

Atomic Structure and Periodicity

Wave Partilce Duality

** Not Part of class**

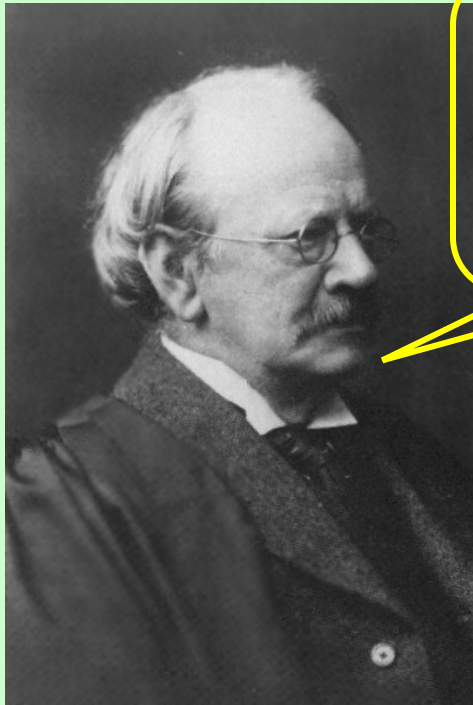
The Puzzle of the Atom

- ❖ Protons and electrons are attracted to each other because of opposite charges
- ❖ Electrically charged particles moving in a curved path give off energy
- ❖ Despite these facts, atoms don't collapse

Wave-Particle Duality

JJ Thomson won the Nobel prize for describing the electron as a particle.

His son, George Thomson won the Nobel prize for describing the wave-like nature of the electron.



The
electron is
a particle!

The
electron is
an energy
wave!



Confused??? You've Got Company!



"No familiar conceptions can be woven around the electron; something unknown is doing we don't know what."

Physicist Sir Arthur Eddington

The Nature of the Physical World

1934

The Wave-like Electron



Louis deBroglie

The electron propagates through space as an energy wave. To understand the atom, one must understand the behavior of electromagnetic waves.

The de Broglie relation:

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

Diagram illustrating the de Broglie relation: $\lambda = \frac{h}{mv}$. The variables are labeled with arrows: λ is labeled "wavelength", h is labeled "Planck's Constant", m is labeled "mass", and v is labeled "velocity".

Every particle has wave nature as well, but it is only truly evident when a particle is very light, such as an electron ($m = 9.11 \times 10^{-28} \text{ g}$)



Light Travels through space as a wave

Light transmits energy as a particle

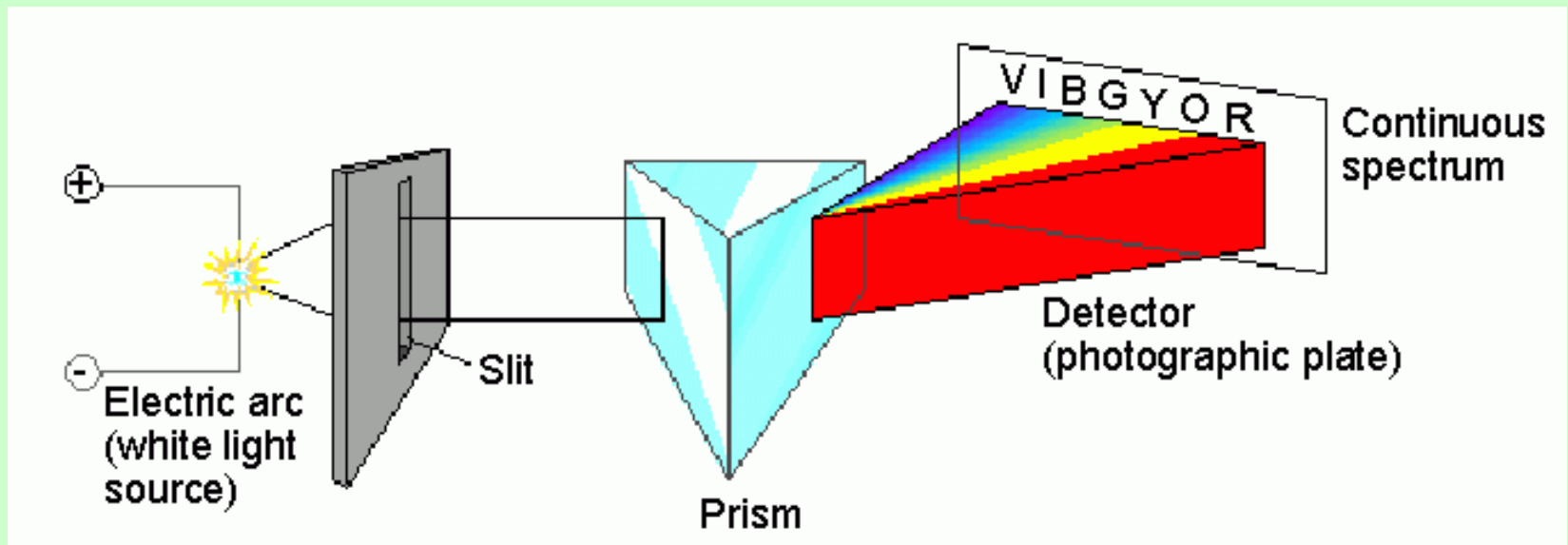
Particles have wavelength, exhibited by diffraction patterns

