

# Atomic Physics / Lecture Three

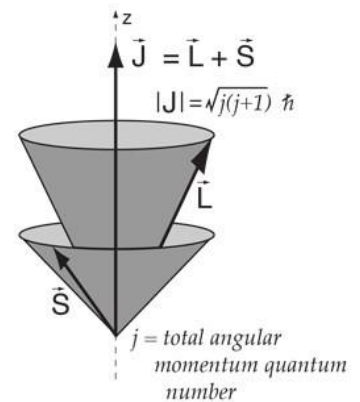
## Spin Orbit Coupling

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L-S coupling or Russell-Saunders coupling predicts results in good agreement with the observed spectral details for many light atoms. In such cases of multi-electron atoms the spin-orbit coupling is weak. In this coupling scheme it is presumed that the orbital angular momenta of the individual electrons add to form a resultant orbital angular momentum  $\mathbf{L}$ .

Similarly, the individual spin angular momenta should couple to produce a resultant spin angular momentum

$\mathbf{S}$ . Then  $\mathbf{L}$  and  $\mathbf{S}$  combine to form the total angular momentum.



This scheme of coupling may be visualized in terms of a vector model of angular momentum.

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

## 2- Quantum Numbers and Atomic Orbitals

**From** the solution of Schrödinger equation for hydrogen atom in spherical coordinates, we obtained a set of mathematical equations, called wave functions, which describe the probability of finding electrons at certain energy levels within an atom.

A wave function for an electron in an atom is called an *atomic orbital*; this atomic orbital describes a region of space in which there is a high probability of finding the electron. Energy changes within an atom are the result of an electron changing from a wave pattern with one energy to a wave pattern with a different energy (usually accompanied by the absorption or emission of a photon of light).

Each electron in an atom is described by four different quantum numbers. The first three ( $n, \ell, m_\ell$ ) specify the particular orbital of interest, and the fourth ( $m_s$ ) specifies how many electrons can occupy that orbital.

### 1. **Principal Quantum Number ( $n$ ):** $n = 1, 2, 3, \dots, \infty$

Specifies the energy of an electron and the size of the orbital (the distance from the nucleus of the peak in a radial probability distribution plot). All orbitals that have the same value of  $n$  are said to be in the same shell (level). For a hydrogen atom with  $n=1$ , the electron is in its *ground state*; if the electron is in the  $n=2$  orbital, it is in an *excited state*. The total number of orbitals for a given  $n$  value is  $n^2$ .

**2. Angular Momentum (Secondary, Azimunthal) Quantum Number ( $\ell$ ):  $\ell = 0, 1, \dots, (n-1)$ .**

Specifies the shape of an orbital with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of orbitals called subshells (sublevels). Usually, a letter code is used to identify ( $\ell$ ) to avoid confusion with ( $n$ ):

$\ell$	0	1	2	3	4	5	...
Letter	s	p	D	f	g	h	...

**3. Magnetic Quantum Number ( $m_\ell$ ):  $m_\ell = -\ell, \dots, 0, \dots, +\ell$**

Specifies the orientation in space of an orbital of a given energy ( $n$ ) and shape ( $\ell$ ). This number divides the subshell into individual orbitals which hold the electrons; there are ( $2\ell + 1$ ) orbitals in each subshell. Thus the s subshell has only one orbital, the p subshell has three orbitals, and so on.

**4. Spin Quantum Number ( $m_s$ ):  $m_s = +1/2$  or  $-1/2$ .**

Specifies the orientation of the spin axis of an electron. An electron can spin in only one of two directions (sometimes called *up* and *down*).

The Pauli exclusion principle (Wolfgang Pauli, Nobel Prize 1945) states that “*no two electrons in the same atom can have identical values for all four of their quantum numbers.*”, What this means is that no more than two electrons can occupy the same orbital, and that two electrons in the same orbital must have opposite spins.

Because an electron spins, it creates a magnetic field, which can be oriented in one of two directions. For two electrons in the same orbital, the spins must be opposite to each other; the spins are said to be paired. These substances are not attracted to magnets and are said to be *diamagnetic*. Atoms with more electrons that spin in one direction than another contain unpaired electrons. These substances are weakly attracted to magnets and are said to be *paramagnetic*.

### Table of Allowed Quantum Numbers

Relationship Among Values of  $n$ ,  $l$ , and  $m_l$  Through  $n = 4$

$n$	Possible Values of $l$	Subshell Designation	Possible Values of $m_l$	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2	0	2s	0	1	4
	1	2p	1, 0, -1	3	
3	0	3s	0	1	9
	1	3p	1, 0, -1	3	
	2	3d	2, 1, 0, -1, -2	5	
4	0	4s	0	1	16
	1	4p	1, 0, -1	3	
	2	4d	2, 1, 0, -1, -2	5	
	3	4f	3, 2, 1, 0, -1, -2, -3	7	

### Electron Configurations of Several Lighter Elements

Element	Total Electrons	Orbital Diagram					Electron Configuration
		1s	2s	2p			
Li	3	$\uparrow\downarrow$	$\uparrow$				$1s^2 2s^1$
Be	4	$\uparrow\downarrow$	$\uparrow\downarrow$				$1s^2 2s^2$
B	5	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$			$1s^2 2s^2 2p^1$
C	6	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$		$1s^2 2s^2 2p^2$
N	7	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$	$\uparrow$	$1s^2 2s^2 2p^3$
NE	10	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$1s^2 2s^2 2p^6$
Na	11	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$1s^2 2s^2 2p^6 3s^1$

**EX1: Select the Quantum number of last electron in  ${}_6\text{C}$ .**

Sol:

Electron Configuration of C Carbon:

**$1s^2 2s^2 2p^2$**

$n=2$  ,  $l=1$  ,  $m_l=0$  ,  $m_s= \frac{1}{2}$

**EX2: Select the z of element which have  $n=3$  ,  $l=1$  ,  $ms=-1/2$  for last electron .**

**Sol:**

**$n=3$  ,  $l=1$  >>>>  $3p$**

**$1s^2 2s^2 2p^6 3s^2 3p^6$**

**$Z=2+2+6+2+6 =18$**

# Homework :

Q.1) Rank the following electrons with quantum numbers  $(n, l, m_l, m_s)$  from lowest energy to highest energy.

- A.  $(2, 1, 1, +1/2)$
- B.  $(1, 0, 0, -1/2)$
- C.  $(4, 1, -1, +1/2)$

Q.2) What is wrong with the quantum numbers  $(n, l, m_l, m_s)$  of the following electrons?

- a.  $(2, 2, 0, +1/2)$
- b.  $(3, 1, -1, -1/2)$
- c.  $(3, 1, -2, 1)$

Q.4) Rank the following from highest energy to lowest energy.

$3s, 5p, 4d, 1s, 5d, 3p$