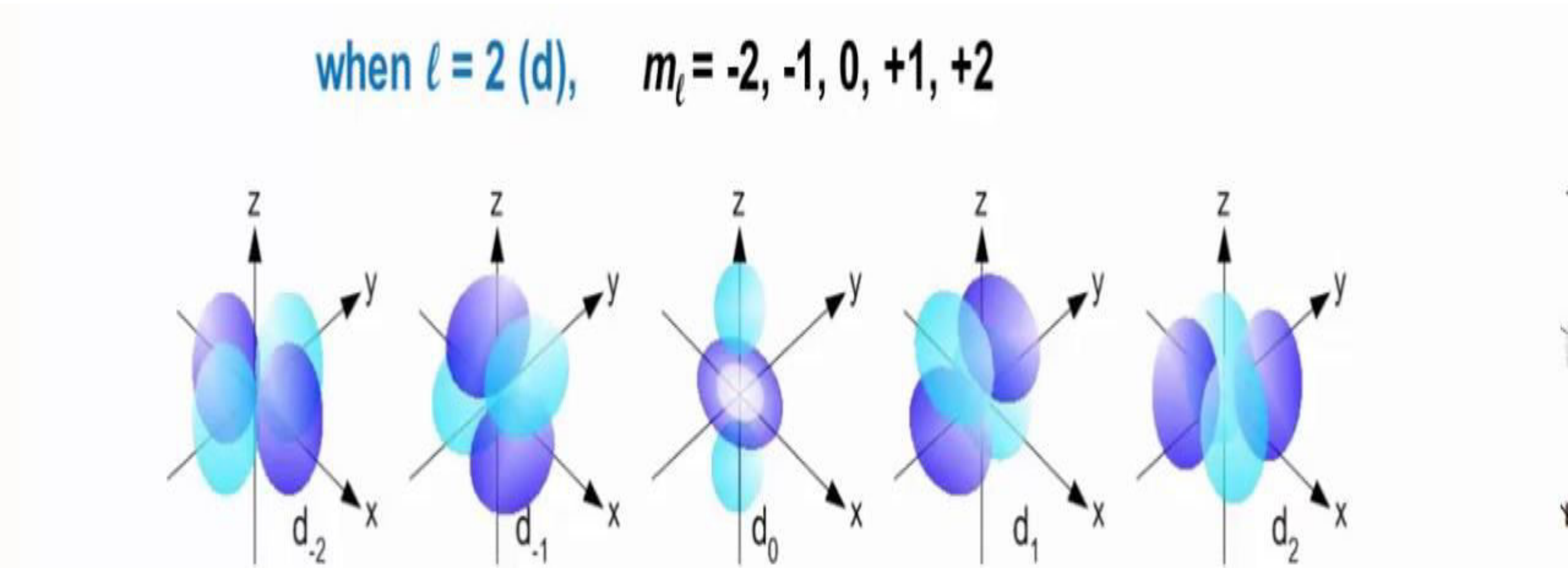
Structure Of Atom



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SIGNIFICANCE OF ψ and ψ^2

- S.W.E is a second order partial differential equation.
- The symbol ψ in the equation is called the **wave function and** represents **the amplitude** of the electron wave**.**
- The symbol **ψ** has no physical significance.
- It is just a mathematical function.
- The wave function **ψ** is not a observable quantity.

- In case of light waves,

  Intensity of light ∞ [Amplitude]^2

- It means that the intensity of light is proportional to the density of photons at that point in space.

- Applying the same concept to electron wave function

  [Amplitude]^2 ∞ Intensity of electrons at that point

- Acc. to uncertainty principle, it is not possible to determine the position of electron accurately.

- So, **ψ^2** determines the **probability density** of finding the electron at that point.

- **Higher** the value of **ψ^2** , **higher** will be the probability of finding the electron at that point.

- **Lower** the value of **ψ^2** , **lesser** will be the probability of finding the electron at that point.

- For a volume element having volume dV where (dV = dx, dy, dz) , the **probability** of finding the electron in this volume dV will be **$\psi^2 dV$.**

- The probability of finding an electron can be large, small, zero but **it can never be imaginary**.