Large particles have very short wavelength

All Matter exhibits both particle and wave properties

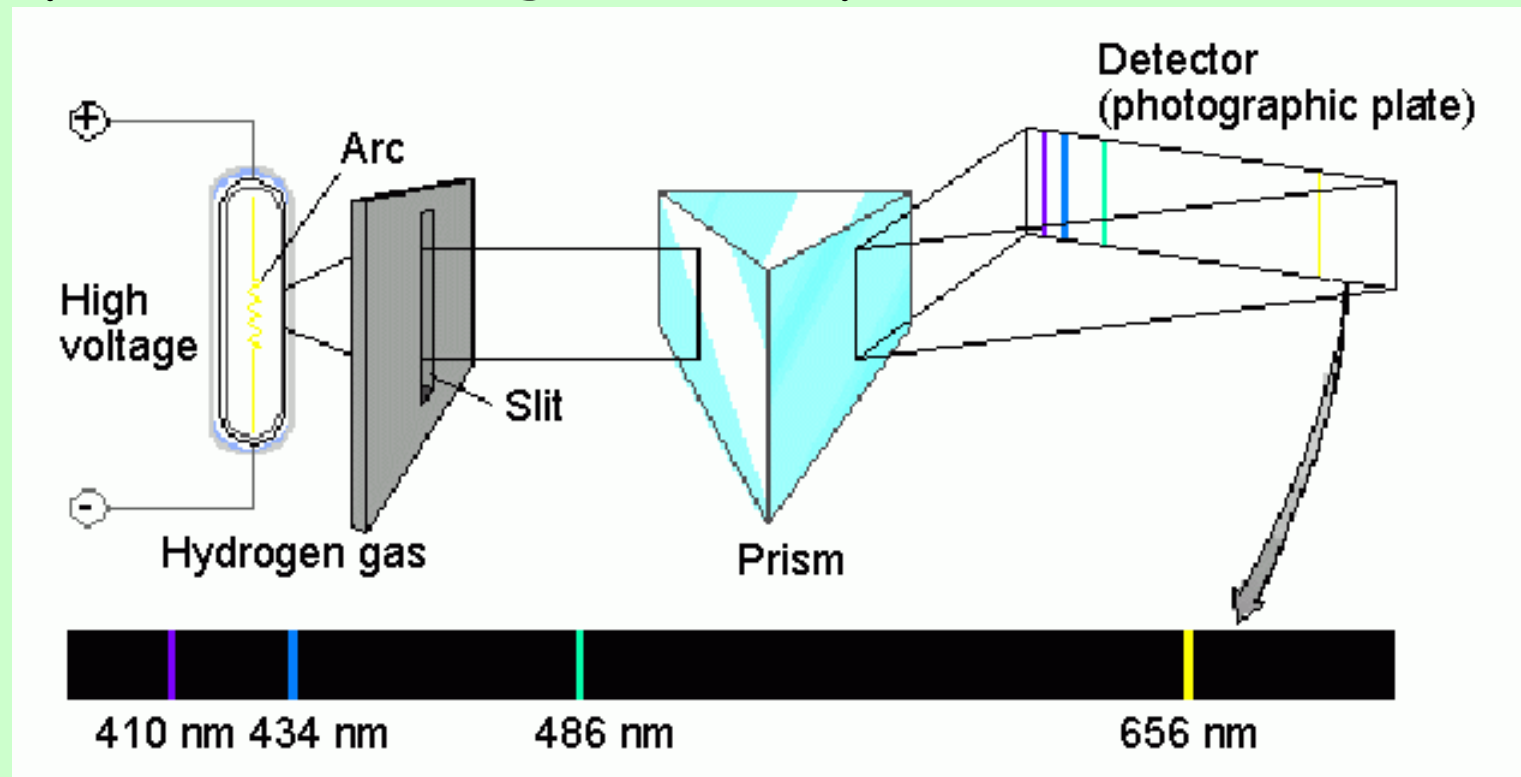
Spectroscopic analysis of the visible spectrum...

...produces all of the colors in a continuous spectrum



Spectroscopic analysis of the hydrogen spectrum...

...produces a “bright line” spectrum



Electron Energy in Hydrogen

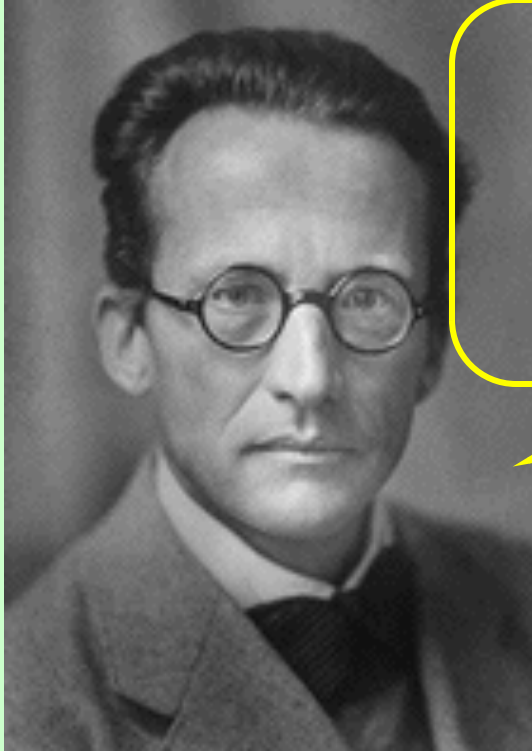
The Bohr Model

- Bohr Model
 - The electron moves around the nucleus only in certain allowed circular orbits
 - Bright line spectra confirms that only certain energies exist in the atom, and atom emits photons with definite wavelengths when the electron returns to a lower energy state
 - Energy levels available to the electron in the hydrogen atom

Shortcomings of Bohr Model...

