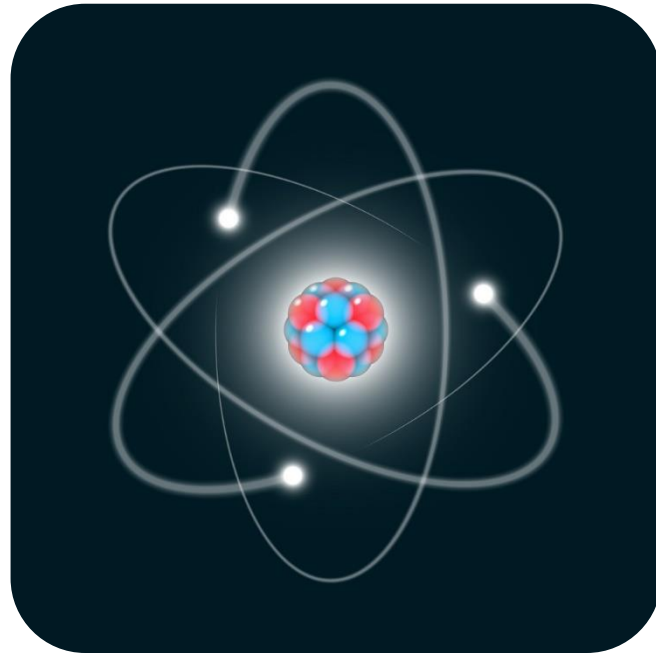


Quantum Theory & Atomic Structure



The contents of this presentation is made to provide a brief idea about the topic, details will be discussed in the classes. Contents have been collected from multiple textbooks and internet.