Normal Wave function: Is the integration of ψ^2 and $\psi\psi^*$ (if is imaginary) over whole space is equal to one

$$\int_{-\infty}^{+\infty} \psi^2 dx\, dy\, dz = 1$$

$$\int_{-\infty}^{+\infty} \psi\psi^* dx\, dy\, dz = 1$$

If $\boldsymbol{\psi}$ has imaginary value, then it is multiplied by its complex conjugate $\boldsymbol{\psi^*}$, so that the product gives real values.

$$\int_{-\infty}^{+\infty} (N\psi)(N\psi) dx\, dy\, dz = 1$$

$$N^2 \int_{-\infty}^{+\infty} \psi^2 dx\, dy\, dz = 1$$

$$\int_{-\infty}^{+\infty} \psi^2 dx\, dy\, dz = N^{-2}$$

$$\int_{-\infty}^{+\infty} (N\psi)(N\psi^*) dx\, dy\, dz = 1$$

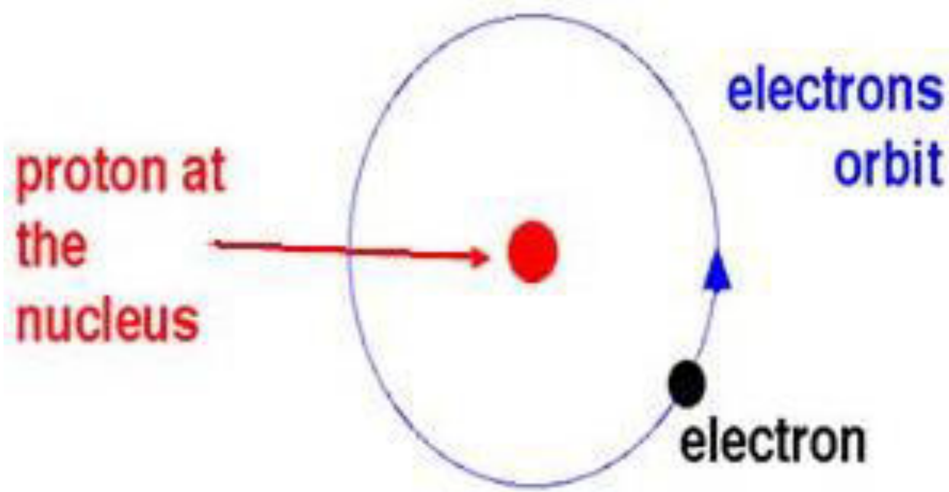
$$\int_{-\infty}^{+\infty} \psi\psi^* \, dx\, dy\, dz = N^{-2}$$

Orthogonal Wave Function: The orthogonality means that the product of two wave function , integration over whole space is zero.

$$\int_{-\infty}^{+\infty} (\psi_1)(\psi_2{}^*)dx\,dy\,dz = 0$$

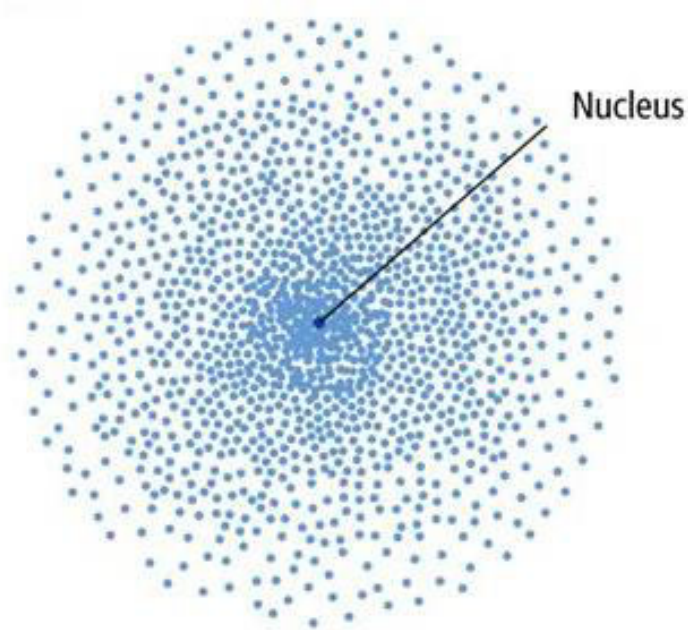
$$\int_{-\infty}^{+\infty} (\psi_2)(\psi_1{}^*)dx\,dy\,dz = 0$$

