Lesson Overview
Quantum Mechanics

Objective: The student will be able to define the wave nature of matter and how this definition lead to the location of electrons in an electronic cloud.

Lesson Outline:

I. The Wave Behavior of Matter
II. Quantum Mechanics & Atomic Orbitals
III. Representations of Orbitals
IV. Quantum Numbers

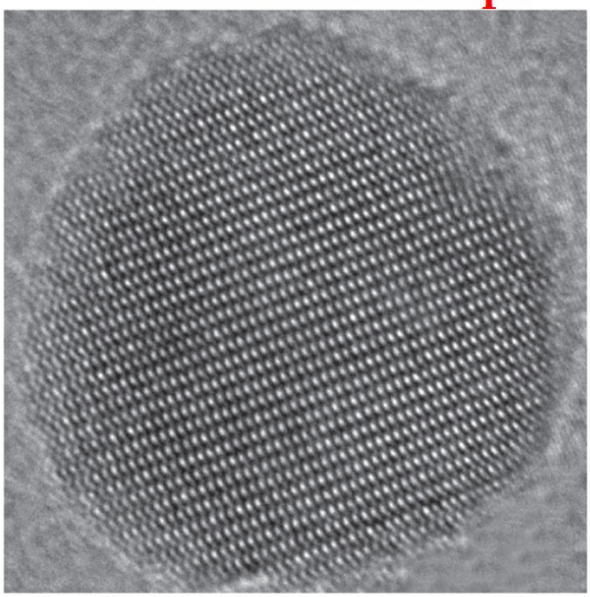
The Wave Behavior of Matter

Louis de Broglie: Wave-Particle Duality

$$\lambda = \frac{h}{mv}$$

His ideas were confirmed a dew years later with experiments in X-ray diffraction.

Electron Microscope



The Heisenberg Uncertainty Principle

The dual nature of matter places a fundamental limitation on how precisely one can know the location and momentum simultaneously.

$$\Delta x \cdot \Delta m \geq \frac{h}{4\pi}$$

Only important when we look at incredibly small matter (subatomic level)

Uncertainty Principle Illustration

Calculate the uncertainty in the position, given the following:

$$\Delta x \cdot \Delta m \geq \frac{h}{4\pi}$$

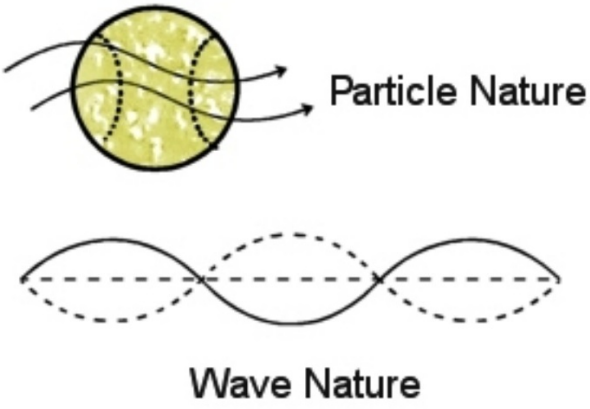
mass of e^-: 9.11×10^{-31} kg

avg. speed of e^- in H atom: 5×10^6 m/s (with 1% uncertainty)

Significance of de Broglie & Heisenberg

"De Broglie's hypothesis and Heisenberg's uncertainty principle set the stage for a new and more broadly applicable theory of atomic structure."

- Brown, Lemay, Bursten (12 edition)

