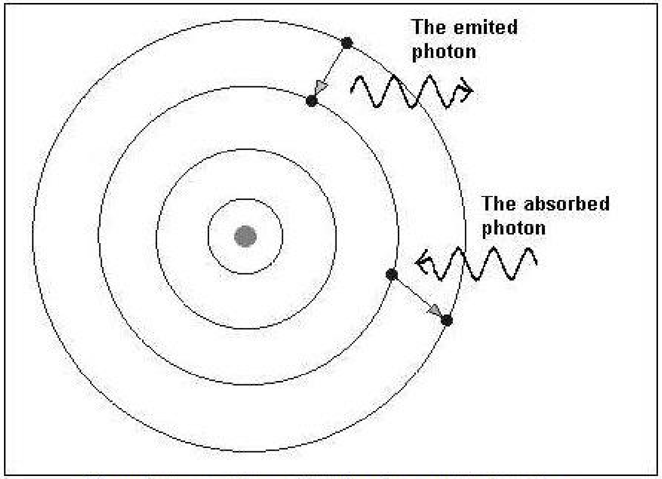
UNIT 1: STRUCTURE AND PROPERTIES

QUANTUM MECHANICS

Development of the Modern Atomic Theory

Problems with the Bohr Model

- Bohr's theory only fit the observed spectra of hydrogen.
- In addition, the Bohr model could not explain WHY these fixed orbits or energy levels even existed!



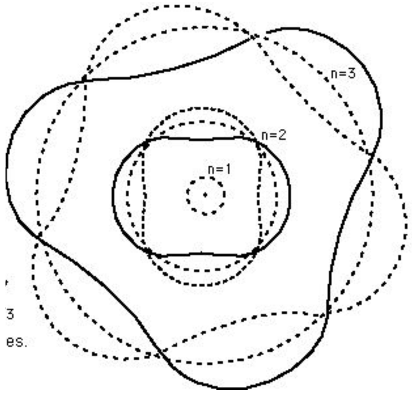
The electron emits or absorbs the energy changing the orbits.

???

de Broglie Waves

- Louis de Broglie (1923) proposed that the dual wave-particle properties of light may also apply to matter.
- Proposed that electrons exist as "matter waves" around the nucleus, with only complete integer values of the electron wavelength permitted.
- This number was the the principal quantum number (***n***).

View this animation to see the connection between electron orbits and their wavelength.



Video: Quantum Model of the Atom

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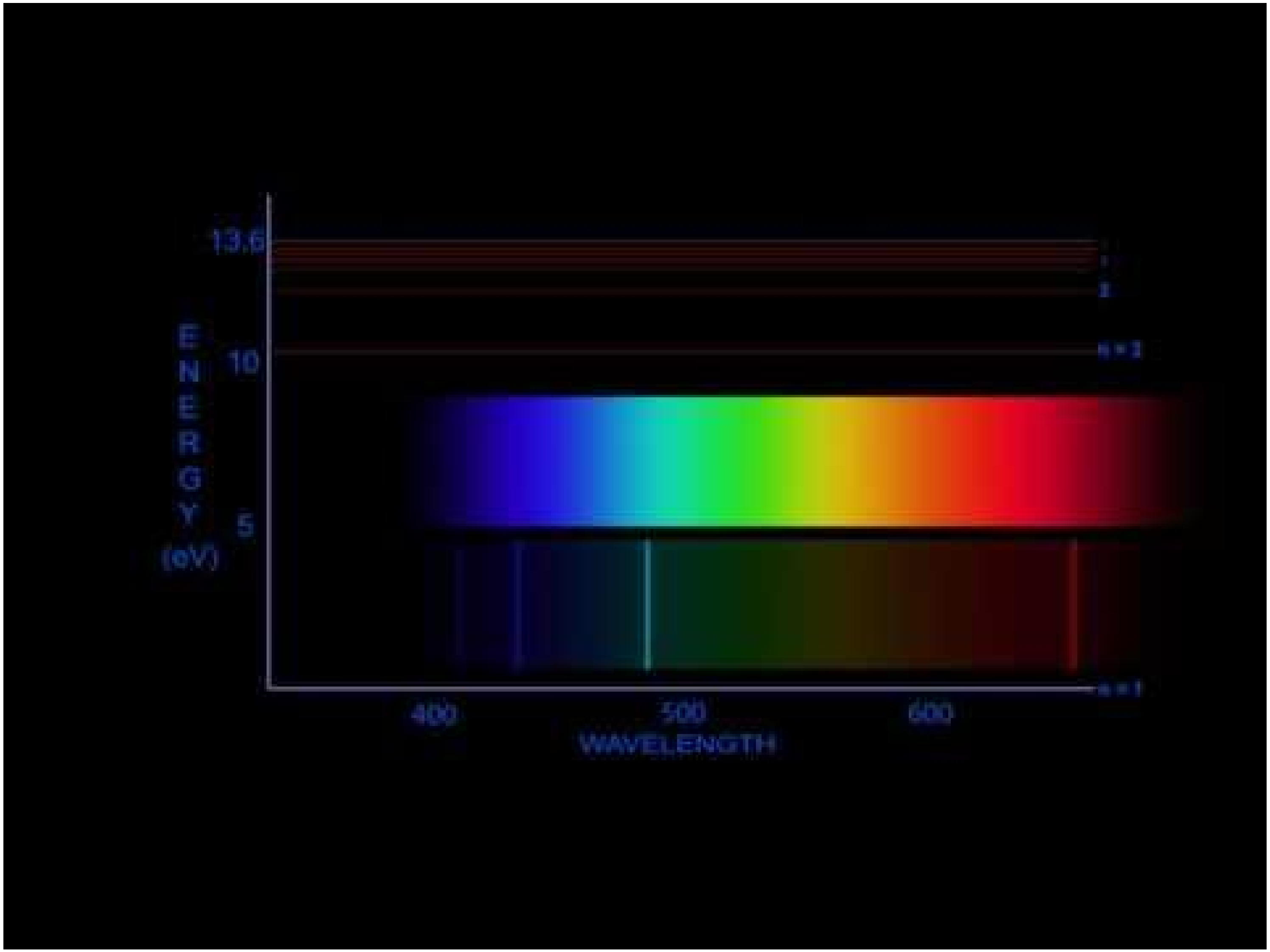