CONCEPT OF ATOMIC ORBITALS



Orbit - Bohr's concept

Orbital – Uncertainty principle



Orbit	Orbital
1. Orbit is a well defined circular path followed by revolving electrons around the nucleus.	1. Orbital is a region of space around the nucleus of an atom where the electron is most likely to be found.
2. It represents planar motion of electron.	2. It represents three dimensional motion of electron around nucleus.
3. Orbits are circular in shape.	3. Orbitals have different shapes.
4. Orbit can accommodate $2n^2$ electrons, where n is the number of orbit.	4. An orbital can accommodate only two electrons.
5. Orbits are non-directional in nature.	5. Orbitals (except *s*-orbital) are directional in nature.
6. Concept of orbits does not comply with Heisenberg's principle.	6. Concept of orbitals is in accordance with Heisenberg's principle.

Quantum Numbers

Each electron in an atom has a unique set of 4 quantum numbers which describe it.

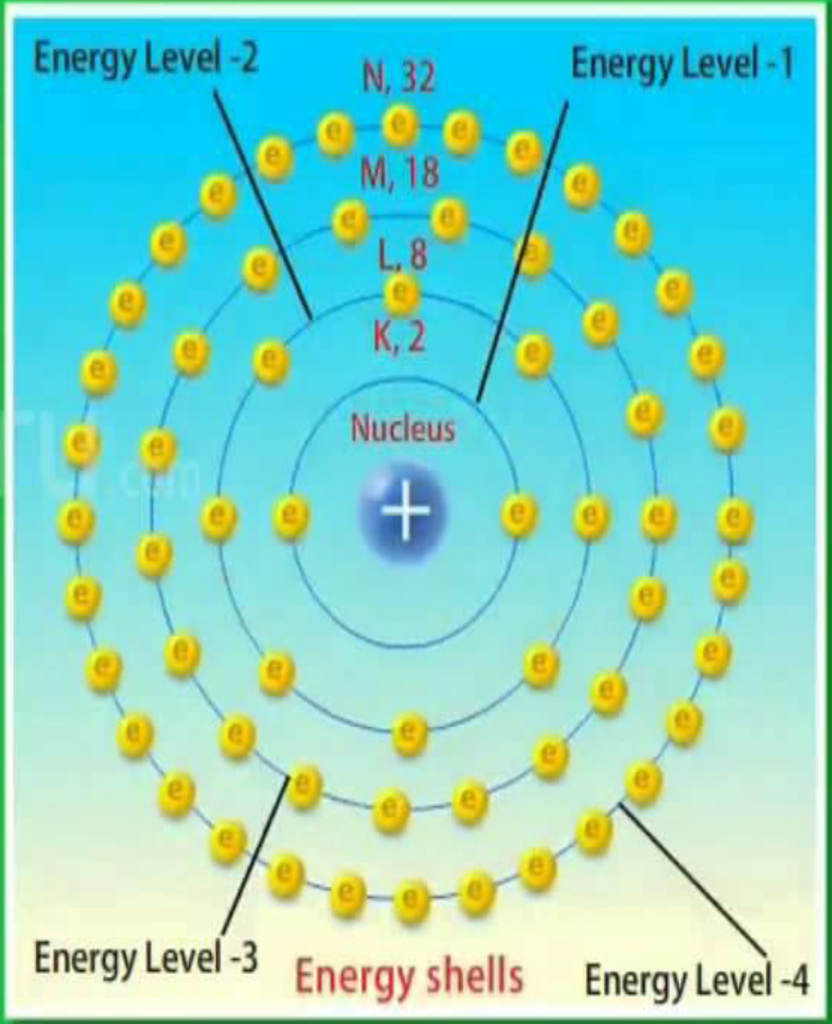
- Principal quantum number
- Angular momentum quantum number
- Magnetic quantum number
- Spin quantum number

The Principal Quantum Number (n)

Principal quantum number tells us in which principal energy level the electron is present. It can have any whole number value such as 1, 2, 3, 4 etc. The energy levels or energy shells corresponding to these numbers are designated as K, L, M, N, etc.