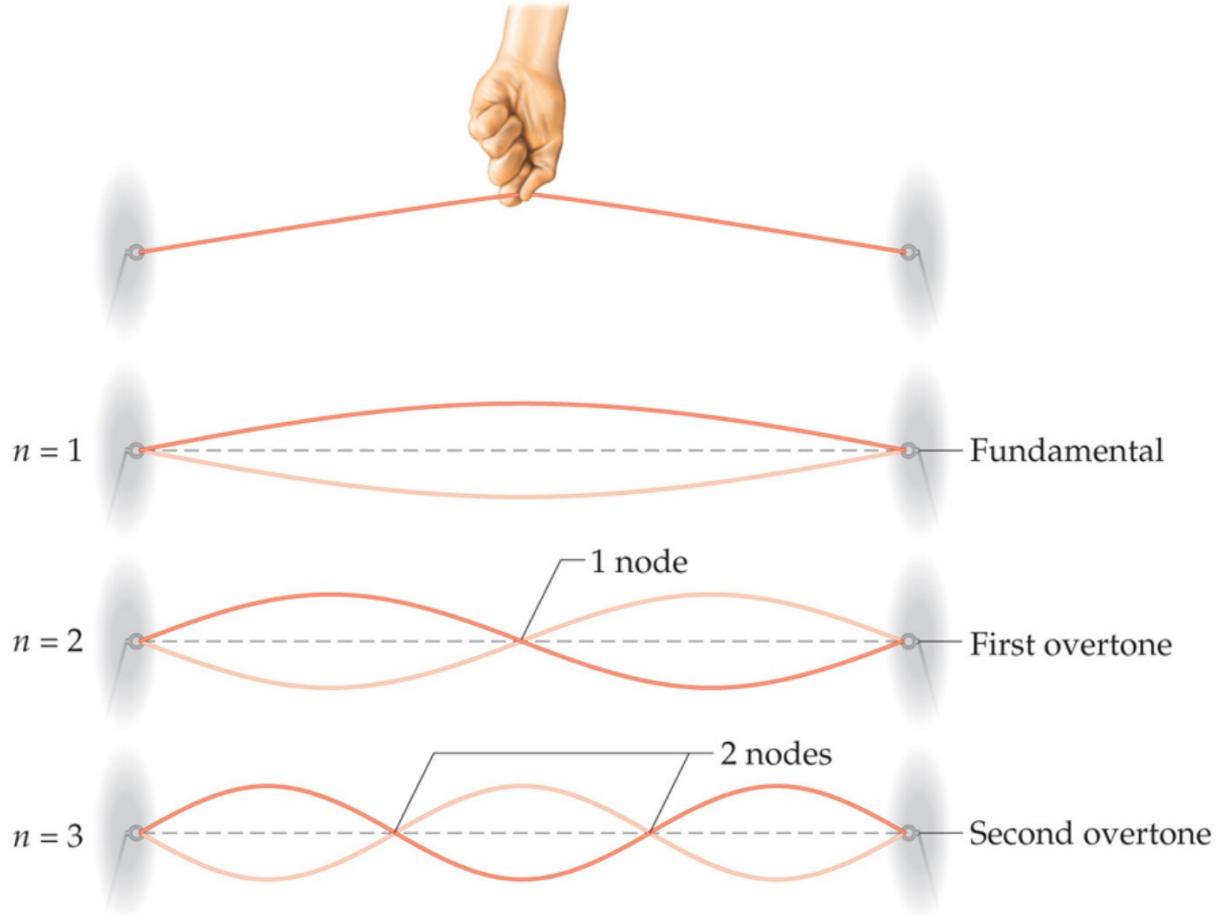


Quantum Mechanics & Atomic Orbitals

- Schrödinger and Equation

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{\delta^2\Psi}{\delta y^2} + \frac{\delta^2\Psi}{\delta z^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

- **incorporates both the wave-like and particle-like behaviors of the electron.**
- **treated the electron in Hydrogen as a plucked guitar string.**

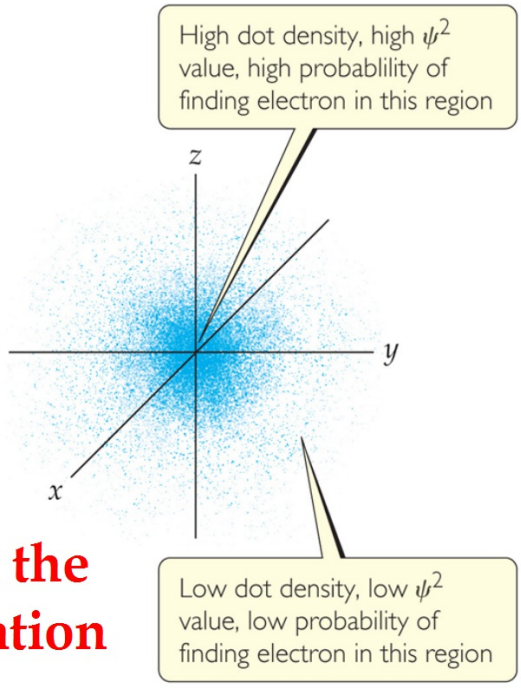


An electron is like a plucked guitar string.

The Schrödinger Equation

Solving the equation leads to a series of mathematical functions called wave functions that describe the electron in the atom.