1. Bohr's model does not work for atoms other than hydrogen
2. Electron's do not move in circular orbits

Schrodinger Wave Equation



Erwin Schrodinger

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

Equation for probability of a single electron being found along a single axis (x-axis)

Heisenberg Uncertainty Principle



Werner
Heisenberg

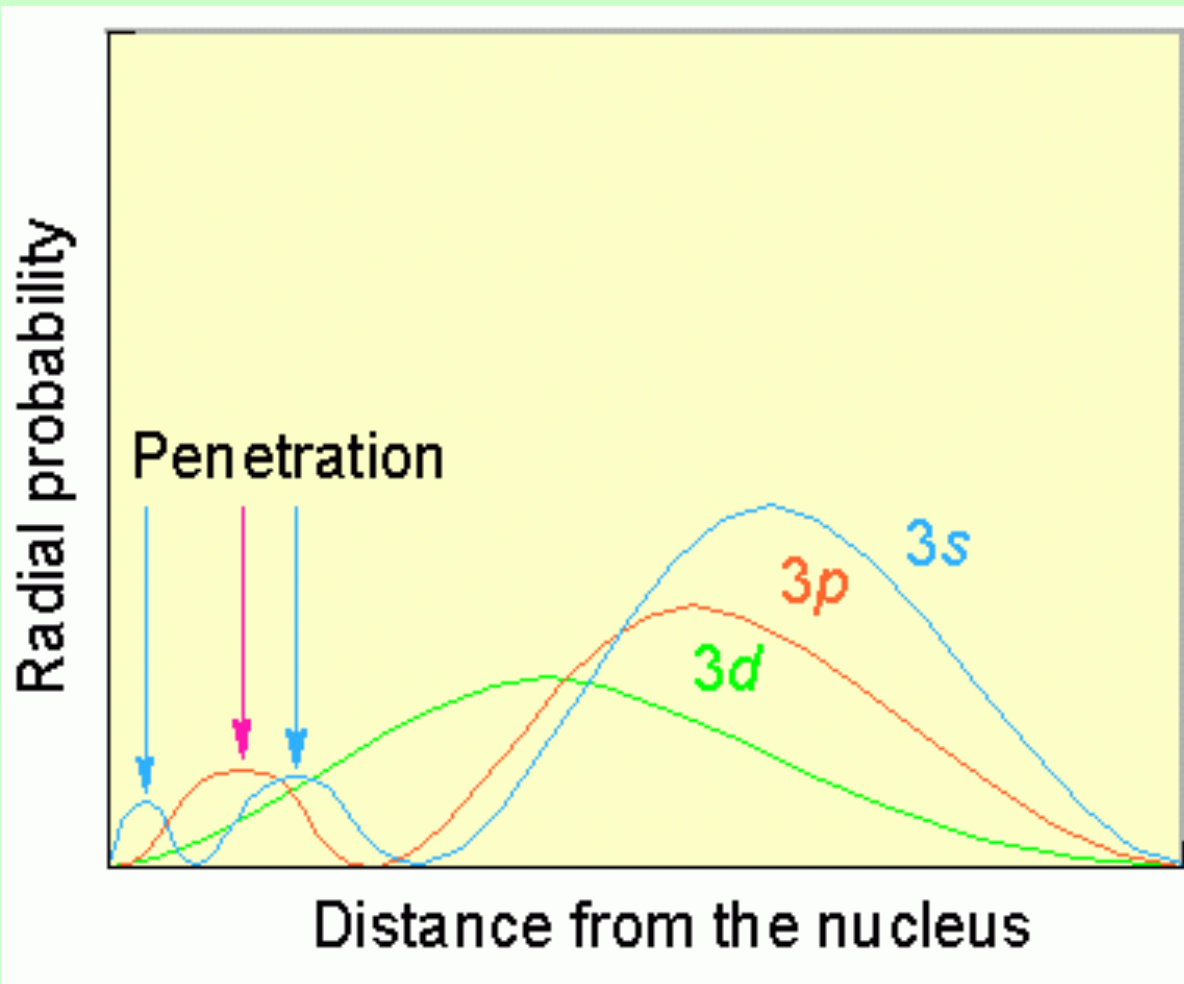
"One cannot simultaneously determine both the position and momentum of an electron."

You can find out where the electron is, but not where it is going.

OR...

You can find out where the electron is going, but not where it is!

Which of the orbital types in the 3rd energy level does not seem to have a “node”?



WHY NOT?

Penetration #2

Quantum Numbers

Each electron in an atom has a unique set of 4 quantum numbers which describe it.