Wave-Mechanical Model of the Atom

- Since the wavelength of an electron must be a whole number, only certain quantized energies are allowed.
- Erwin Schrodinger developed the wave-mechanical equation (1925):

$$\left(\frac{\partial^2 \Psi}{\partial x^2}\right) + \frac{8\pi^2 m}{h^2}(E - V)\Psi(x) = 0$$

- δ = derivative
- Ψ = wave function
- *x* = position in 1 dimension

h = Plank's constant
E = total energy
V = potential energy

Schrodinger's Equations

- This equation describes the energy and position of an electron around the hydrogen atom in 1 dimension (*x*).
- Schrodinger's equation can be solved to obtain wave functions (Ψ) which describe the location in space (*x*, *y*, *z*) where an electron is likely to be found.
- These regions are known as **orbitals**.

Video: Development of Schrodinger's Equations

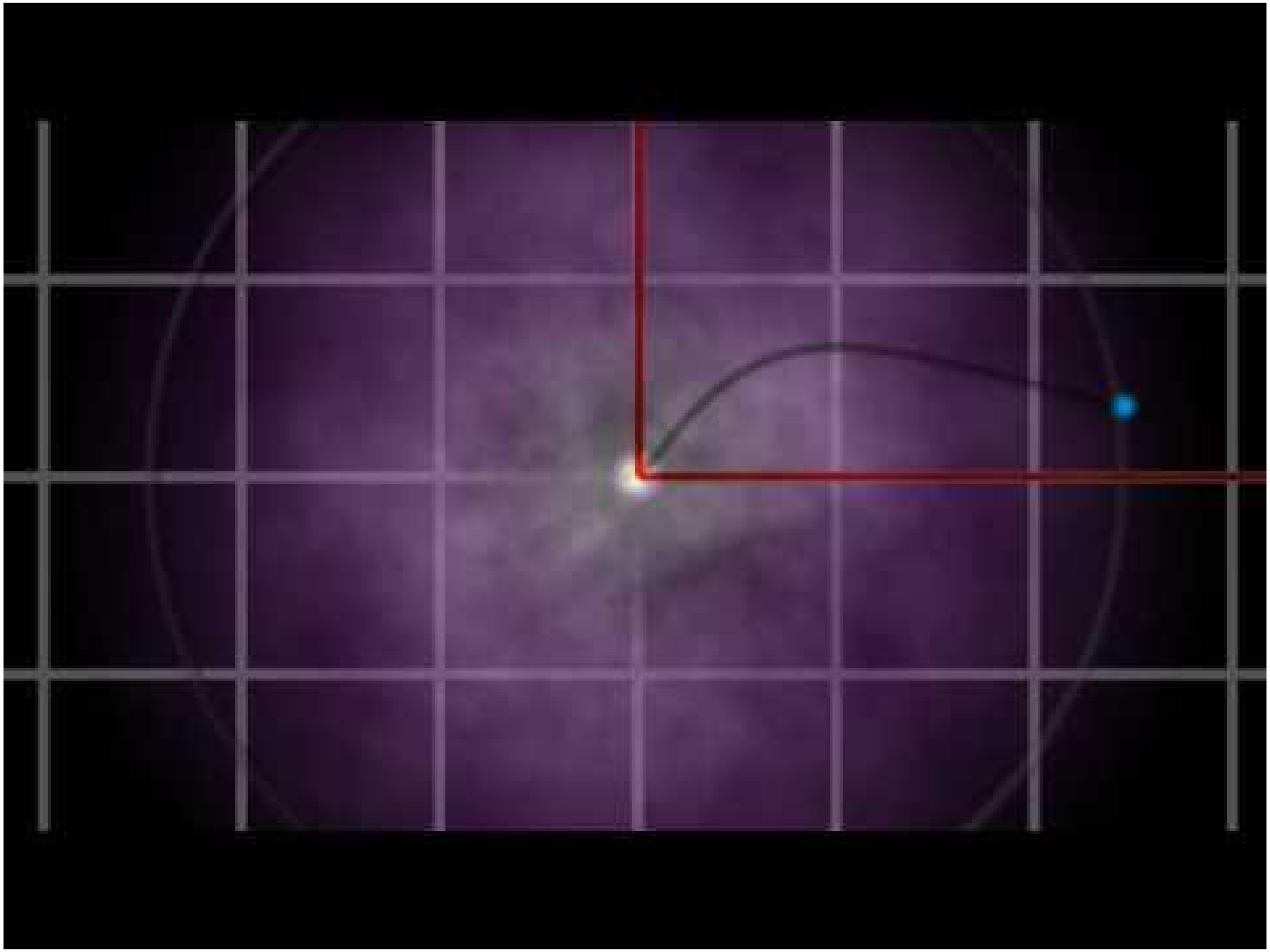
Development of Schrodinger's Equations

The Uncertainty Principle

- Werner Heisenberg (1927) proposed that it is impossible to simultaneously determine the exact position and velocity (energy) of a single subatomic particle.
- Schrodinger's wave functions actually describe probability distributions for where an electron ***may*** be found.