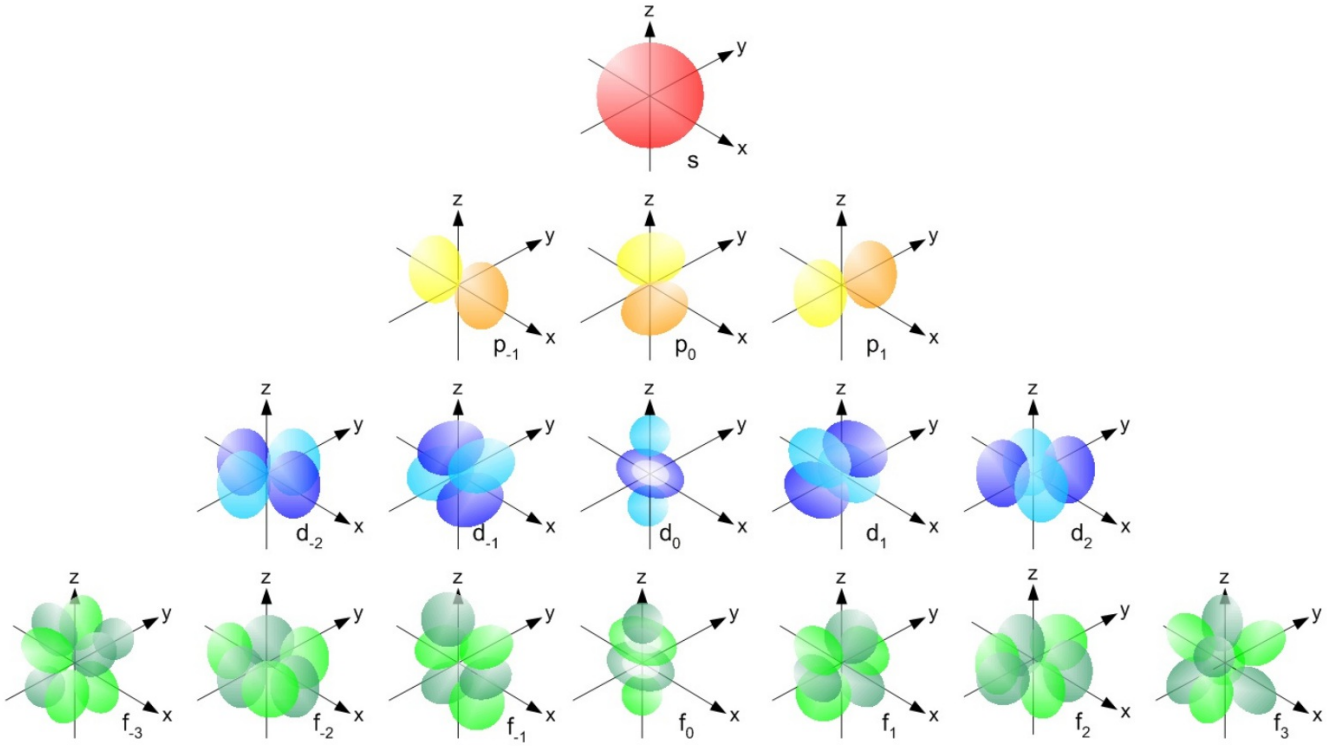
The actual solution of the value ψ has no significance, it is the square of the wave function, ψ^2, that has meaning.



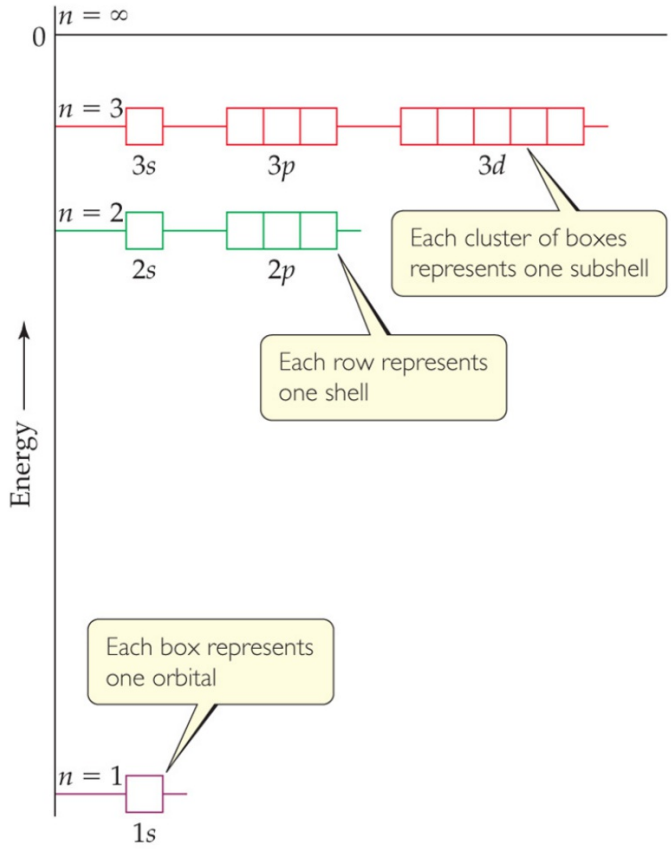
ψ^2 represents the probability that the electron will be found in that location

