Atomic and Molecular Physics

Presented by

Lec. Dr. Sarah Mahdi Obaid

Department of Medical Physics,

Al-Mustaqbal University,

Babil, Iraq

Email: sarah.mahdi@uomus.edu.iq

Second-year students

Lecture 5

Many electron atom

5.1 Quantum Numbers and Atomic Orbitals

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, ℓ, m_ℓ) 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, …, ∞ 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 (ℓ): $\ell = 0, 1, \cdots, (n-1)$.**

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 (ℓ) to avoid confusion with (*n*):

ℓ	**0**	**1**	**2**	**3**	**4**	**5**	**...**
Letter	***s***	***p***	***d***	***f***	***g***	***h***	**...**

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

Specifies the orientation in space of an orbital of a given energy (*n*) and shape (ℓ). 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=+½ or -½.**

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.

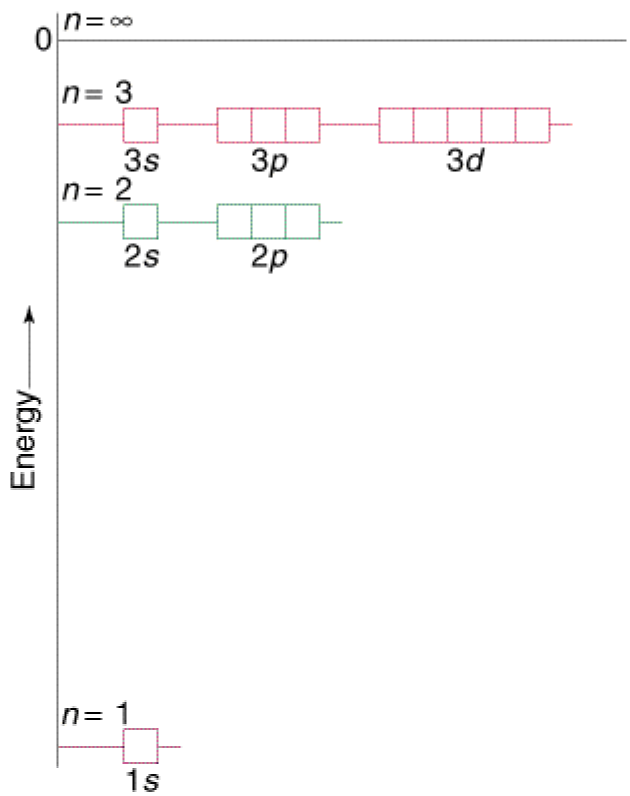
Because an electron spins, it creates a magnetic field, which can be oriented in one of two directions. For two electrons in the same orbital, the spins must be opposite to each other; the spins are said to be paired. These substances are not attracted to magnets and are said to be *diamagnetic*. Atoms 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	1*s*	0	1	1
2	0	2*s*	0	1	
	1	2*p*	1, 0, −1	3	4
3	0	3*s*	0	1	
	1	3*p*	1, 0, −1	3	
	2	3*d*	2, 1, 0, −1, −2	5	9
4	0	4*s*	0	1	
	1	4*p*	1, 0, −1	3	
	2	4*d*	2, 1, 0, −1, −2	5	
	3	4*f*	3, 2, 1, 0, −1, −2, −3	7	16

The energy of the orbitals of a one-electron atom depends only on $1/n^2$, so the energy spectrum looks like this, where all orbitals with the same n quantum number 'shell' are *degenerate* (i.e. have the same energy).