Energy of the electron in a hydrogen atom is related to principal quantum number by the following relation:

$$E_n = -k^2 \frac{2\pi^2 m e^4}{n^2 h^2} = -\frac{2.18 \times 10^{-18}}{n^2}\ \text{J}$$



Principal Quantum Number

- main **<u>energy level</u>** of an orbital.
- Indicates the relative size of the orbital
- an increase in n also means increase in the energy of the electron in the orbital.

  n= 1, 2, 3….

AZIMUTHAL QUANTUM NUMBERS

- Azimuthal Quantum Numbers*(l)*, is also known as Orbital Angular Momentum or Subsidiary Quantum Numbers.
- It defines the three dimensional shape of the orbital.
- We obtain the following information from the Azimuthal Quantum Numbers:-
- It designates the sub shell to which the electron belongs.
- It tells about the shape of the orbitals.
- For a given value *n, l* can have n values ranging from 0 to n-1, i.e., the possible values of *l* = 0, 1, 2, 3, ……, (n-1).
- Each shell consists of one or more sub-shells or sub-levels. The sub-shell in the principal shell is equal to the value of *n*.

Azimuthal Quantum Number, ℓ

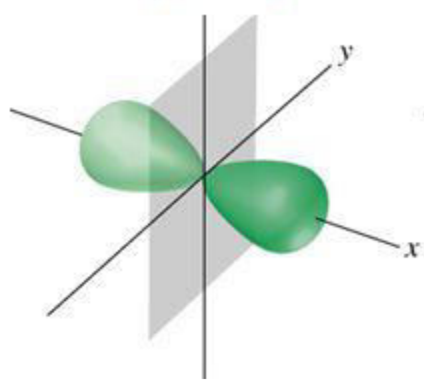
- This quantum number defines the **shape of the orbital**.
- Allowed values of ℓ are integers ranging from 0 to $n - 1$.
- We also use letter designations:

Value of ℓ	0	1	2	3
Type of orbital	*s*	*p*	*d*	*f*

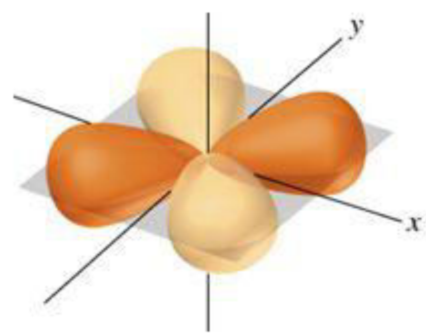
$\ell = 0$

1*s*

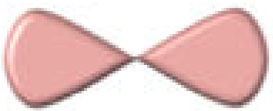
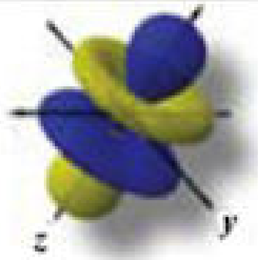
$\ell = 1$



$\ell = 2$



$\ell = 3$

Angular Momentum Quantum Number, ℓ	**Name of Subshell**	**Shape**	
0	s	Sphere	
1	p	Dumbbell	
2	d	Complex/double dumbbell	
3	f	More complex/ multiple lobes	

Principal Quantum Number, *n*	**Angular Momentum Quantum Number, ℓ ℓ = 0, 1, 2… n-1**	**Subshells**
1	$\ell = 0$	s (1 subshell)
2	$\ell = 0$ $\ell = 1$	s p (2 subshells)
3	$\ell = 0$ $\ell = 1$ $\ell = 2$	s p d (3 subshells)
4	$\ell = 0$ $\ell = 1$ $\ell = 2$ $\ell = 3$	s p d f (4 subshells)

- Azimuthal quantum number gives the energy of the electron due to angular momentum of the electron.