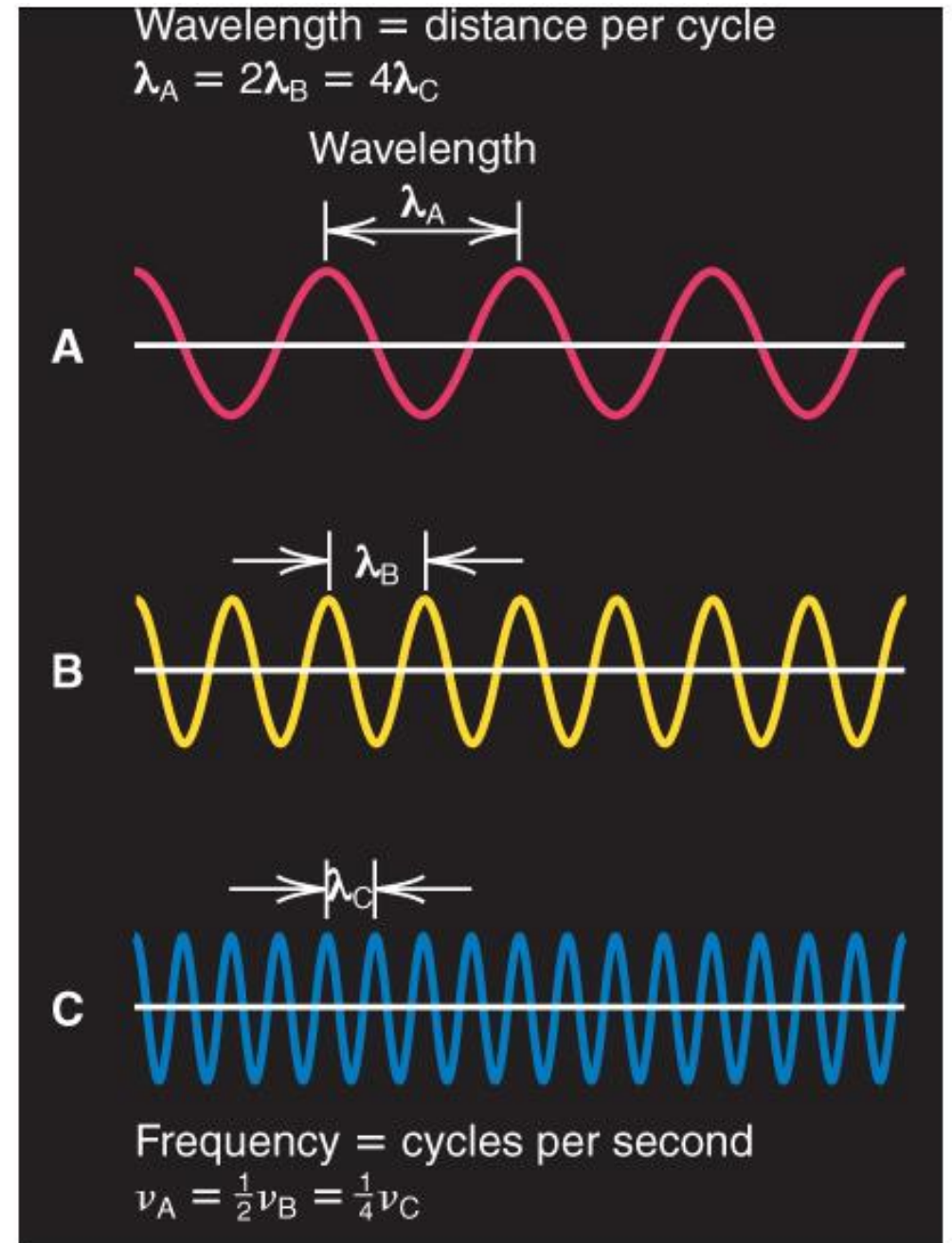
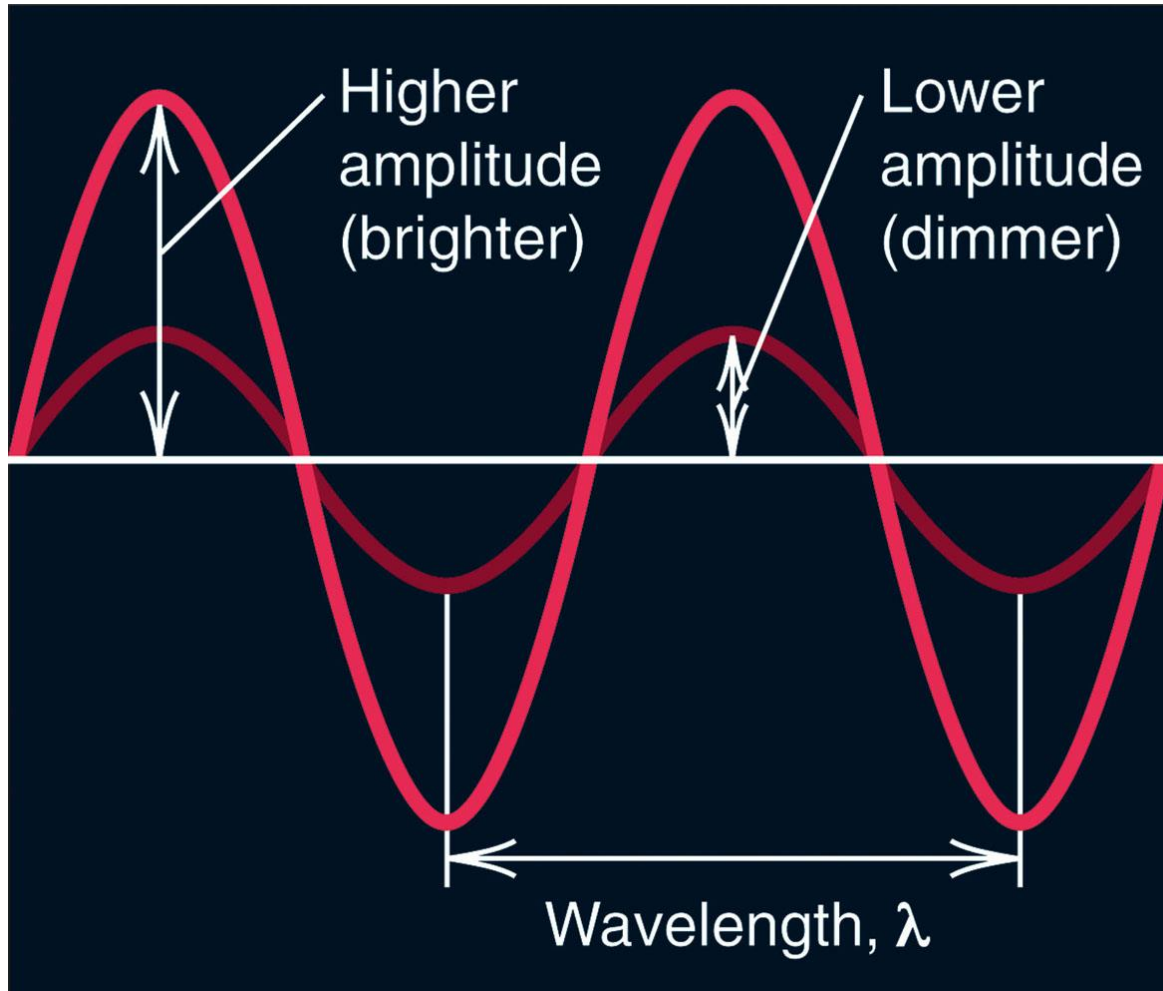
The Wave nature of Light

- Visible light is a type of *electromagnetic radiation*.
- The wave properties of electromagnetic radiation are described by **three variables** -
 - ✓ *frequency* (n), cycles per second
 - ✓ *wavelength* (l), the distance a wave travels in one cycle
 - ✓ *amplitude*, is the vertical distance from the midline of a wave to the peak.