- ❖ Principal quantum number, n
- ❖ Angular momentum quantum number, l
- ❖ Magnetic quantum number, m or m_l
- ❖ Spin quantum number, s or m_s

Pauli Exclusion Principle



Wolfgang
Pauli

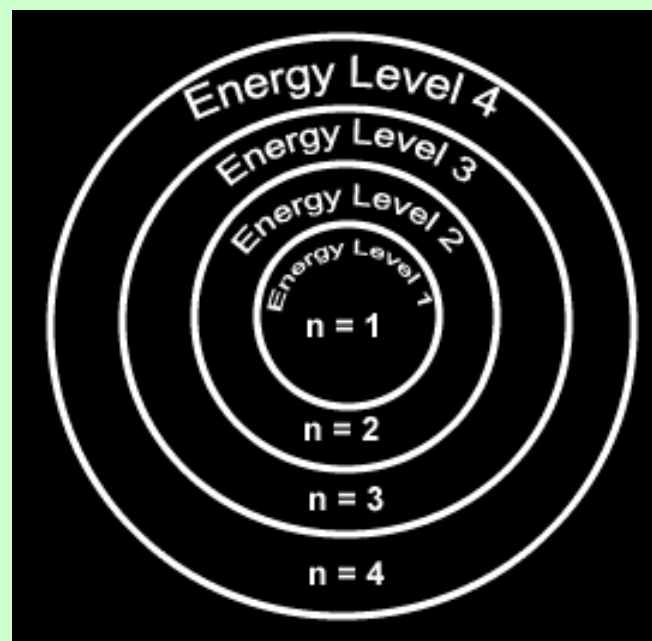
No two electrons in an atom can have the same four quantum numbers.

Principal Quantum Number

Generally symbolized by n , it denotes the shell (energy level) in which the electron is located.

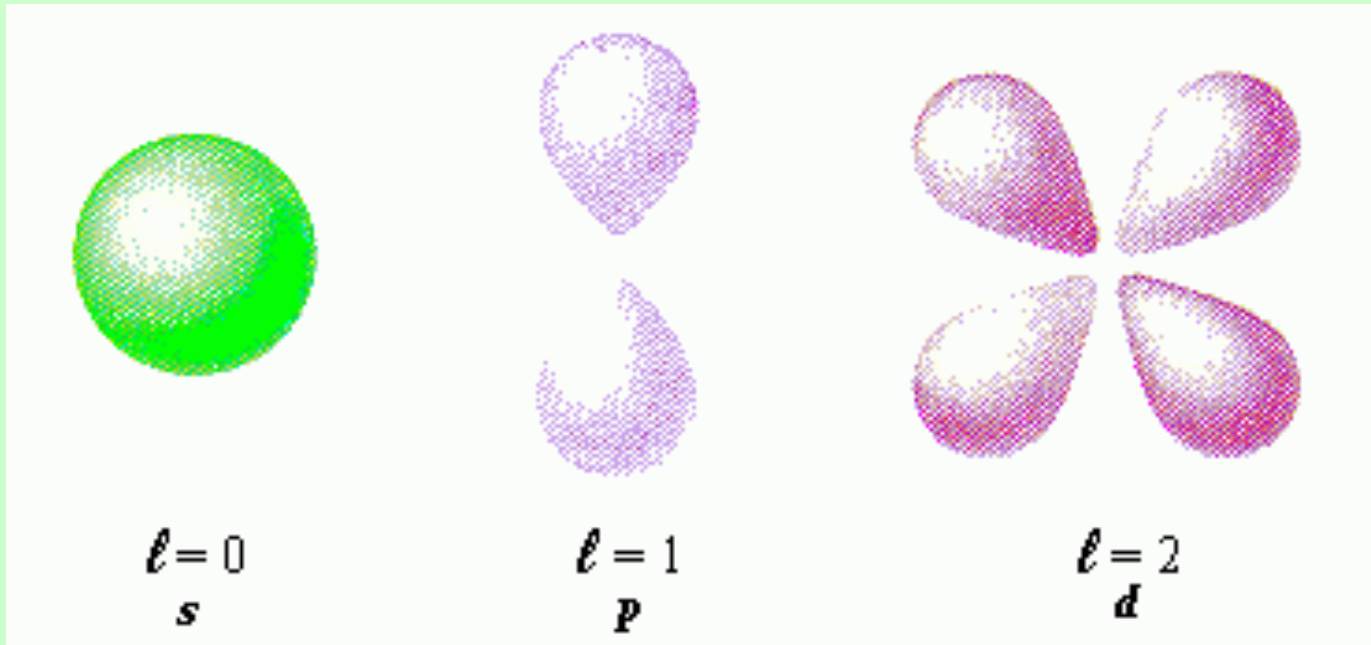
Number of electrons
that can fit in a shell:

$$2n^2$$



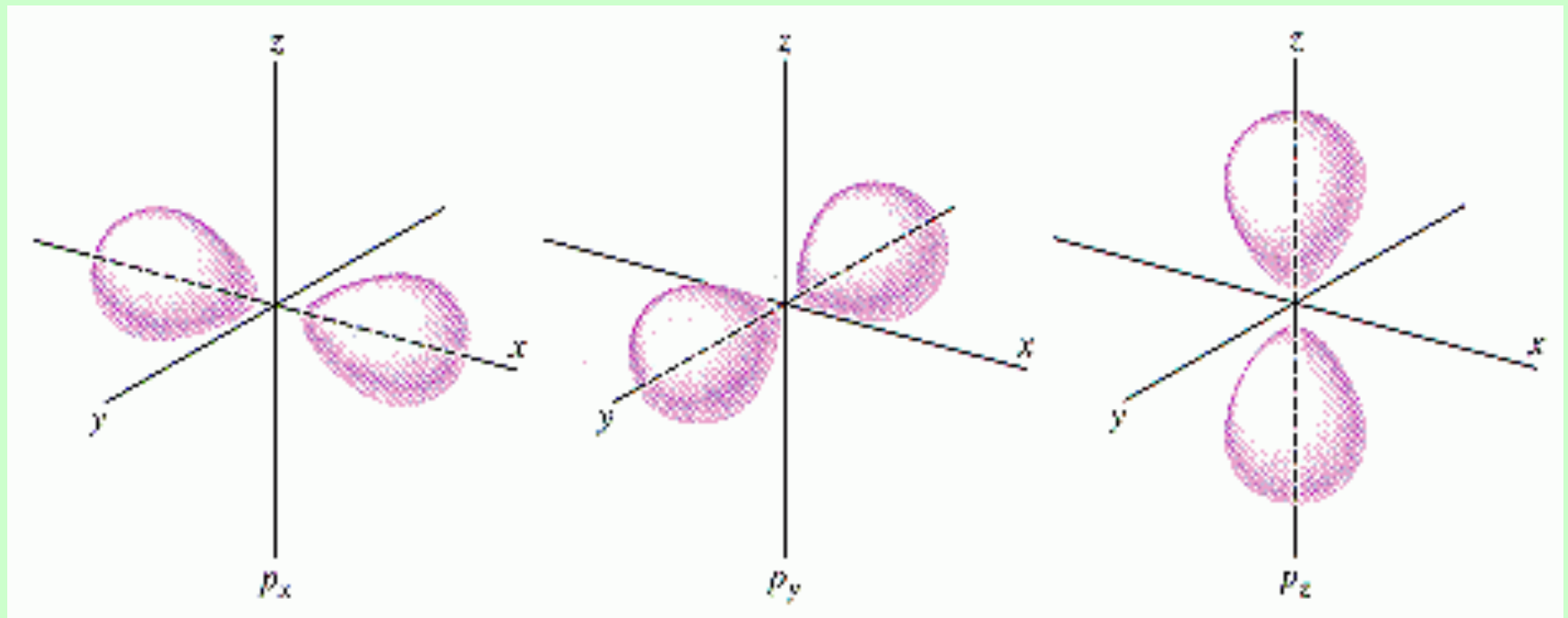
Angular Momentum Quantum Number

The angular momentum quantum number, generally symbolized by l , denotes the orbital (subshell) in which the electron is located.



Magnetic Quantum Number

The magnetic quantum number, generally symbolized by m , denotes the orientation of the electron's orbital with respect to the three axes in space.



Spin Quantum Number

Spin quantum number denotes the behavior (direction of spin) of an electron within a magnetic field.

Possibilities for electron spin:

$$+\frac{1}{2} \qquad -\frac{1}{2}$$

Assigning the Numbers

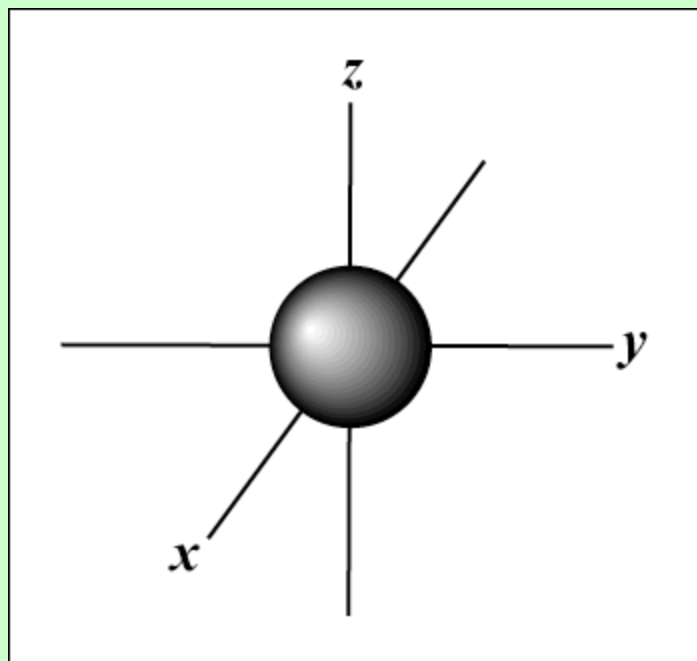
- ❖ The three quantum numbers (n , l , and m) are integers.
- ❖ The principal quantum number (n) cannot be zero.
- ❖ n must be 1, 2, 3, etc.
- ❖ The angular momentum quantum number (l) can be any integer between 0 and $n - 1$.
- ❖ For $n = 3$, l can be either 0, 1, or 2.
- ❖ The magnetic quantum number (m_l) can be any integer between $-l$ and $+l$.
- ❖ For $l = 2$, m can be either -2, -1, 0, +1, +2.