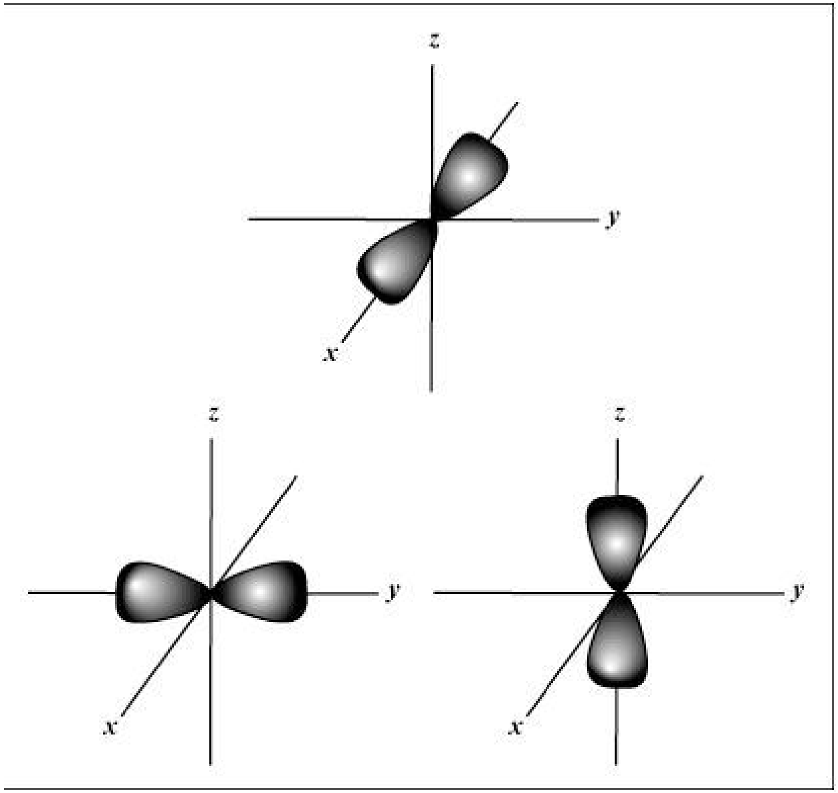
$$\text{Angular momentum (mvr)} = \frac{h\,[\,l(\,l + 1)]^{1/2}}{2\pi}$$

- The s, p ,d ,f designations arise from the characteristic of spectral lines produced in a spectra.

Value of *l*	Symbol	Designation
0	s	sharp
1	p	principal
2	d	diffuse
3	f	fundamental

Magnetic Quantum Number

- The **magnetic quantum number (*m_l*)** describes how the various orbitals are oriented in space.
  - Orbitals can be oriented along x, y, and z axes.
  - Examples: $2p_x$, $2p_y$, $2p_z$



Why are electrons or subshells oriented in different directions in space ?

- The movement of charged particle i.e. electron around the nucleus generates an **electric field**.

- This electric field generates a **magnetic field**.

- When an external magnetic field is applied **, interaction occurs** between the external magnetic field and the magnetic field of the electron.

- Due to this interaction electrons tend to **orient themselves in some preferred direction** in space around the nucleus.

- These orientations or regions of space are called **orbitals**.

- Magnetic quantum number determines the **preferred orientations** of the electrons present in a subshell.