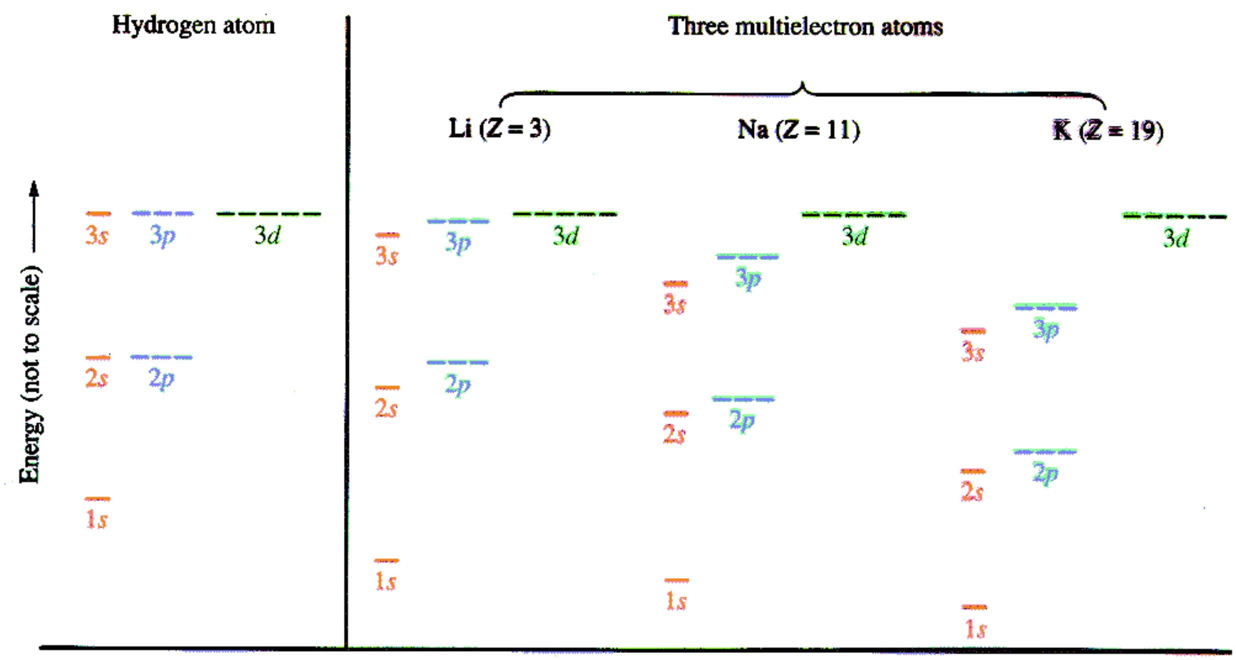


When describing any element other than Hydrogen, the structure of that atom will by more complicated than the simple Bohr picture can predict.

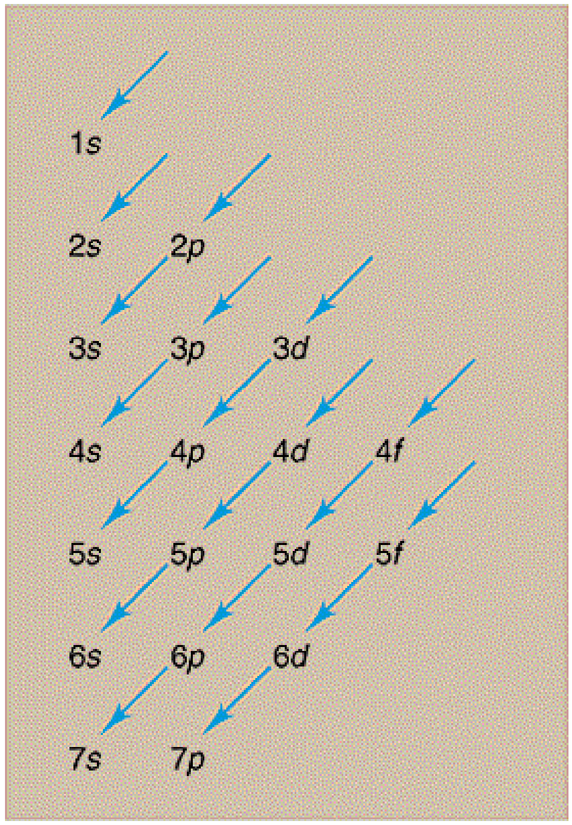
- **First, the charge on the nucleus will be larger than +1e. The increased electrostatic attraction of the electrons to the nucleus will have a tendency to draw those electrons closer to the nucleus (and as a result closer to each other). This will lower the total energy of the atom (the Bohr model can handle this effect)**
- **Except for positive ions that contain only a single electron, the electrons of the atom or ion will interact with each other *repulsively*, since they have like charges. This will raise the total energy of the atom and 'spread out' the electrons. The Bohr model cannot describe electron-electron repulsion and therefore fails for any multiple electron atom or ion**

The description of how most elemental atoms and ions behave is a balance of the two above phenomena.