Principle, angular momentum, and magnetic quantum numbers: n , l , and m_l

Table 7.2 Quantum numbers for the first four levels of orbitals in the hydrogen atom

n	l	Orbital designation	m_l	# of orbitals
1	0	1s	0	1
2	0	2s	0	1
	1	2p	-1, 0, 1	3
3	0	3s	0	1
	1	3p	-1, 0, 1	3
	2	3d	-2, -1, 0, 1, 2	5
4	0	4s	0	1
	1	4p	-1, 0, 1	3
	2	4d	-2, -1, 0, 1, 2	5
	3	4f	-3, -2, -1, 0, 1, 2, 3	7

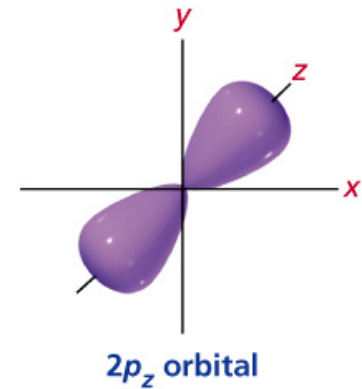
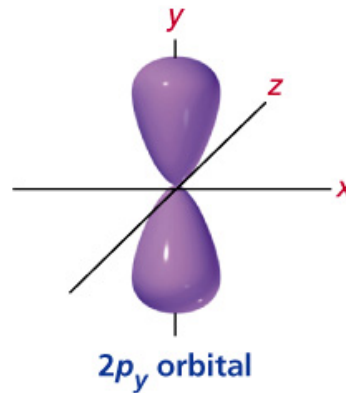
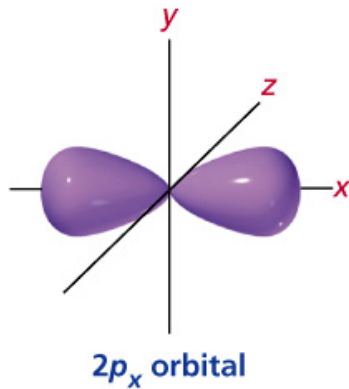
The s orbital has a spherical shape centered around the origin of the three axes in space.

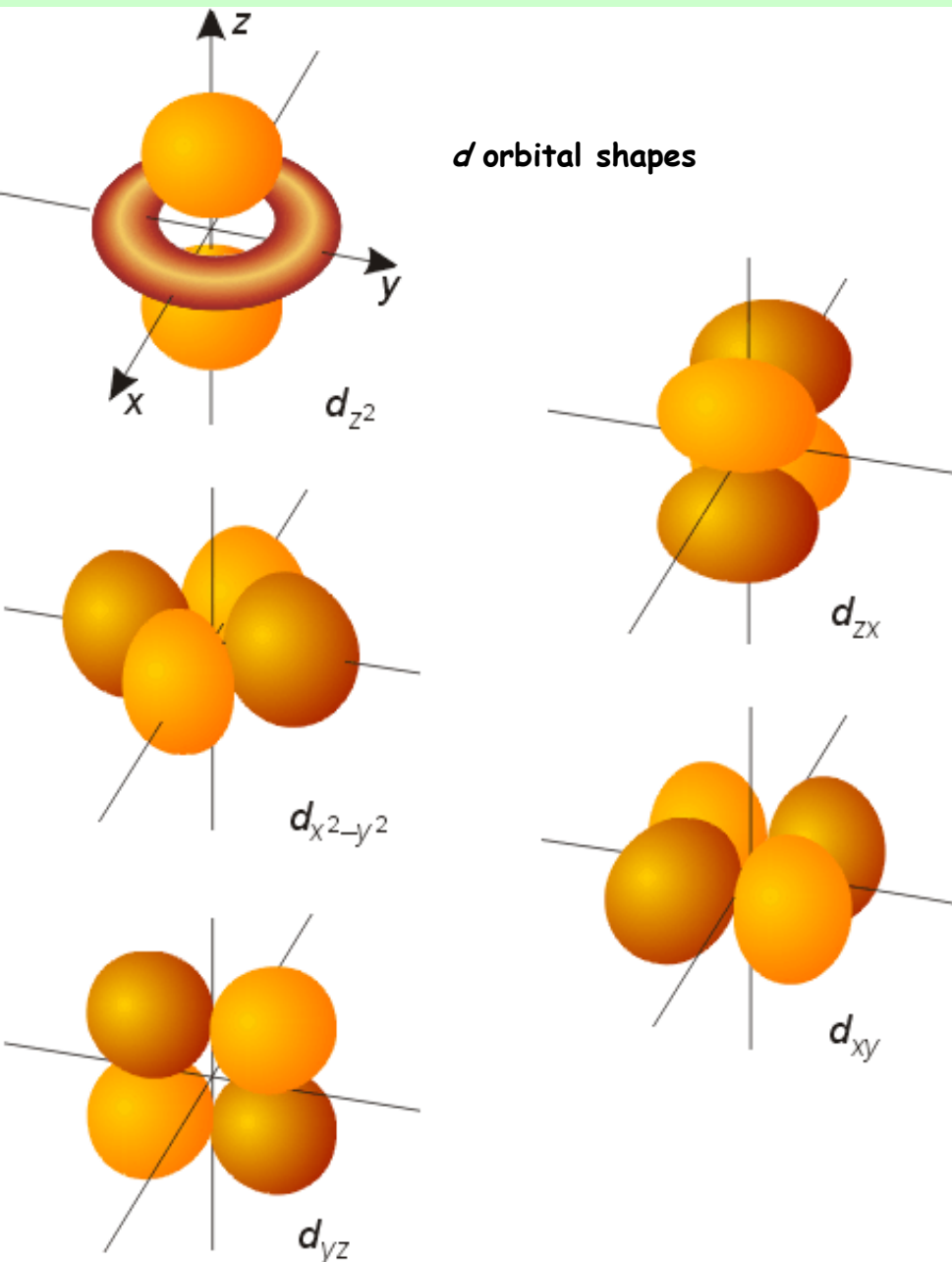


s orbital shape

p orbital shape

There are three dumbbell-shaped p orbitals in each energy level above $n = 1$, each assigned to its own axis (x , y and z) in space.