Orbitals and their Shapes

The solution to Schrödinger's equation for the hydrogen atom yields a set of wave functions called orbitals.



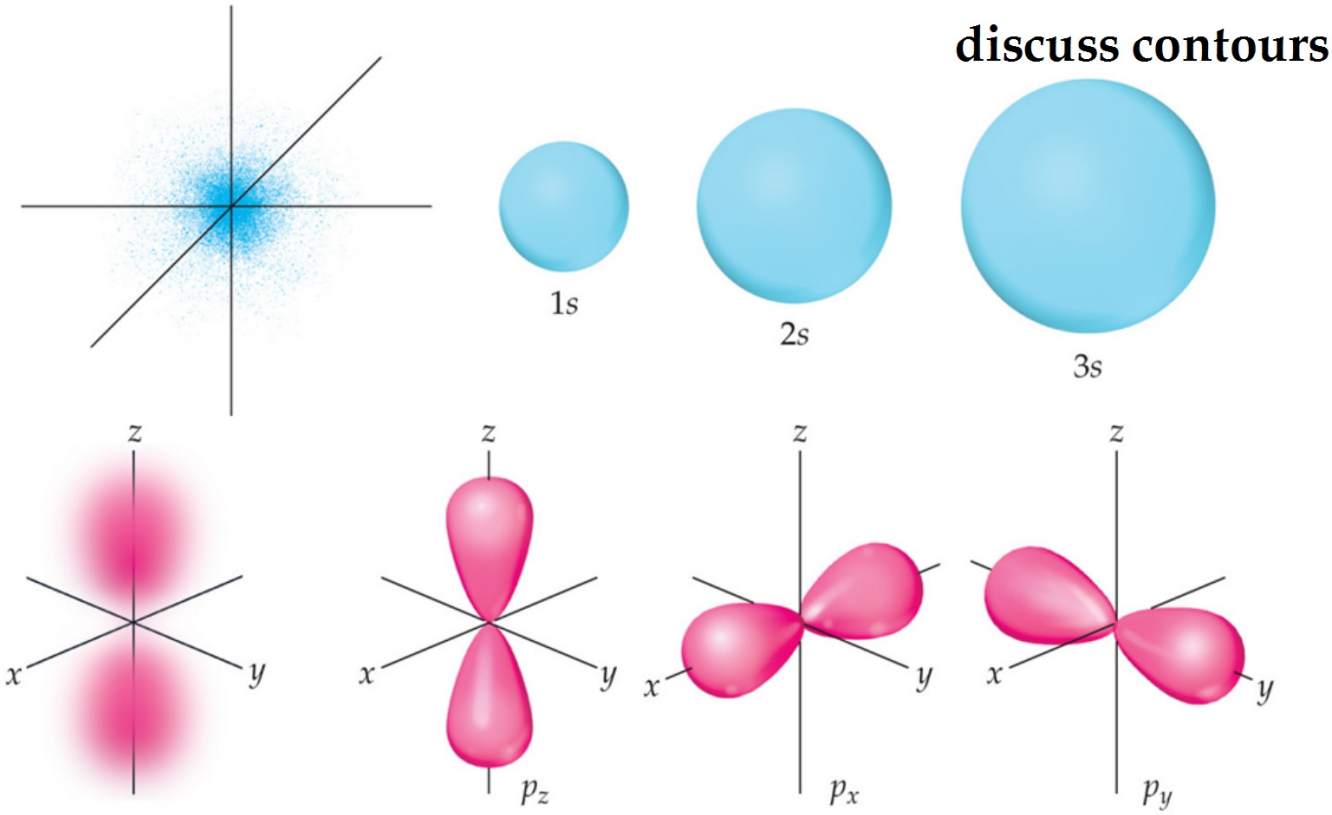
Orbital Diagrams



$n = 1$ shell has one orbital
$n = 2$ shell has two subshells composed of four orbitals
$n = 3$ shell has three subshells composed of nine orbitals