We will treat the way in which the whole atom behaves as the cumulative behavior of each individual electron. Each individual electron is a 'wave' and has a wavefunction, which may be described approximately with at orbitals of Hydrogen. The energy of each of these wavefunctions (orbitals) is qualitatively different from that of the one-electron atom, however, because of the discriminatory effects of electron-electron repulsion.



The order of filling of the orbitals (the order in energy from low to high) can be remembered by the following chart:



We can now 'build' atoms by filling the orbitals expected from a one-electron model 'perturbed' by what we know about electron-electron repulsion. This is called atomic 'Aufbau'. The first elements are easy if we postulate two 'rules':

- **Each electron has one of two possible 'flavors': up or down which are described by a quantum number called m_s, which has values +1/2 or -1/2, respectively.**

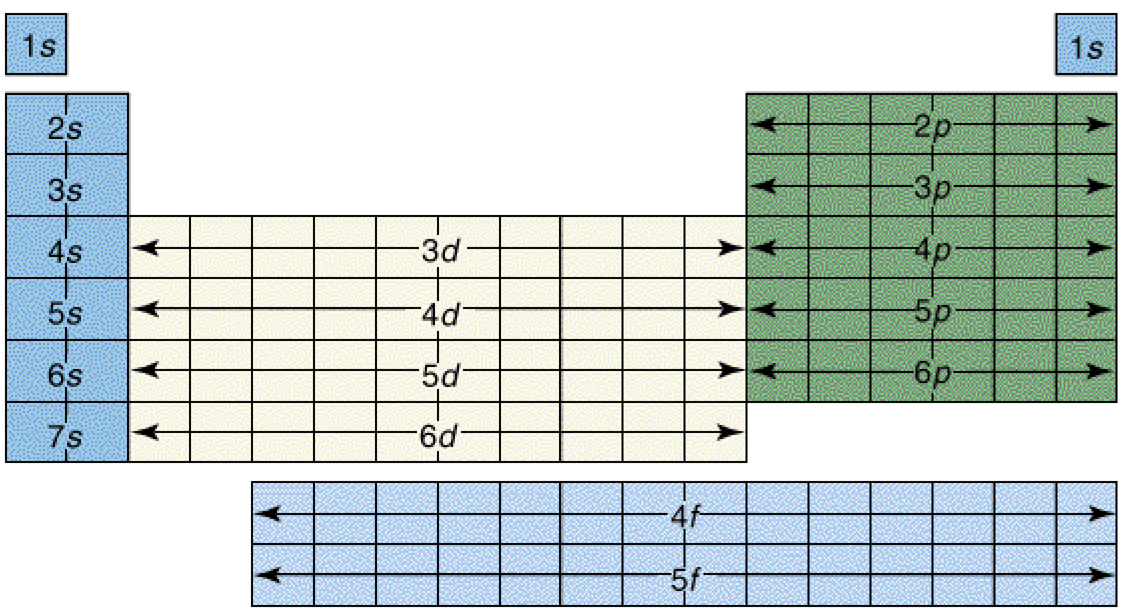
- **Electrons 'exclude' each other in that no two electrons can occupy the same 'state' at the same time. Thus, no two electrons in the same atom can have the same quantum numbers. This is called the *Pauli Exclusion Principle.***

If it were not for the *spin* (the 'up' or 'down' flavor) of the electron, many electron atoms would be filled by putting one electron in each hydrogen-like orbital, to satisfy the Pauli exculsion principle. But, as it is, each spatial orbital can two electrons in it, as long as they are spin paired (one up, one down).