- It is impossible to know everything about a system at the quantum scale; this is not a failure of our ability to measure a system precisely enough (the classical view) but rather is a property of microscopic particles such as electrons and protons.

Video: The Uncertainty Principle

Video: The Uncertainty Principle



Quantum Weirdness

- Matter at the quantum scale of the atom has no reasonable analogy in our world.
- Dr. Quantum's Double Slit Experiment
- Quantum Entanglement

Thoughts on Quantum Theory

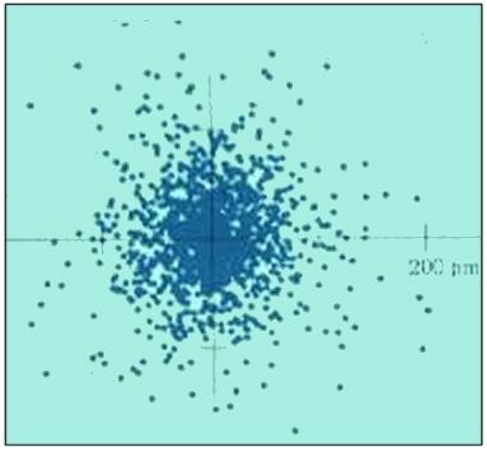
- "[T]he atoms or elementary particles themselves are not real; they form a world of potentialities or possibilities rather than one of things or facts.“ *Werner Heisenberg*

- Anyone not shocked by quantum mechanics has not yet understood it.“ *Neils Bohr*

- [I can't accept quantum mechanics because] "I like to think the moon is there even if I am not looking at it." *Albert Einstein*

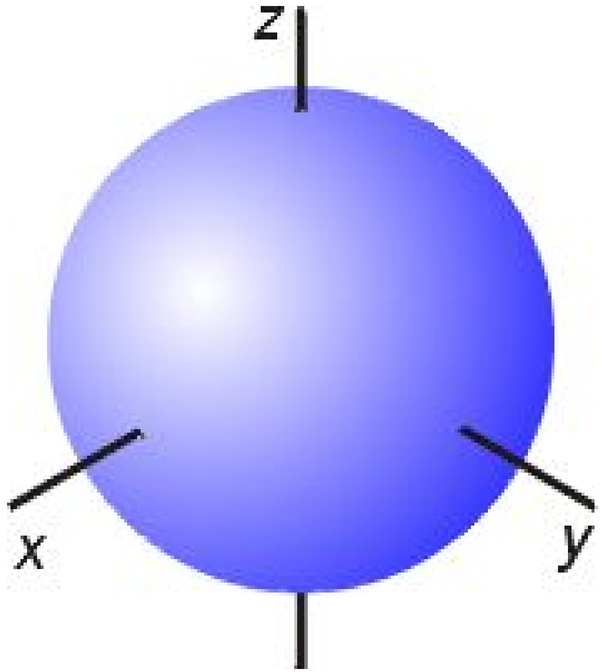
Orbitals

- At each energy level, ***n***, there is a probability distribution for where an electron may be found. These probability distributions are known as **orbitals**.