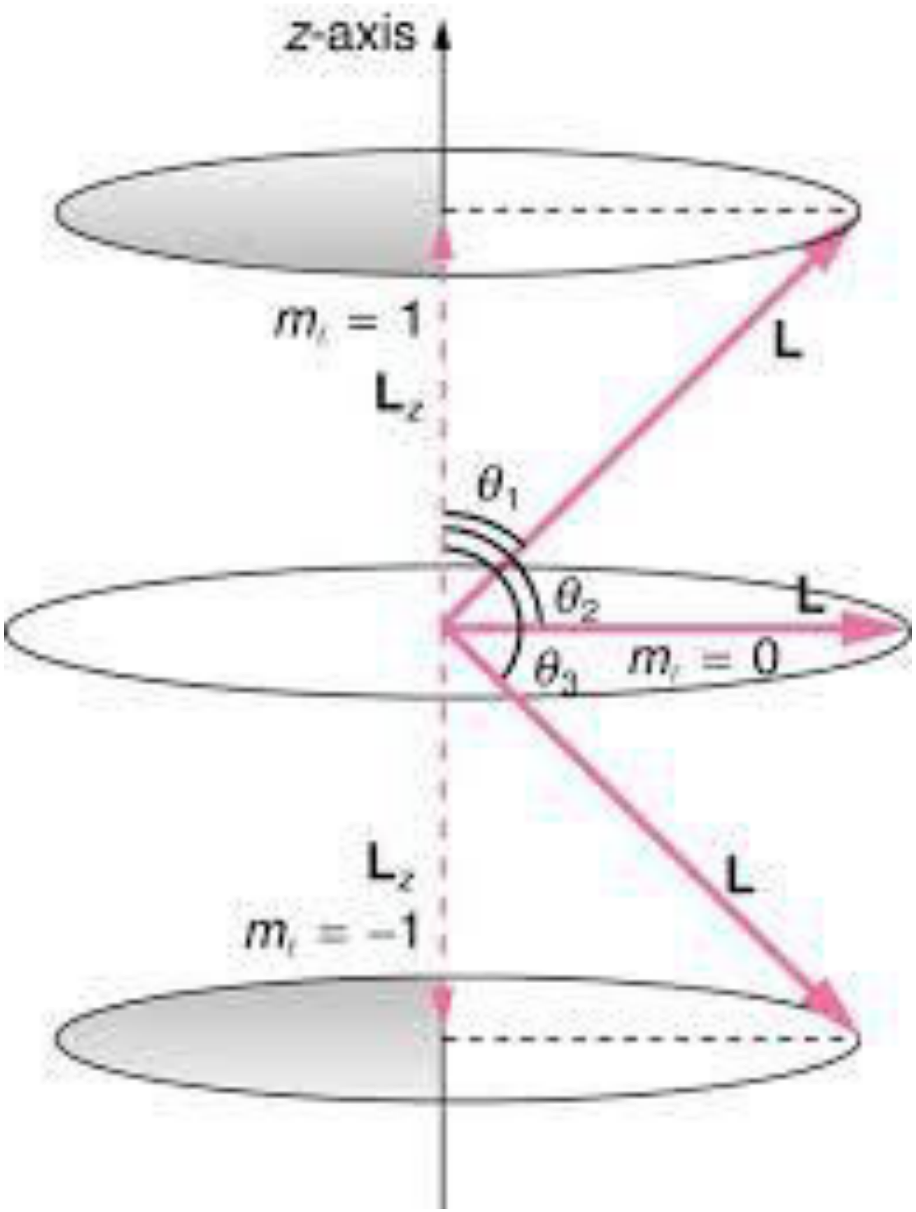
- Each orientation corresponds to a **orbital.**

- So, magnetic quantum number gives the **total number of orbitals** present in a sub shell.

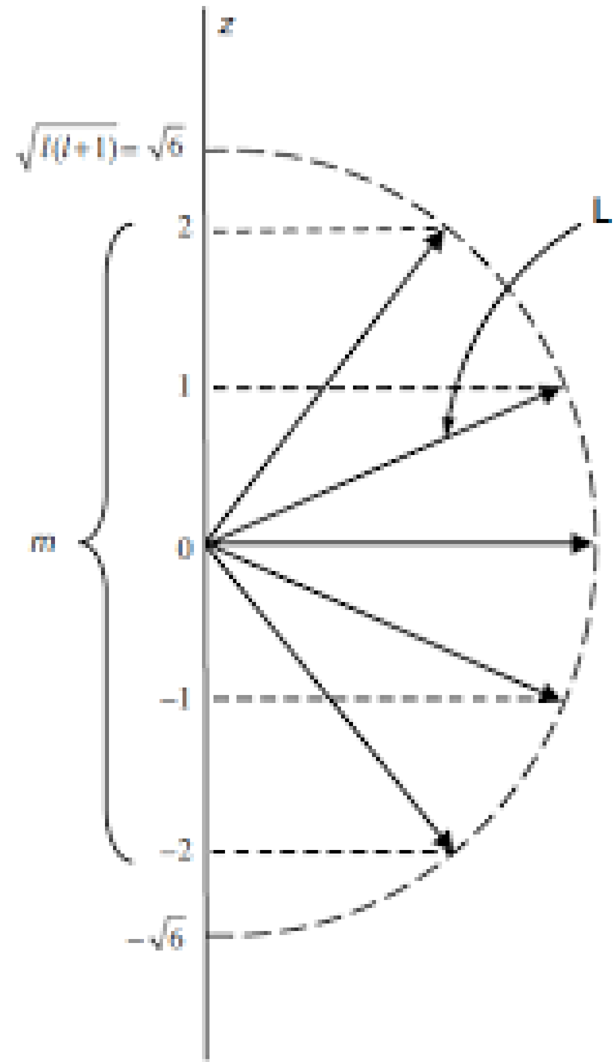
- The value of magnetic quantum number (m) **depends on the value** of azimuthal quantum number (*l*).

