Many-Electron Atoms

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Contents

1 The Pauli Exclusion Principle

- An important rule proposed by Wolfgang Pauli (1925):
  - No two electrons in a single atom can have the same set of quantum numbers (n, l, m_l, m_s)
  - It applies to all "spin 1/2" particles (fermions)
- Examples:
  - Hydrogen: $1e^-$ in ground state: $\left(1, 0, 0, \pm\frac{1}{2}\right)$
  - Helium: $2e^-$: $\left(1, 0, 0, -\frac{1}{2}\right)$ and $\left(1, 0, 0, \frac{1}{2}\right)$
  - Lithium: $\left(1, 0, 0, -\frac{1}{2}\right)$, $\left(1, 0, 0, \frac{1}{2}\right)$, and $(2, l, m_l, m_s)$
    * If the electron has spin 1, this may be different:
    * Lithium: $(1, 0, 0, 1)$, $(1, 0, 0, \pm 1/0)$, and $(1, 0, 0, \pm 1/0)$
- Electron states in many-electron atoms
  - "Filling rule": e^-'s occupy the lowest levels first
  - Orbitals with the same n lie at about the same distance from the nucleus $\Longrightarrow$ $r_n = n^2 a_o$ (an atomic shell)

n	1	2	3	4	5
Shell	K	L	M	N	O

  - According to the Pauli Exclusion Principle, the maximum amount of electrons in each subshell is $2(2l + 1)$
  - Equivalent levels of d are much higher in energy levels because of the "electron screening effect"

2 Outer Electrons: Screening and Optical Transitions

- Screening Effect of Electron Levels
  - Lithium $(1s^2 2s^1)$
    * The ionization energy of Li is only 5.39[eV]
    * For the electron in the $2s$ shell, its ionization energy is 3.4[eV]
    * This is due to interactions between different shells
  - To an outer electron, the charge of the nucleus can be screened or shielded by the electrons in the inner shells — this is the screening effect

- The less penetrating the wave function, the more accurate the screening model is
- The parity of wave functions:

$$\begin{array}{ll} \text{Even:} & \psi(x) = \psi(-x) \\ \text{Odd:} & \psi(-x) = -\psi(x) \end{array}$$

The Selection Rule

- $\Delta l = l_2 - l_1 = \pm 1$
- This means, by optical transition, it is forbidden for an electron to make a transition to a different-numbered, but same-lettered subshell
  * For example, np to ns or vice versa is permitted for any values n