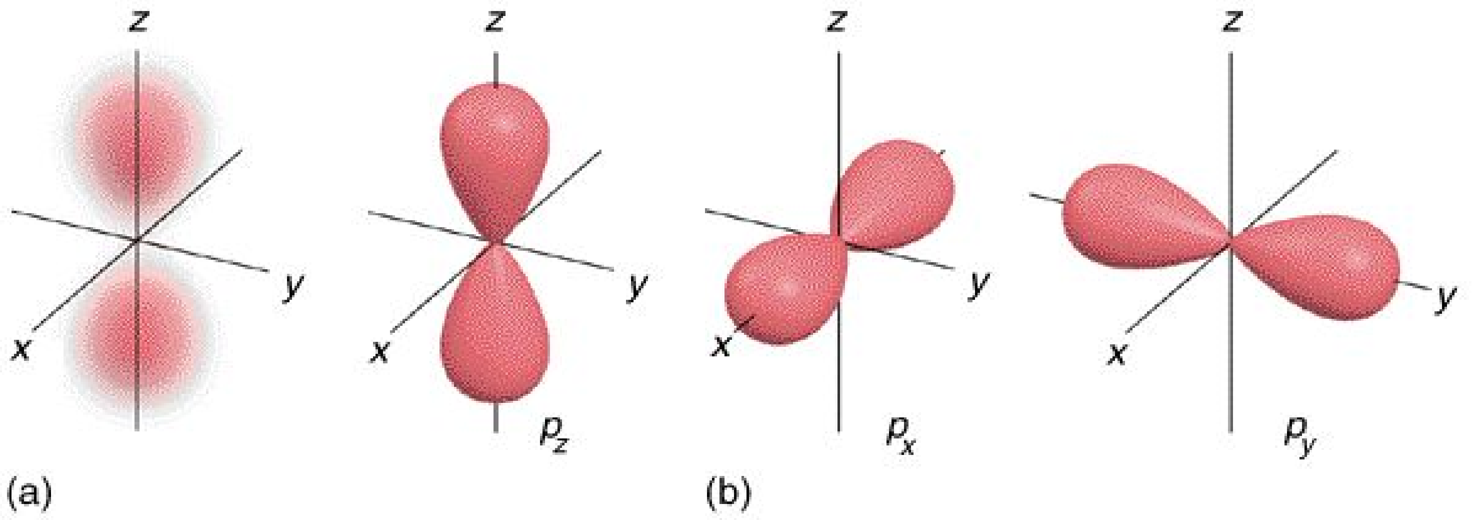


- Each orbital can contain only **2** electrons.
- Orbitals have various 3-D shapes denoted by the letters ***s*** (1 type). ***p*** (3 types), ***d*** (5 types) and ***f*** (7 types).

