Quantum Mechanics 2

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Electron Configurations

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Pick ups from the H-Atom

Multi-electron atoms are much more complicated than the Hydrogen atom not only because of the number of parts involved, but also because there are many more interactions that one has to consider. This includes electron-electron interaction, and magnetic interactions. One has to also take into account the Pauli Exclusion principle.

There are no exact solutions for atoms heavier than Hydrogen. There are however approximate solutions that are reasonably accurate. These solutions are not analytical, and generally requires high computational power.

There are however basic features of atoms that can be gleaned from the results for the Hydrogen atom.

Degeneracy

Atoms are degenerate systems as several eigenstates have the same energy levels. Energy levels of a Hydrogen atom are defined by the principal quantum number

$$E_n = -\frac{Z^2 e^2}{4\pi\varepsilon_0}\frac{1}{2n^2 a_0}$$

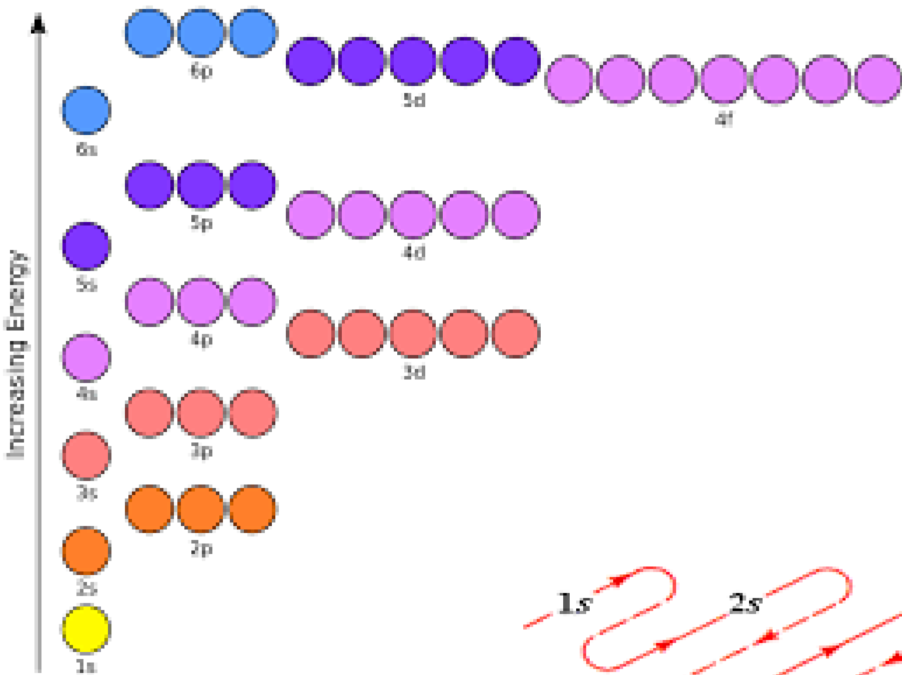
For each energy level, there are $2n^2$ eigenstates* [Hydrogen 3], these being the various $|nlmm_s\rangle$ states. In spectroscopic notation, the principal quantum number $n = 1,2,3,\cdots$ corresponds to the $K, L, M, \cdots$ electron shells of the atom, while the angular quantum number corresponds to the $s, p, d, f\ \cdots$** subshells.

For example:

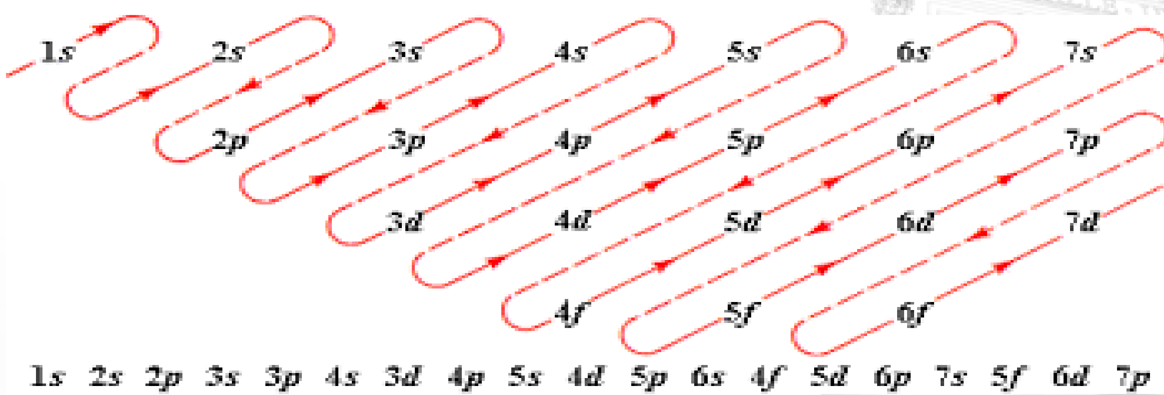
$$|100\rangle: 1s \quad |32,-1\rangle: 3d_{-1} \quad |410\rangle: 4p_0$$

