5.111 Lecture Summary #7

Readings for today: Section 1.10 (1.9 in 3rd ed) – Electron Spin, Section 1.11 (1.10 in 3rd ed) – The Electronic Structure of Hydrogen.

Read for Lecture #8: Section 1.12 (1.11 in 3rd ed) – Orbital Energies (of many-electron atoms), Section 1.13 (1.12 in 3rd ed) – The Building-Up Principle.

Topics:

I. RPD for s-orbitals (continued from Lecture #6)

II. p-orbitals
   A. The shape of p-orbitals
   B. Radial probability distributions

III. Electron spin and the fourth quantum number

IV. Wavefunctions for multielectron atoms

I. RADIAL PROBABILITY DISTRIBUTIONS (RPD) FOR S-ORBITALS

Radial Probability Distribution: The probability of finding an electron in a spherical shell of thickness dr at a distance r from the origin.

\[
\Psi^2 x 4\pi r^2 dr = \text{RPD}
\]

\[
\text{probability} \times \frac{4\pi r^2 dr}{\text{volume}} = \text{probability}
\]

Knowing only probability is one of main consequences of Quantum Mechanics. Unlike CM, QM is non-deterministic. The uncertainty principle forbids us from knowing r exactly.

\[
\Psi_{200} \quad (2s) \quad \Psi_{300} \quad (3s)
\]

II. P ORBITALS

- For any subshell of \( l = 1 \), there are three p-orbitals, _____, _____, and _____.
- \( m = \pm 1 \) states combine to give \( p_x \) and \( p_y \) orbitals. \( m = 0 \) is called the \( p_z \) orbital.
A. THE SHAPE OF P-ORBITALS

- Unlike s orbitals, p-orbitals have θ, φ dependence. P-orbitals ______________ spherically symmetrical.
- p orbitals consist of two lobes (of opposite sign) separated by a ___________ plane on which \( \Psi = 0 \) (and \( \Psi^2 = 0 \)).
- There is zero probability of finding a p-electron in a nodal plane. Thus, there is ________ probability of finding a p-electron at the nucleus.

Probability density maps of p orbitals:

\[ \Psi_{2p_x}^2 \]
\[ \Psi_{2p_y}^2 \]
\[ \Psi_{2p_z}^2 \]

HIGHEST PROB Along _________ Along _____ axis Along ____ axis

POSITIVE \( \Psi \) where z is _________ where x is positive where y is positive

NODAL PLANE \( \theta = 90^\circ \) _______ plane \( \phi = 90^\circ \) _______ plane \( \phi = 0^\circ \)

Nodal planes (planes that have no electron density) arise from angular nodes in the wavefunction.

- Angular nodes: values of ______ or ______ at which \( \Psi \) (and \( \Psi^2 \)) = 0.
- Recall from Lecture #6: Radial nodes are values of r at which \( \Psi \) (and \( \Psi^2 \)) = 0.

In general, an orbital has:

- \( n - 1 \) total nodes
- _________ angular nodes
- _________ radial nodes

For 2s: _________ = ___ total nodes For 2p: _________ = ___ total nodes
- _________ = ___ angular nodes
- _________ = ___ angular nodes
B. RADIAL PROBABILITY DISTRIBUTIONS

Interpreting RPD plots

- As \( n \) increases (from 1 to 2 to 3), the orbital \( r_{mp} \) “size” ________.

- As \( l \) increases (from \( s \) to \( p \) to \( d \)) for a given \( n \), the orbital \( r_{mp} \) “size” ________.

- Only electrons in \( s \) states have a substantial probability of being very close to nucleus. This means that although the “size” of \( s \) orbitals is larger than \( p \) or \( d \) orbitals, \( s \)-electrons are the ________ shielded.

III. ELECTRON SPIN AND THE FOURTH QUANTUM NUMBER

From quantum mechanics, a fourth quantum number appears that describes the spin of an electron within an orbital.

Spin magnetic quantum number, ______
There is no classical analogy to spin.

- An electron can have two spin states:
  \[ m_s = \_\_\_\_\_\_ (\text{spin up}) \quad \text{or} \quad m_s = \_\_\_\_\_\_ (\text{spin down}). \]

- Similar to the angular momentum quantum number, \( l \), \( m_s \) describes the magnitude of an angular momentum. However, \( m_s \) completes the description of an ____________ and is NOT dependent on the orbital.

The property of electron spin was first proposed by S. Goudsmit and G. Uhlenbeck in 1925 to explain tiny deviations from the expected frequencies of spectral lines:

\[
\begin{array}{cc}
\text{expected } \nu & \text{observed } \nu \\
\end{array}
\]

So we can describe a given orbital using three quantum numbers \((n, l, m_l)\) and a given electron using 4 quantum numbers \((n, l, m_l, m_s)\).

\[
\begin{array}{cc}
\Psi_{n/l/m_l} & \Psi_{n/l/m_l/m_s} \\
\text{describes an } & \text{describes an } \\
\end{array}
\]

**PAULI EXCLUSION PRINCIPLE**

No two electrons in the same atom can have the same four quantum numbers. In other words, no two electrons can be in the same orbital and have the same spin.

The Pauli exclusion principle limits an atom to _______ electrons per orbital.

ie. How many *electrons* in a single atom can have the following two quantum numbers: \( n = 4 \) and \( m_l = -2 \)? _______