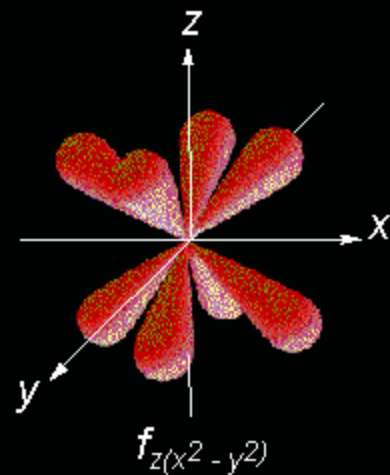
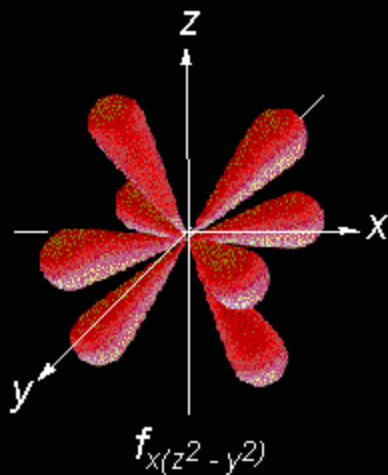
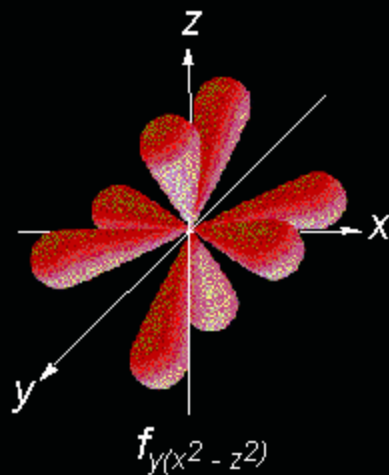
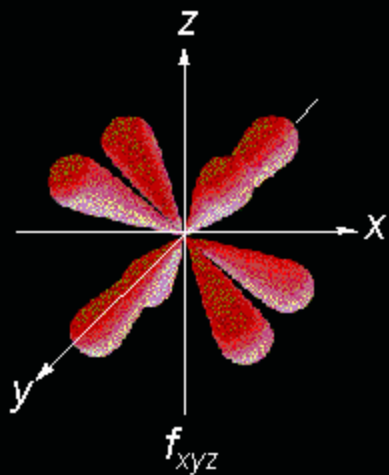
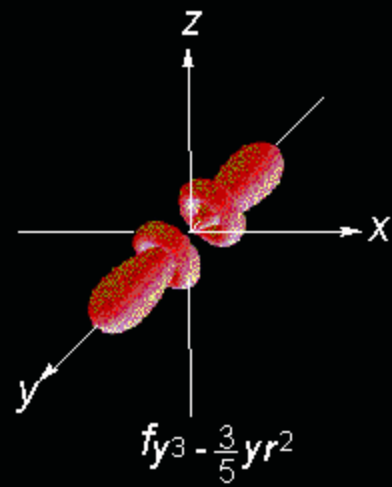
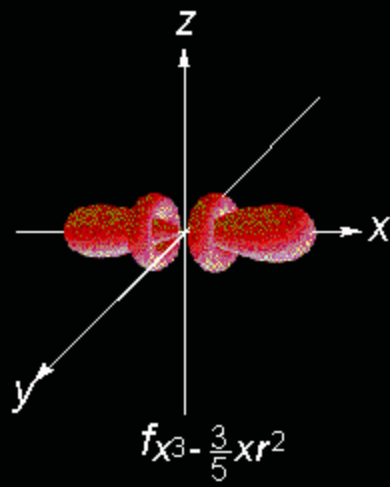
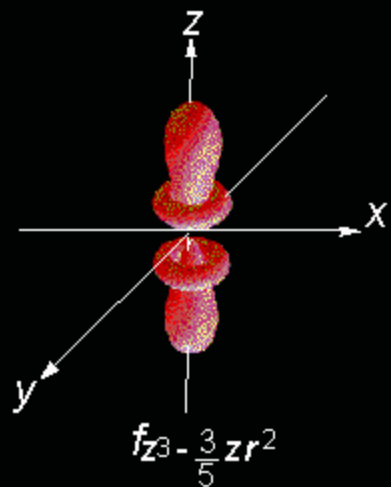


Things get a bit more complicated with the five *d* orbitals that are found in the *d* sublevels beginning with $n = 3$. To remember the shapes, think of:

“double dumbells”

...and a “dumbell with a donut”!