The *speed of light* is a constant:

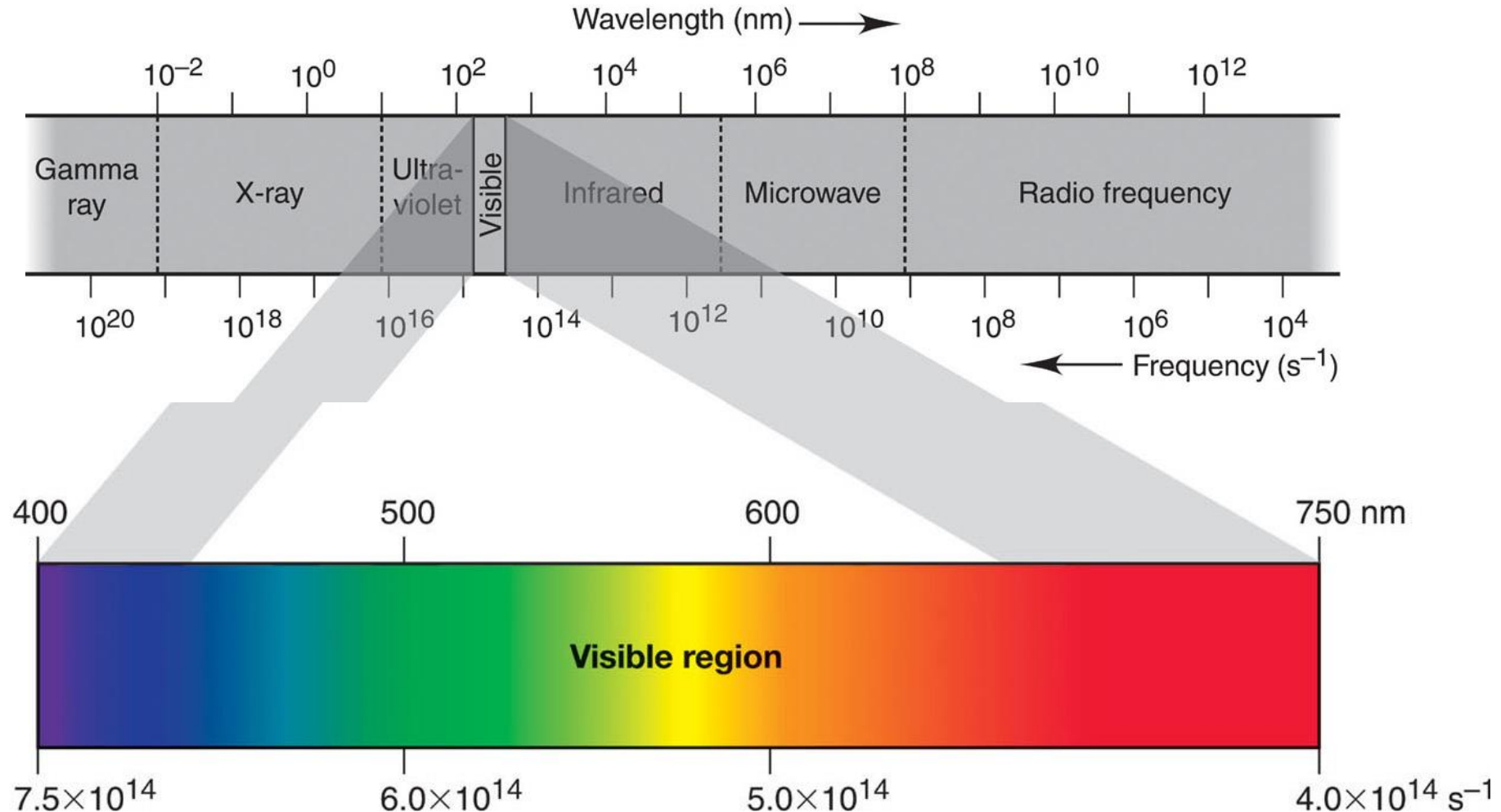
$$c = n \times l$$
$$= 3.00 \times 10^8 \text{ m/s in a vacuum}$$

The Wave nature of Light



Electromagnetic Spectrum

- The range of frequencies or wavelengths of electromagnetic radiation is called the electromagnetic spectrum.