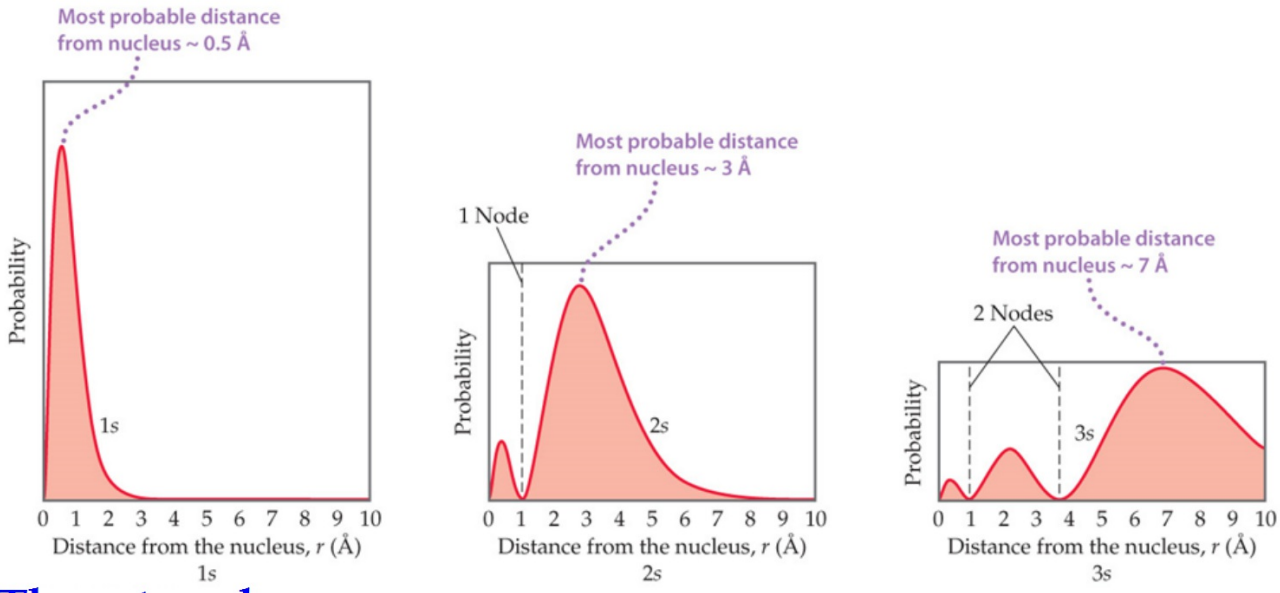
Representations of Orbitals

discuss contours



How do these orbitals change based on the energy level?