Electron Configurations of Several Lighter Elements

Element	Total Electrons	Obital Diagram 1s	2s	2p			3s	Electron Configuration
Li	3	↑↓	↑					$1s^2 2s^1$
Be	4	↑↓	↑↓					$1s^2 2s^2$
B	5	↑↓	↑↓	↑				$1s^2 2s^2 2p^1$
C	6	↑↓	↑↓	↑	↑			$1s^2 2s^2 2p^2$
N	7	↑↓	↑↓	↑	↑	↑		$1s^2 2s^2 2p^3$
NE	10	↑↓	↑↓	↑↓	↑↓	↑↓		$1s^2 2s^2 2p^6$
Na	11	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^6 3s^1$

The electron configuation of the elements are what give rise to the shape of the periodic table and the names of the blocks that compose it.



Many-Electron Atom — MCQs

1. The wave function that describes the region of space where an electron is likely to be found is called a:
   (a) Energy level
   (b) Atomic orbital
   (c) Shell
   (d) Subshell

2. Energy changes within an atom occur when an electron:
   (a) Spins in a new direction
   (b) Moves to another atom
   (c) Changes from one wave pattern to another
   (d) Stops spinning

3. How many quantum numbers are required to describe an electron completely?
   (a) Two
   (b) Three
   (c) Four
   (d) Five

4. The principal quantum number n primarily determines:
   (a) The shape of an orbital
   (b) The energy level and size of the orbital
   (c) The spin of the electron
   (d) The number of orbitals in a subshell

5. For a given value of n, the total number of orbitals is equal to:
   (a) n
   (b) n^2
   (c) $2n$
   (d) n^3

6. The angular momentum quantum number ℓ defines:
   (a) The orientation of the orbital
   (b) The spin direction

(c) The shape of the orbital
(d) The size of the orbital

7. Which subshell corresponds to $\ell = 2$?

(a) s
(b) p
(c) d
(d) f

8. The magnetic quantum number m_ℓ specifies:

(a) The energy of the orbital
(b) The orientation of the orbital in space
(c) The size of the atom
(d) The total number of electrons

9. The number of orbitals in a subshell is given by:

(a) $2\ell + 1$
(b) ℓ^2
(c) n^2
(d) $\ell + n$

10. The spin quantum number m_s can have values of:

(a) $+1$ or -1
(b) $+\frac{1}{2}$ or $-\frac{1}{2}$
(c) 0 or $+1$
(d) 0 or -1

11. The Pauli exclusion principle states that:

(a) Electrons in the same orbital must have the same spin
(b) No two electrons can have identical sets of four quantum numbers
(c) All electrons in an atom have opposite spins
(d) Electrons occupy orbitals singly before pairing

12. Substances with all electrons paired are said to be:

(a) Paramagnetic
(b) Ferromagnetic

(c) Diamagnetic
(d) Superconductive

13. In many-electron atoms, electron–electron repulsion tends to:
    (a) Increase total energy
    (b) Decrease total energy
    (c) Eliminate electron spin
    (d) Neutralize the nucleus

14. The Bohr model fails for multi-electron atoms because it cannot:
    (a) Describe circular orbits
    (b) Handle electron–electron repulsion
    (c) Predict energy levels
    (d) Explain light emission

15. The Aufbau principle is used to:
    (a) Predict atomic mass
    (b) Determine order of orbital filling
    (c) Measure ionization energy
    (d) Explain nuclear charge

16. According to the Aufbau principle, electrons fill orbitals in order of:
    (a) Increasing atomic number
    (b) Increasing energy
    (c) Increasing distance from the nucleus only
    (d) Random distribution

17. If two electrons occupy the same orbital, they must have:
    (a) The same spin
    (b) Opposite spins
    (c) Different principal quantum numbers
    (d) Different shapes

18. The paramagnetism of an atom is due to:
    (a) Paired electrons
    (b) Unpaired electrons

(c) Circular orbits
(d) High nuclear charge

19. The term *degenerate orbitals* refers to orbitals that have:
    (a) Different energies
    (b) The same energy
    (c) Opposite spins
    (d) Different shapes

20. The periodic table's structure arises mainly from:
    (a) Nuclear mass differences
    (b) Electron configuration of atoms
    (c) Atomic size only
    (d) Isotopic distribution