Obtaining the Wavelength of Light from its Frequency

Problem: What is the wavelength of the yellow sodium emission, which has a frequency of $5.09 \times 10^{14}/s$?

Solution The frequency and wavelength are related by the formula $c = \nu\lambda$. You rearrange this formula to give

$$\lambda = \frac{c}{\nu}$$

in which c is the speed of light (3.00×10^8 m/s). Substituting yields

$$\lambda = \frac{3.00 \times 10^8 \text{ m/s}}{5.09 \times 10^{14}/s} = 5.89 \times 10^{-7} \text{ m, or } \mathbf{589 \text{ nm}}$$

Similarly, you can obtain the frequency of light from its wavelength

Obtaining the Frequency of Light from its Wavelength

Problem: Calculate the wavelength (in nm) of the red light emitted by a barcode scanner that has a frequency of $4.62 \times 10^{14} \text{ s}^{-1}$.

Solution:

$$v = \frac{c}{\lambda}$$

$$\lambda = \frac{c}{v} = \frac{3.00 \times 10^8 \text{ m/s}}{4.62 \times 10^{14} / \text{s}}$$

$$= 6.49 \times 10^{-7} \text{ m}$$

$$= 6.49 \times 10^{-7} \text{ m} \times \frac{1 \text{ nm}}{10^{-9} \text{ m}} = 649 \text{ nm}$$

Problem:

A laser dazzles the audience in a rock concert by emitting green light with a wavelength of 515 nm. Calculate the frequency of the light.

Obtaining the Frequency of Light from its Wavelength

Problem: A dental hygienist uses x-rays ($\lambda = 1.00\text{\AA}$) to take a series of dental radiographs while the patient listens to a radio station ($\lambda = 325\text{ cm}$) and looks out the window at the blue sky ($\lambda = 473\text{ nm}$). What is the frequency (in s^{-1}) of the electromagnetic radiation from each source? (Assume that the radiation travels at the speed of light, $3.00 \times 10^8\text{ m/s}$.)

Solution:

$$\text{For the x-rays: } \lambda = 1.00\text{\AA} \times \frac{10^{-10}\text{ m}}{1\text{\AA}} = 1.00 \times 10^{-10}\text{ m}$$

$$\nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8\text{ m/s}}{1.00 \times 10^{-10}\text{ m}} \quad \boxed{= 3.00 \times 10^{18}\text{ s}^{-1}}$$

Obtaining the Frequency of Light from its Wavelength

Problem: A dental hygienist uses x-rays ($\lambda = 1.00\text{\AA}$) to take a series of dental radiographs while the patient listens to a radio station ($\lambda = 325\text{ cm}$) and looks out the window at the blue sky ($\lambda = 473\text{ nm}$). What is the frequency (in s^{-1}) of the electromagnetic radiation from each source? (Assume that the radiation travels at the speed of light, $3.00 \times 10^8\text{ m/s}$.)

Solution:

$$\text{For the radio signal: } \nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m/s}}{325 \text{ cm} \times \frac{10^{-2} \text{ m}}{1 \text{ cm}}} \quad \boxed{= 9.23 \times 10^7 \text{ s}^{-1}}$$

$$\text{For the blue sky: } \nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m/s}}{473 \text{ nm} \times \frac{10^{-9} \text{ m}}{1 \text{ cm}}} \quad \boxed{= 6.34 \times 10^{14} \text{ s}^{-1}}$$

Quantization of Energy

- When solids are heated, they emit electromagnetic radiation over a wide range of wavelengths.

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



© Ravi/Shutterstock.com

Smoldering coal

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



© The McGraw-Hill Companies, Inc./Charles Winters Photographer

Electric heating element

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



© Feng Yu/Shutterstock.com

Lightbulb filament

- It is assumed that atoms and molecules could emit (or absorb) any arbitrary amount of radiant energy.

Quantization of Energy

- Planck said that atoms and molecules could emit (or absorb) energy only in discrete quantities, like small packages or bundles.