- For a given value of ***l***, ***m*** can have values ranging from
–l……..0……+l

- For any value of ***l***, total **m** values will be equal to **2*l* + 1**.



z-axis
$m_l = 1$
L_z
L
θ_1
θ_2
L
θ_3
$m_l = 0$
L
L_z
$m_l = -1$



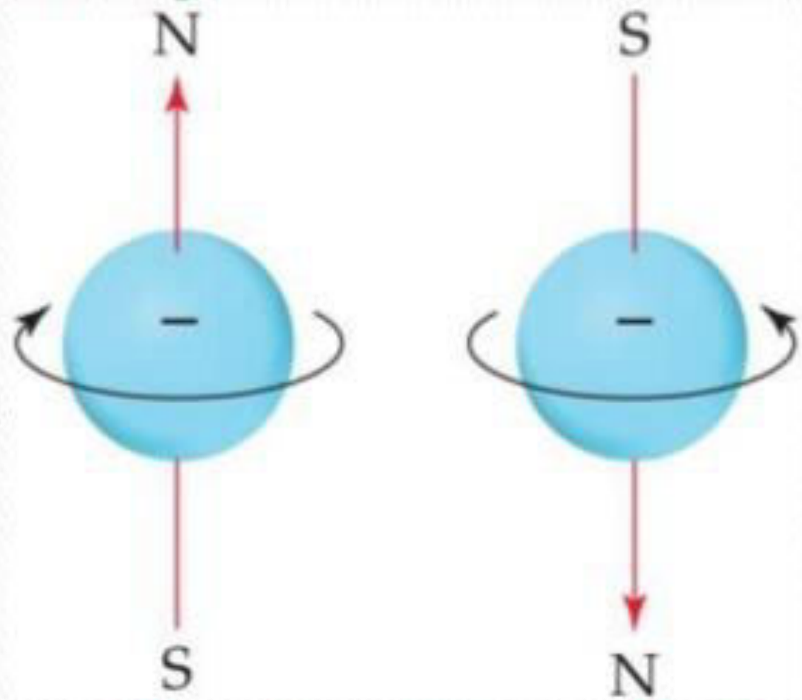
z
$\sqrt{l(l+1)} = \sqrt{6}$
L
2
1
m
0
−1
−2
$-\sqrt{6}$

Quantum Numbers

n	l	m_l	Orbital	Elements		Shell
$n = 1$	0	0	1s	2	2	K
$n = 2$	0	0	2s	2	8	L
	1	−1, 0, 1	2p	6		
$n = 3$	0	0	3s	2	18	M
	1	−1, 0, 1	3p	6		
	2	−2, −1, 0, 1, 2	3d	10		
$n = 4$	0	0	4s	2	32	N
	1	−1, 0, 1	4p	6		
	2	−2, −1, 0, 1, 2	4d	10		
	3	−3, −2, −1, 0, 1, 2, 3	4f	14		

Spin Quantum Number, m_s

- In the 1920s, it was discovered that two electrons in the same orbital do not have exactly the same energy.
- The "spin" of an electron describes its magnetic field, which affects its energy.
- No two electrons in the same atom can have exactly the same energy.
- For example, no two electrons in the same atom can have identical sets of quantum numbers.



The spin quantum number has only 2 allowed values:
m_s = +1/2 and −1/2.

Pauli Exclusion Principle

It states, no two electrons in an atom can have identical set of four quantum numbers.

The maximum number of electrons in s subshell is 2, p subshell is 6 d subshell is 10 and f subshell is 14.

MODERN QUANTUM NUMBERS NOTATION

principal quantum number	period notation	orbital quantum number	orbital notation	magnetic quantum number	spin	maximal number of electrons in	
n	symbol	l = 0…n-1	symbol	m_l	m_s	shell	period
1	K	0	1s	0	+ , -	2	2
2	L	0	2s	0	+ , -	2	8
		1	2p	-1,0,+1	+ , -	6	
3	M	0	3s	0	+ , -	2	18
		1	3p	-1,0,+1	+ , -	6	
		2	3d	-2,-1,0,+1,+2,	+ , -	10	
4	N	0	4s	0	+ , -	2	32
		1	4p	-1,0,+1	+ , -	6	
		2	4d	-2,-1,0,+1,+2,	+ , -	10	
		3	4f	-3,-2,-1,0,+1,+2,+3	+ , -	14	
5	O	0	5s	0	+ , -	2	50
		1	5p	-1,0,+1	+ , -	6	
		2	5d	-2,-1,0,+1,+2,	+ , -	10	
		3	5f	-3,-2,-1,0,+1,+2,+3	+ , -	14	
		4	5g	-4,-3,-2,-1,0,+1,+2,+3+4	+ , -	18	