Radial Probability (function) Density

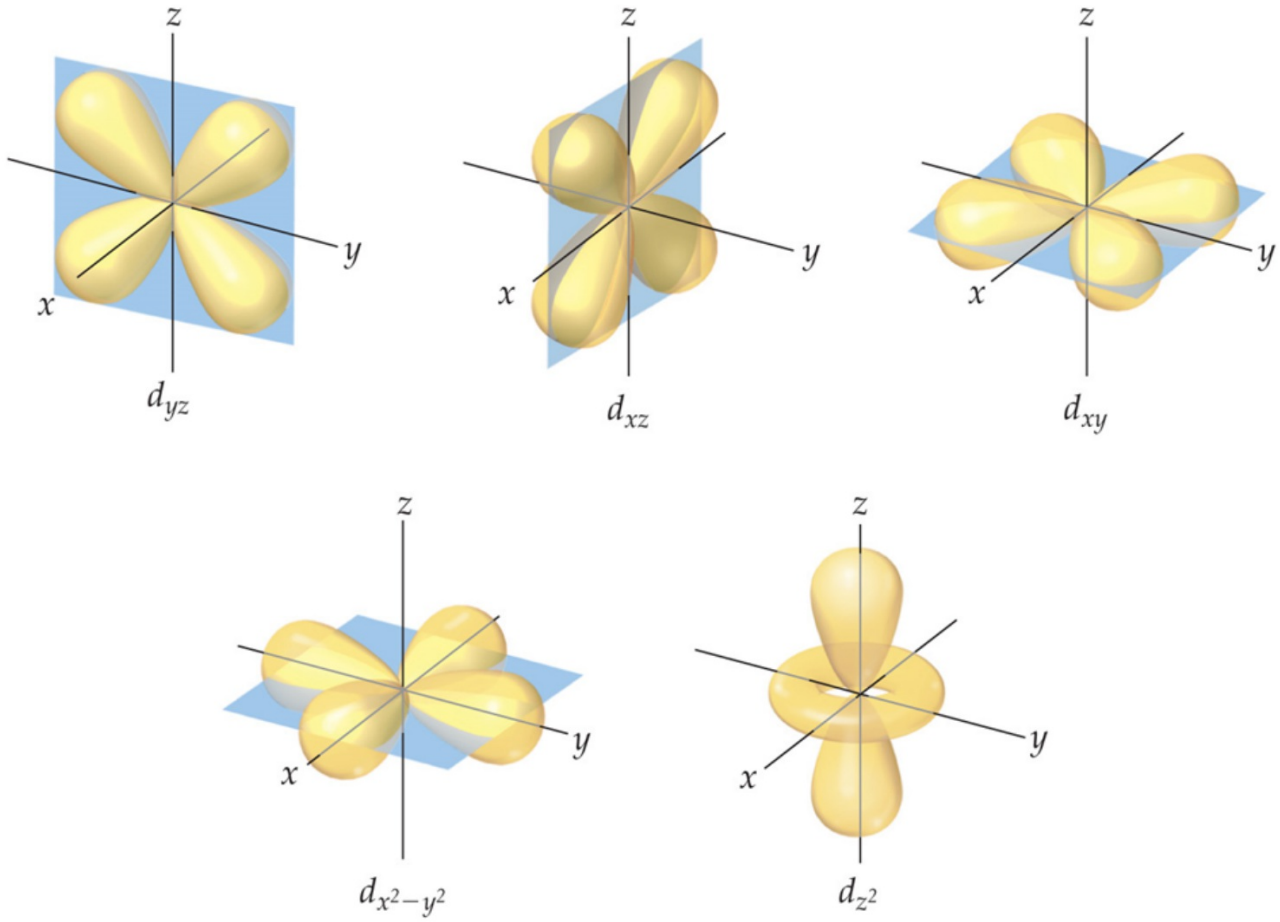


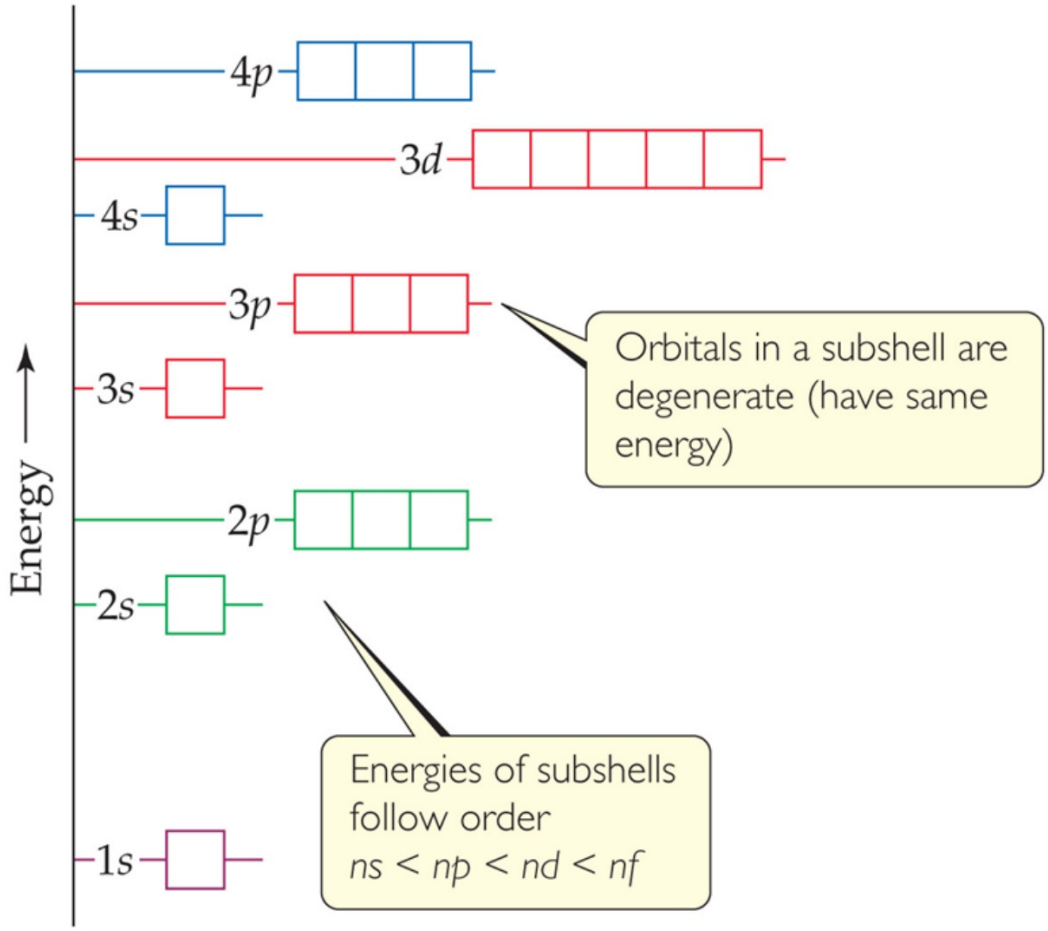
Three trends:

1. The # of peaks increases with increasing "n", the outermost peak being larger than the inner ones.

2. The # of nodes increases with increasing "n".

3. The electron density becomes more spread out with increasing "n".


z
y
x
d_{yz}
z
y
x
d_{xz}
z
y
x
d_{xy}
z
y
x
$d_{x^2-y^2}$
z
y
x
d_{z^2}

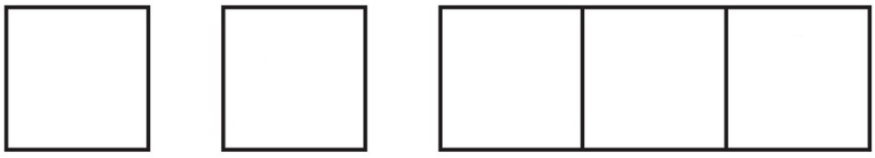

4p
3d
4s
3p
3s
2p
2s
1s
Energy
Orbitals in a subshell are degenerate (have same energy)
Energies of subshells follow order
ns < np < nd < nf

Rules for Filling Orbital Diagrams

Aufbau Principal: Electrons occupy the **lowest energy level** possible (are as close to the nucleus as possible)

Hund's Rule: Electrons will occupy each orbital with the same spin (direction) before occupying an orbital with the opposite spin (direction)

Pauli Exclusion Principal: No two electrons can have the same quantum number. (They must be traveling in opposite directions if they are in the same orbital.



1*s* 2*s* 2*p*

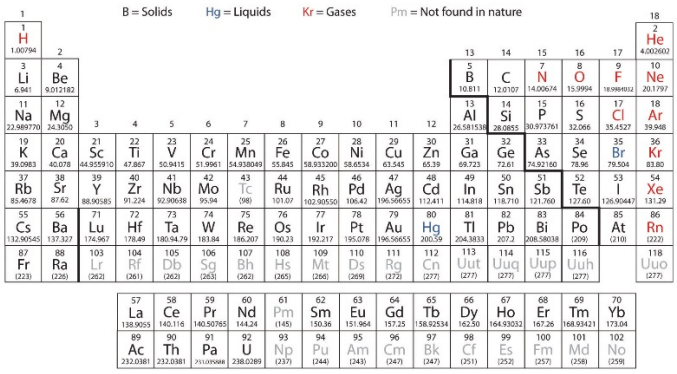
Quantum Numbers

Summary of Quantum Numbers of Electrons in Atoms

Name	Symbol	Permitted Values	Property
principal	n	positive integers(1,2,3,…)	orbital energy (size)
angular momentum	l	integers from 0 to n-1	orbital shape (The l values 0, 1, 2, and 3 correspond to s, p, d, and f orbitals, respectively.)
magnetic	m_l	integers from $-l$ to 0 to $+l$	orbital orientation
spin	m_s	+1/2 or -1/2	direction of e^- spin

Example 1

What is the set of quantum numbers for the last electron in a neutral carbon atom?



Example 2

What is the set of quantum numbers for the last electron in arsenic?

Note: save time. Only draw the sublevel where the electron exists.