Shape of f orbitals



Orbital filling table

The diagram illustrates the periodic table with orbitals distributed across periods and groups. The table is color-coded: light blue for s-orbitals, light green for p-orbitals, light orange for d-orbitals, and light pink for f-orbitals. The periods are labeled 1 through 7 on the left. The groups are labeled 1A through 8A at the top. The orbitals are distributed as follows:

- Period 1:** 1s (1A, 2A)
- Period 2:** 2s (1A, 2A), 2p (3A, 4A, 5A, 6A, 7A, 8A)
- Period 3:** 3s (1A, 2A), 3p (3A, 4A, 5A, 6A, 7A, 8A)
- Period 4:** 4s (1A, 2A), 3d (3A, 4A, 5A, 6A, 7A, 8A), 4p (3A, 4A, 5A, 6A, 7A, 8A)
- Period 5:** 5s (1A, 2A), 4d (3A, 4A, 5A, 6A, 7A, 8A), 5p (3A, 4A, 5A, 6A, 7A, 8A)
- Period 6:** 6s (1A, 2A), La (3A), 5d (3A, 4A, 5A, 6A, 7A, 8A), 6p (3A, 4A, 5A, 6A, 7A, 8A)
- Period 7:** 7s (1A, 2A), Ac (3A), 6d (3A, 4A, 5A, 6A, 7A, 8A), 7p (3A, 4A, 5A, 6A, 7A, 8A)

The lanthanide and actinide series are shown as insets at the bottom, connected by arrows to their positions in the main table. The lanthanide series (La to Lu) is shown in the inset below the main table, and the actinide series (Ac to Lr) is shown in the inset below the lanthanide series.

Electron configuration of the elements of the first three series

H 1s ¹																He 1s ²	
Li 2s ¹	Be 2s ²											B 2p ¹	C 2p ²	N 2p ³	O 2p ⁴	F 2p ⁵	Ne 2p ⁶
Na 3s ¹	Mg 3s ²											Al 3p ¹	Si 3p ²	P 3p ³	S 3p ⁴	Cl 3p ⁵	Ar 3p ⁶

Irregular confirmations of Cr and Cu

Chromium steals a 4s electron to **half fill** its 3d sublevel,
no longer part of this class...

Copper steals a 4s electron to **FILL** its 3d sublevel

K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
$4s^1$	$4s^2$	$3d^1$	$3d^2$	$3d^3$	$4s^1 3d^5$	$3d^5$	$3d^6$	$3d^7$	$3d^8$	$4s^1 3d^{10}$	$3d^{10}$	$4p^1$	$4p^2$	$4p^3$	$4p^4$	$4p^5$	$4p^6$

Quantum Number Practice

Ex #1: phosphorus

P

Rule 1: identify the principle energy level, n (same as period)

In period 3

In the p-block
3rd one in $\therefore 1$

Rule 2: identify the orbital type, / (block the e^- is in)

Is 1st half of block, $\therefore +1/2$

Rule 3: identify the orientation (- / to /).

Answer:

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

(3, 1, 1, $+1/2$)

Quantum Number Practice

Ex #2: Iron

Fe

Rule 1: identify the principle energy level, n (same as period)

In period 3

Rule 2: identify the orbital type, l (block the e^- is in)

In the d-block

6th one in $\therefore -2$

Rule 3: identify the orientation ($-l$ to l).

Is 2nd half of block, $\therefore -1/2$

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

Answer:

(3, 2, -2, -1/2)

Quantum Number Practice

Ex #3: Barium

Ba

Rule 1: identify the principle energy level, n (same as period)

In period 6

Rule 2: identify the orbital type, l (block the e^- is in)

In the s-block

2nd one in $\therefore 0$

Is 2nd half of block, $\therefore -1/2$

Rule 3: identify the orientation ($-l$ to l).

Answer:

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

(6, 0, 0, $-1/2$)

Quantum Number Practice

Ex #4: Tin

Sn

Rule 1: identify the principle energy level, n (same as period)

In period 5

Rule 2: identify the orbital type, l (block the e^- is in)

In the p-block

2nd one in $\therefore 0$

Rule 3: identify the orientation ($-l$ to l).

Is 1st half of block, $\therefore +1/2$

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

Answer:

(5, 1, 0, $+1/2$)

Quantum Number Practice

Ex #5: Silver

Ag

Rule 1: identify the principle energy level, n (same as period)

In period 4

Rule 2: identify the orbital type, l (block the e^- is in)

In the d-block
9th one in $\therefore 1$

Is 2nd half of block, $\therefore -1/2$

Rule 3: identify the orientation ($-l$ to l).

Answer:

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

(4, 2, 1, $-1/2$)

Quantum Number Practice

Ex #6: Oxygen

O

Rule 1: identify the principle energy level, n (same as period)

In period 2

In the p-block
4th one in $\therefore -1$

Rule 2: identify the orbital type, l (block the e^- is in)

Is 2nd half of block, $\therefore -1/2$

Rule 3: identify the orientation ($-l$ to l).

Answer:

Rule 4: 1st half have $+1/2$ spin, 2nd half have $-1/2$ spin

(2, 1, -1, -1/2)

Electron Energy in Hydrogen

The Bohr Model

$$E_{electron} = -2.178 \times 10^{-18} J \left(\frac{Z^2}{n^2} \right)$$

Z = nuclear charge (atomic number)

n = energy level

***Equation works only for atoms or ions with 1 electron (H, He⁺, Li²⁺, etc).

Calculating Energy Change, ΔE , for Electron Transitions

$$\Delta E = -2.178 \times 10^{-18} \text{ J} \left(\frac{Z^2}{n_{final}^2} - \frac{Z^2}{n_{initial}^2} \right)$$

Energy must be absorbed from a photon (**$+\Delta E$**) to move an electron away from the nucleus

Energy (a photon) must be given off (**$-\Delta E$**) when an electron moves toward the nucleus