* The factor of 2 takes into account the two spin states
** standing for sharp, principal, diffuse and fine

Energy Levels



A certain amount of degeneracy is however broken if electron-electron or magnetic interactions are taken into account. These interactions have r^s dependencies, and as seen in [hydrogen 5], expectation values $\langle r^s \rangle$ would have dependence on the quantum numbers n and l. As such $2s$ and a $2p$ state will no longer have the same energy level.



Diagonal Rule

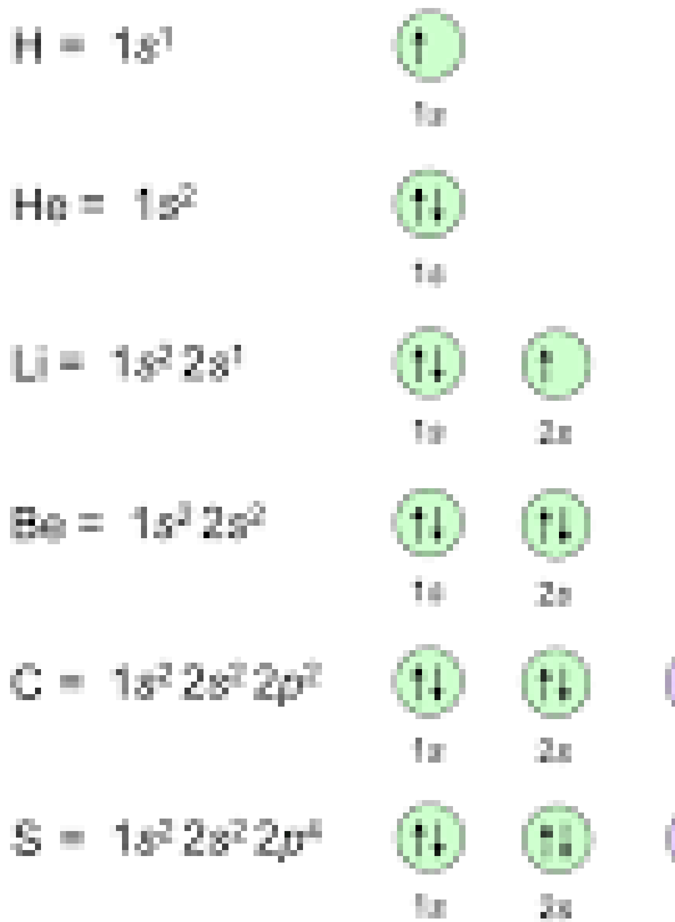
Because of the Pauli Exclusion Principle, electrons could occupy higher energy levels even if the atom is in the ground state. In this state, electrons will fill up the lower energy states first, following the sequence shown on the right.

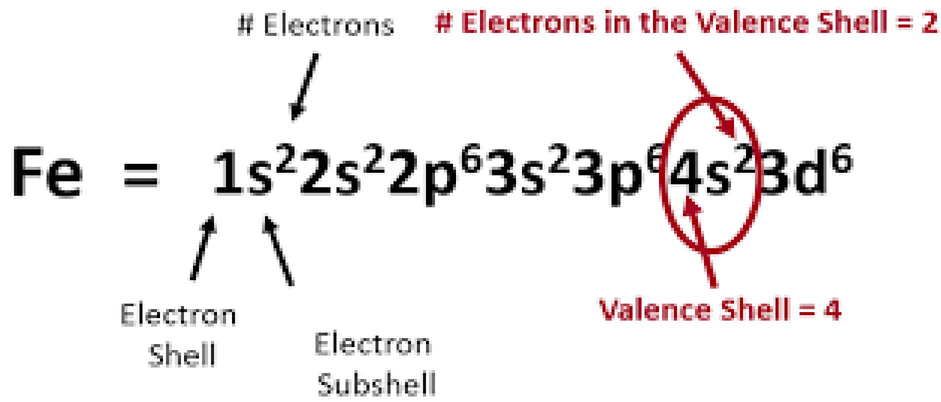
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$
$3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2$
$4f^{14}\ 5d^{10}\ 6p^6\ 7s^2\ 5f^{14}\ 6d^{10}\ 7p^6$