s orbital

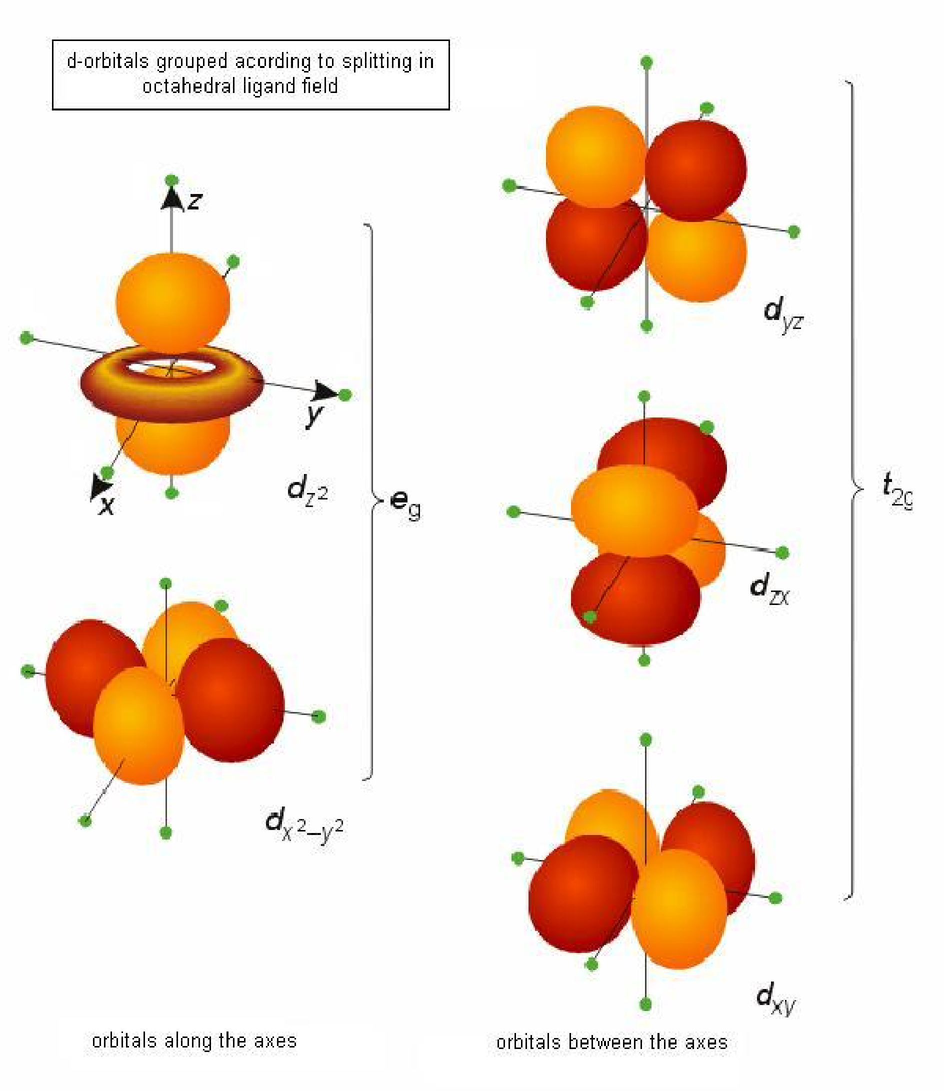


p orbitals



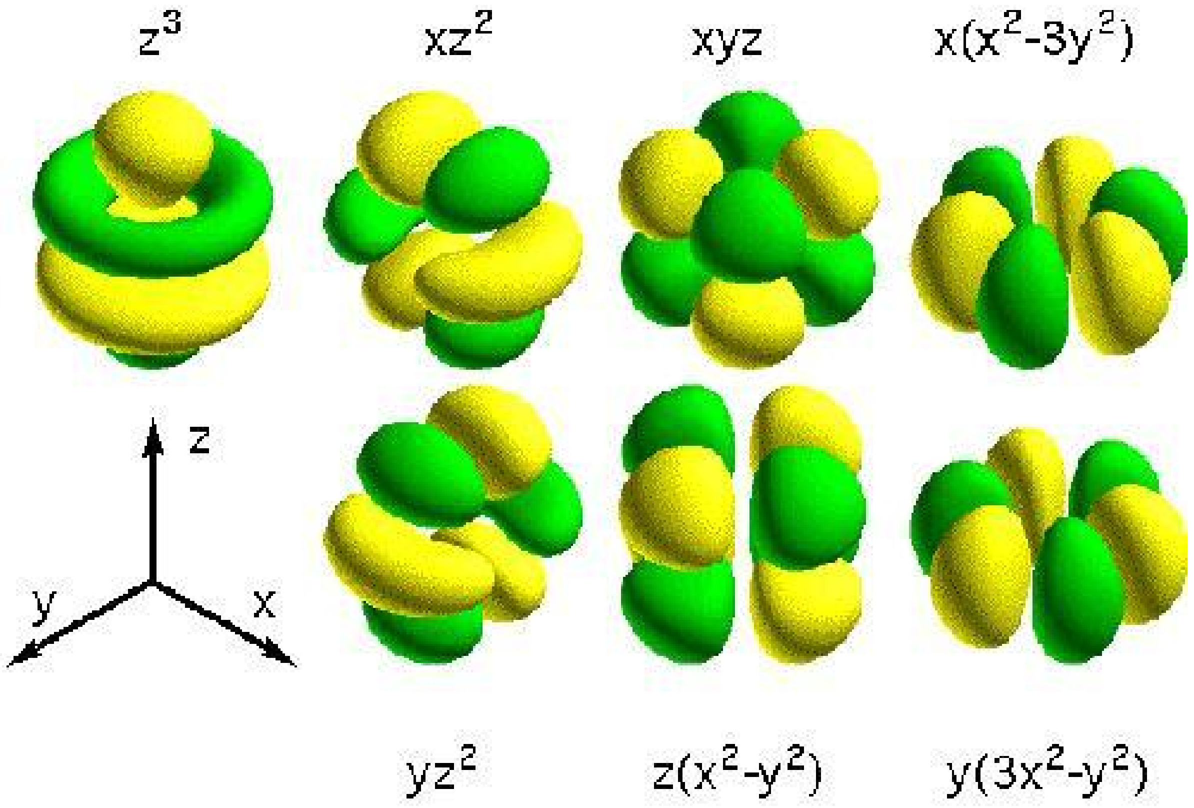
- View what a full set of orbitals look like.