Example 13. *Which of the following sets of quantum numbers (in order of n, l, m, s) are impossible for an electron in an atom, and why ?*

(*i*) 4, 2, 0, + ½

(*ii*) 3, 3, – 2, – ½

(*iii*) 2, 0, 0, + ½

(*iv*) 4, 0, 1, – ½

(*v*) 3, 2, – 2, 0

(Pbi. U. 2011)

Solution : (*i*) $n = 4$, $l = 2$, $m = 0$, $s = +½$

This set of quantum numbers is *possible.*

(*ii*) $n = 3$, $l = 3$, $m = -2$, $s = -½$

This is *not possible* because for $n = 3$, l cannot be 3. It can have values only 0, 1 and 2.

(*iii*) $n = 2$, $l = 0$, $m = 0$, $s = +½$

This is *possible.*

(*iv*) $n = 4$, $l = 0$, $m = 1$, $s = -½$

This is *not possible* because for $l = 0$, m cannot have value equal to 1.

(*iv*) $n = 3$, $l = 2$, $m = -2$, $s = 0$

This is *not possible* because s cannot have value equal to 0. It can have only + ½ or – ½ value.

Example 14. *An electron is in a 4f-orbital. What possible values for the quantum numbers n, l, m and s can it have ?* (C.D.L.U. 2012)

Solution : For 4*f*-orbital

$n = 4$

$l = 3$ (for *f*-subshell $l = 3$)

$m = -3, -2, -1, 0, +1, +2, +3$

$s = +\frac{1}{2}$ and $-\frac{1}{2}$ for each value of m.

Example 15. *Which of the following orbitals are not possible ?*

1p, 2s, 2p, 3f.

Give reasons. (G.N.D.U. 2002)

Solution : 1*p* is not possible because for $n = 1$, l has only one value, $l = 0$ and therefore only *s*-subshell is possible.

(*ii*) 2*s*—possible.

(*iii*) 2*p*—possible.

(*iv*) 3*f*—not possible, because for $n = 3$, l has values $l = 0$ (*s*), 1 (*p*) and 2(*d*). Therefore, *f*-subshell is not possible.

Example 16. *Can we have 5g-subshell ? How many orbitals are there in this subshell ?*

Solution : For $n = 5$, l can have values, $l = 0, 1, 2, 3, 4$. The corresponding subshells are 5*s*, 5*p*, 5*d*, 5*f* and 5*g*.

Therefore, 5*g*-subshell is possible.

For 5*g*-subshell, $l = 4$ and the corresponding values of m are :

$$m = -4, -3, -2, -1, 0, +1, +2, +3, +4$$

There are thus **nine** orbitals in 5*g*-subshell.

(a) *Give the values of n and l for the following subshells :*

5f, 3p, 6s, 4d (H.P.U. 2013)

(b) *Name the various orbitals possible for :*

(i) $n = 3, l = 0$ (ii) $n = 3, l = 1$.

(c) *What is the maximum number of electrons that can be accommodated in :*

(i) 3p-subshell (ii) 4s-subshell (iii) $2p_x$-orbital (iv) orbital designated as $n = 3, l = 2, m = +2$ (v) subshell designated as $n = 3, l = 2$, (vi) $n = 3$ shell.

Solution : (a) (i) 5f : $n = 5,$ $l = 3$

(ii) 3p : $n = 3,$ $l = 1$

(iii) 6s : $n = 6,$ $l = 0$

(iv) 4d : $n = 4,$ $l = 2$

(b) **Names of orbitals :**

(i) $n = 3,$ $l = 0$ 3s-orbitals

(ii) $n = 3,$ $l = 1$ 3p-orbitals ; $3p_x$, $3p_y$, $3p_z$