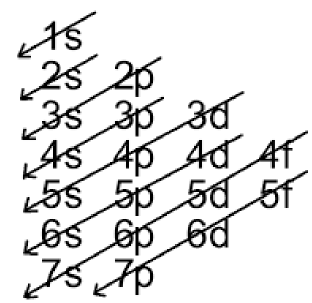
Diagonal Rule

For each angular momentum number, there remains a $2(2l+1)$ degeneracy, owing to the $(2l+1)$ magnetic state m and the two spin states. Thus an s subshell has 2 states, p has 6 states, d has 10 states, f has 14 states, and the g subshell has 18 states.

Electron Configuration



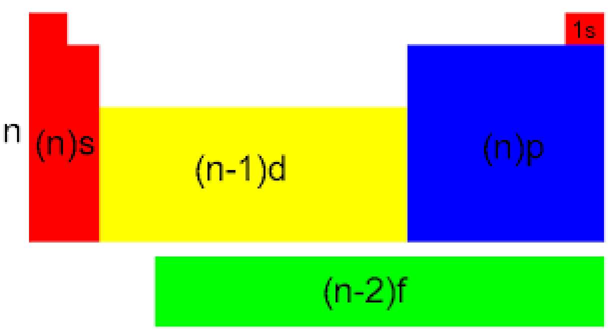




The Periodic Table

The electron configuration of atoms is the “prime mover” of the structure of the periodic table*, and is the primary reason why different atoms behave as they do.

* Except for Helium



ELECTRON CONFIGURATION CHART

s = 2 p = 6 d = 10 f = 14

1	$1s^1$																	$1s^2$
2	$2s^1$	$2s^2$											$2p^1$	$2p^2$	$2p^3$	$2p^4$	$2p^5$	$2p^6$
3	$3s^1$	$3s^2$											$3p^1$	$3p^2$	$3p^3$	$3p^4$	$3p^5$	$3p^6$
4	$4s^1$	$4s^2$	$3d^1$	$3d^2$	$3d^3$	$3d^5$	$3d^5$	$3d^6$	$3d^7$	$3d^8$	$3d^{10}$	$3d^{10}$	$4p^1$	$4p^2$	$4p^3$	$4p^4$	$4p^5$	$4p^6$
5	$5s^1$	$5s^2$	$4d^1$	$4d^2$	$4d^4$	$4d^5$	$4d^5$	$4d^7$	$4d^8$	$4d^{10}$	$4d^{10}$	$4d^{10}$	$5p^1$	$5p^2$	$5p^3$	$5p^4$	$5p^5$	$5p^6$
6	$6s^1$	$6s^2$		$5d^2$	$5d^3$	$5d^4$	$5d^5$	$5d^6$	$5d^7$	$5d^9$	$5d^{10}$	$5d^{10}$	$6p^1$	$6p^2$	$6p^3$	$6p^4$	$6p^5$	$6p^6$
7	$7s^1$	$7s^2$		$6d^2$	$6d^3$	$6d^4$	$6d^5$	$6d^6$	$6d^7$	$6d^8$	$6d^{10}$	$6d^{10}$	$7p^1$	$7p^2$	$7p^3$	$7p^4$	$7p^5$	$7p^6$

$5d^1$	$4f^1$	$4f^3$	$4f^4$	$4f^5$	$4f^6$	$4f^7$	$4f^7$	$4f^9$	$4f^{10}$	$4f^{11}$	$4f^{12}$	$4f^{13}$	$4f^{14}$	$4f^{14}$
$6d^1$	$6d^2$	$5f^2$	$5f^3$	$5f^4$	$5f^6$	$5f^7$	$5f^7$	$5f^9$	$5f^{10}$	$5f^{11}$	$5f^{12}$	$5f^{13}$	$5f^{14}$	$5f^{14}$