d orbitals



d-orbitals grouped acording to splitting in octahedral ligand field
z
y
x
d_{z^2}
$d_{x^2-y^2}$
e_g
d_{yz}
d_{zx}
d_{xy}
t_{2g}
orbitals along the axes
orbitals between the axes

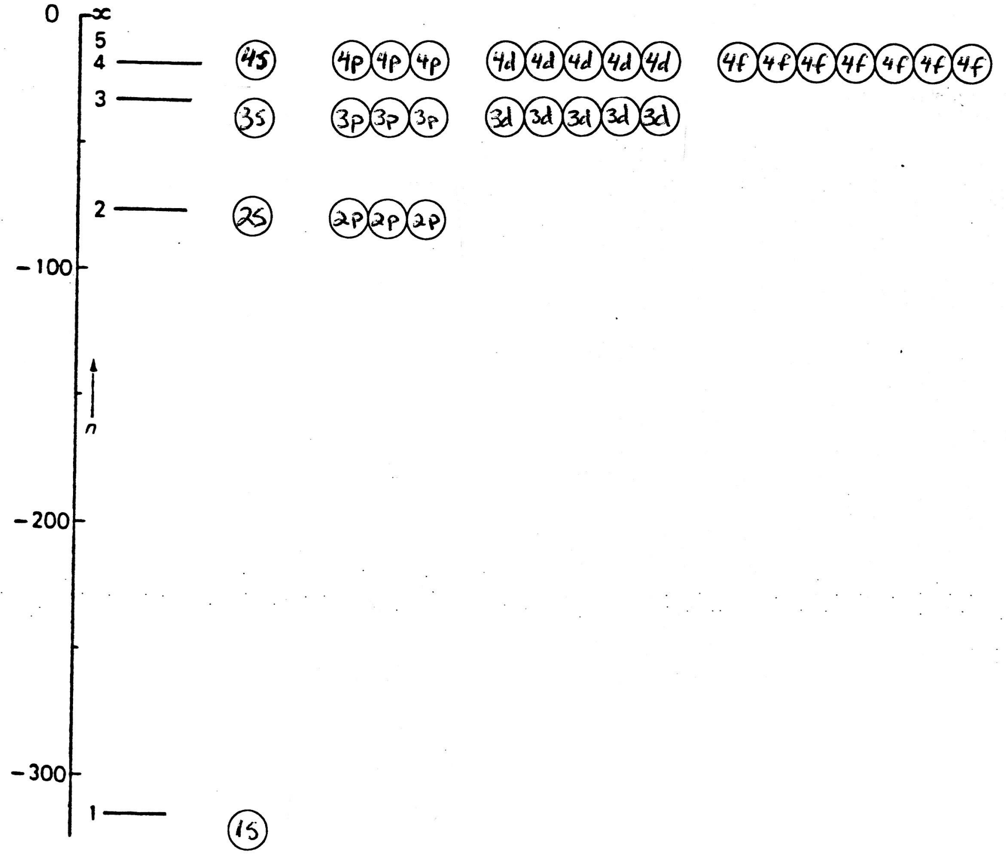
f orbitals



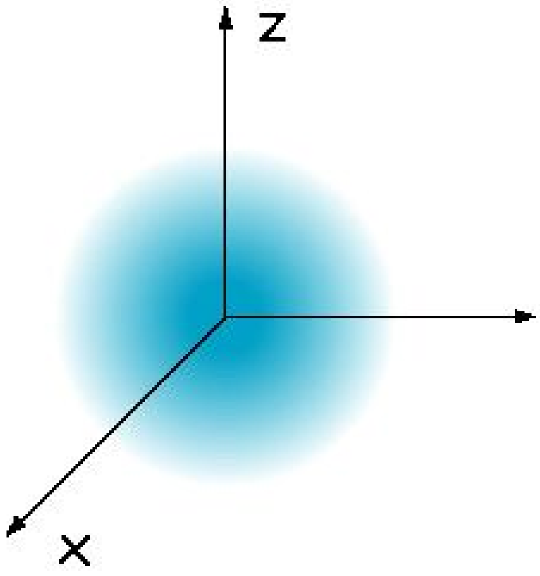
[The Grand Table of Orbitals]

