Quantum Number (ml)**: Describes the orientation of the orbital in space.
- **Spin Quantum Number (ms)**: Represents the spin of the electron.

Roles:

- Define the size(energy), shape, orientation, and energy of atomic orbitals. & spin of electron.

Shapes of Atomic Orbitals:

- Atomic orbitals are regions of space around the nucleus where electrons are likely to be found.

Types of Orbitals:

- **s Orbital**: Spherical in shape, centered around the nucleus.
- **p Orbital**: Dumbbell-shaped with three orientations (px, py, pz) perpendicular to each other.
- **d Orbital**: Complex shapes with five orientations (dxy, dxz, dyz, dx^2-y^2, dz^2).
- **f Orbital**: More complex shapes with seven orientations.

Determined by:

- Angular momentum quantum number (l) dictates the shape and number of orbitals within each subshell.

Generally

- The quantum mechanical model of the atom utilizes wave functions to describe electrons in discrete energy levels, governed by quantum numbers that define orbital shapes and orientations. The Heisenberg Uncertainty Principle imposes limits on the precision of measuring pairs of complementary properties. Quantum numbers (n, l, ml, ms) specify the quantum state of electrons, influencing their spatial distribution within atomic orbitals, each characterized by distinct shapes (s, p, d, f). Together, these concepts form the foundation of modern atomic theory, explaining the structure, behavior, and properties of atoms and molecules.