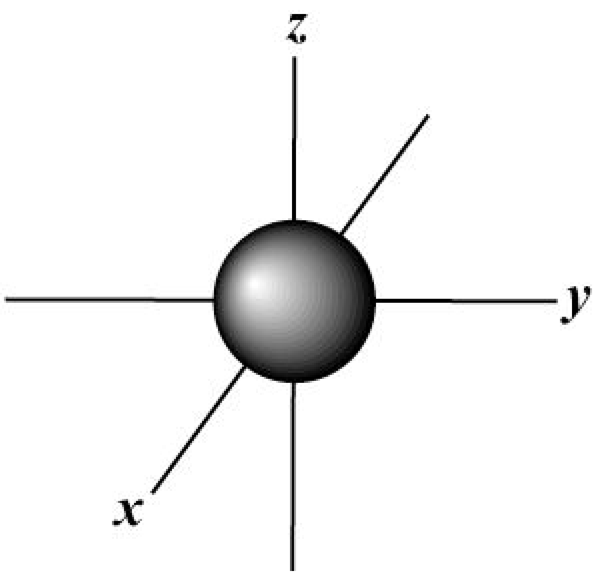
Hydrogen's Orbitals

- The first 4 energy levels of hydrogen contain the following orbitals:



- For hydrogen, the ***ground state*** is ***n*=1** or the first (*1s*) orbital. The "distance" of an electron from the nucleus can only be predicted from the radial probability distribution. In 3 dimensions, the 1s orbital can be imagined as a spherical "cloud" of electrons around the nucleus:





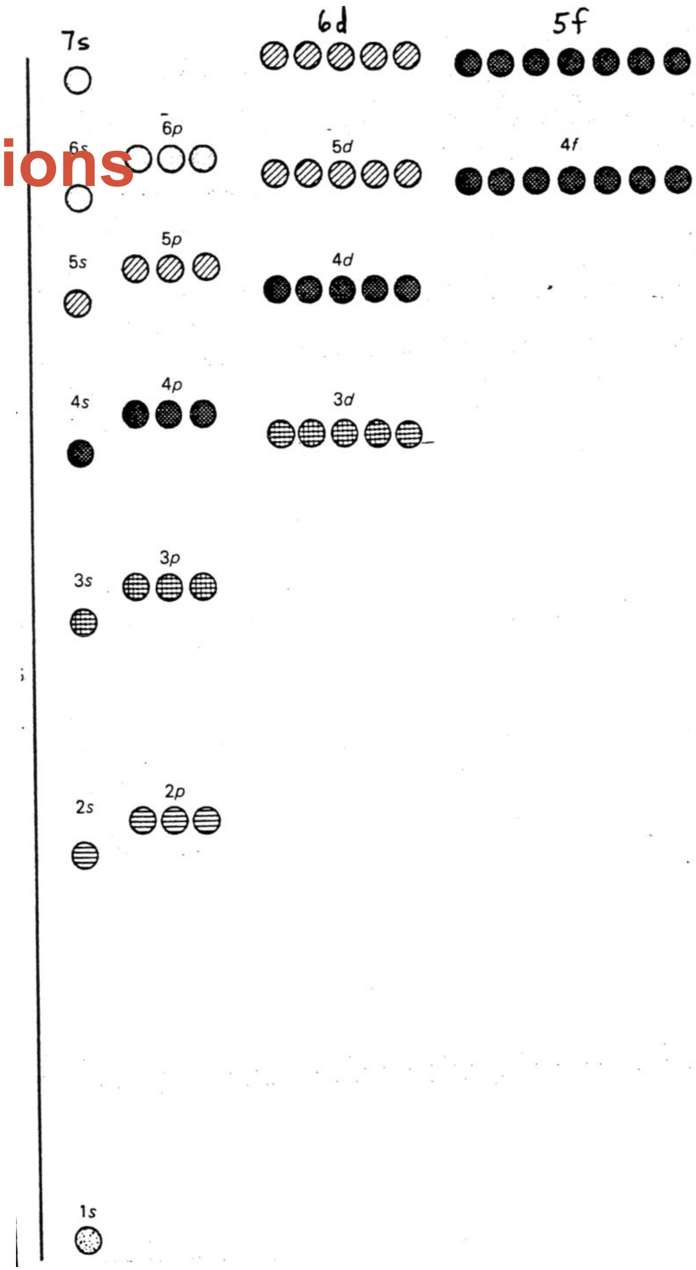
Multi-Electron Atoms and Ions

- With atoms and ions with more than 1 electron, factors such as electron-electron repulsion cause the energy level diagram to be modified.

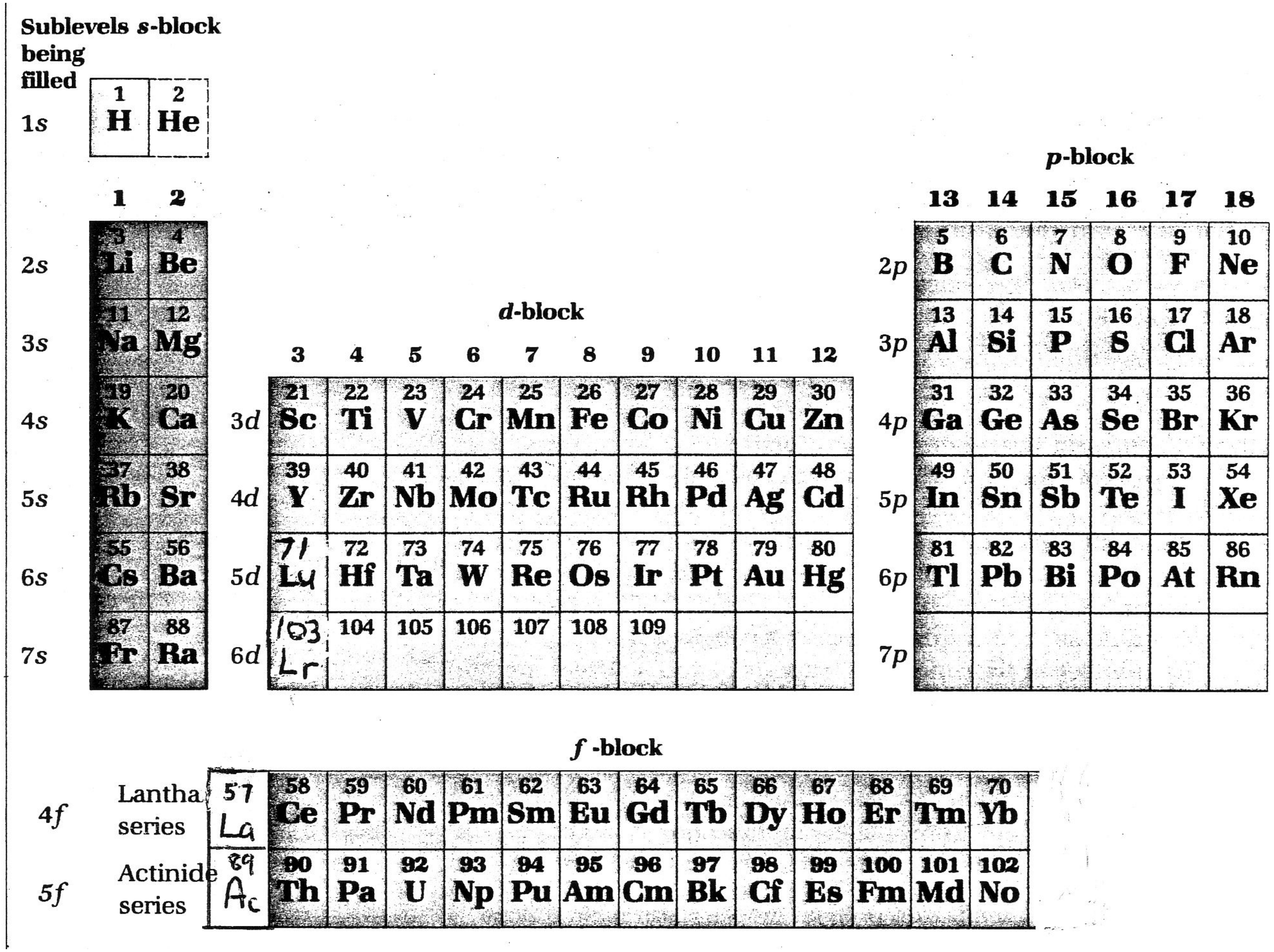
- An energy level diagram shows relative energies of the various orbitals and can be used for dealing with all atoms of the periodic table.

Rules for Writing Energy Level Diagrams & Electron Configurations

- 1. <u>Aufbau Principle</u>: Electrons are added to the lowest energy orbitals that are available
- 2. A maximum of 2 electrons can occupy a single orbital.
- 3. <u>Hund's Rule</u>: Due to electron repulsion, all orbitals of equal energy acquire one electron before any orbital accepts two electrons.
- 4. <u>Pauli Exclusion Principle</u>: Electrons in the same orbital have the opposite spin (up or down).



Writing Electron Configuration Using the Periodic Table



Writing Energy Level Diagrams

1. Write the energy level diagrams for the following atoms:
   a) beryllium
   b) carbon
   c) oxygen
   d) chromium
   e) gold

Writing Electron Configurations

1. Write the ground state electron configurations for the following atoms (the same atoms from the last slide):
   a) beryllium
   b) carbon
   c) oxygen
   d) chromium
   e) gold

2. Write the short form electron configuration for these atoms.

Writing Electron Configurations of Ions

1. Write the ground state electron configurations or energy level diagrams for the following atoms and their ions:

   a) fluorine, F; fluoride ion F^-

   b) sodium, Na; sodium ion, Na^+

   c) iron, Fe; iron(II), Fe^{2+}; iron(III), Fe^{3+}

Practice:

Complete:

Q. 1 – 9 of the worksheet "SP02: The Quantum Mechanical Model of the Atom", and

Q. 1, 2, 7-9 of the worksheet "SP03: Quantum Numbers and Energy Level Diagrams."