Sold at any quantities



Sold only in 1 kg packets

Quantization of Energy

- Planck gave the name quantum to the smallest quantity of energy that can be emitted (or absorbed) in the form of electromagnetic radiation.

$$E = h\nu$$

h is Planck constant, ν is frequency

Allowed

$$1 \text{ quanta} = h\nu$$

$$2 \text{ quanta} = 2h\nu$$

$$3 \text{ quanta} = 3h\nu$$



Not Allowed

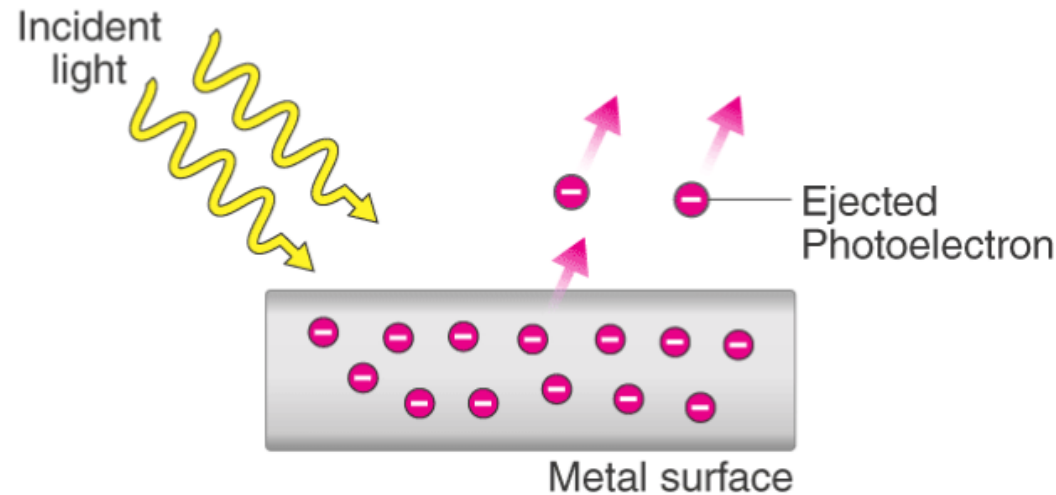
$$\frac{1}{2} \text{ quanta} = \frac{1}{2}h\nu$$

$$\frac{3}{2} \text{ quanta}$$

- Energy is always emitted in integral multiples of $h\nu$; i.e., $E = nh\nu$
Where, $n = 1, 2, 3, \dots$

Photoelectric Effect

- The *photoelectric effect* is the emission of electrons when electromagnetic radiation, such as light, hits a material.



- Electrons emitted in this manner are called *photoelectrons*.
- To cause the emission of electron, the light (now called photon) should have a certain minimum frequency, called the *threshold frequency*.

Calculating Energy of a Photon

$$E = h\nu \text{ and } c = \nu\lambda$$

Problem

The red spectral line of lithium occurs at 671 nm (6.71×10^{-7} m). Calculate the energy of one photon of this light.

Solution The frequency of this light is

$$\nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m/s}}{6.71 \times 10^{-7} \text{ m}} = 4.47 \times 10^{14} \text{ /s}$$

Hence, the energy of one photon is

$$E = h\nu = 6.63 \times 10^{-34} \text{ J}\cdot\text{s} \times 4.47 \times 10^{14} \text{ /s} = 2.96 \times 10^{-19} \text{ J}$$

Answer Check Be sure to use the same systems of units for the wavelength, the speed of light, and Planck's constant. Check that units cancel to give the proper units for energy in the final answer.

Calculating Energy of a Photon

Problem: A cook uses a microwave oven to heat a meal. The wavelength of the radiation is 1.20 cm. What is the energy of one photon of this microwave radiation?

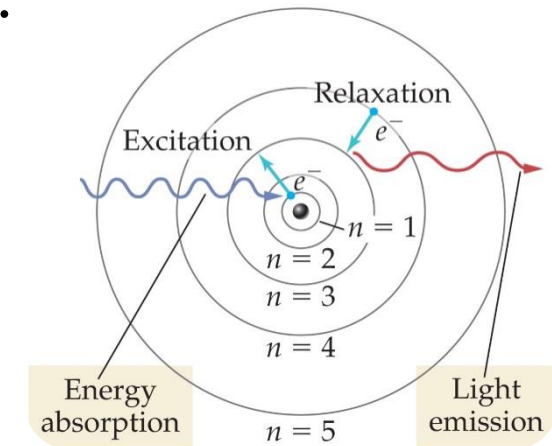
SOLUTION:

$$E = h\nu = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{(1.20 \text{ cm})\left(\frac{10^{-2} \text{ m}}{1 \text{ cm}}\right)} = 1.66 \times 10^{-23} \text{ J}$$

Niels Bohr's Atomic Model

Bohr's postulates

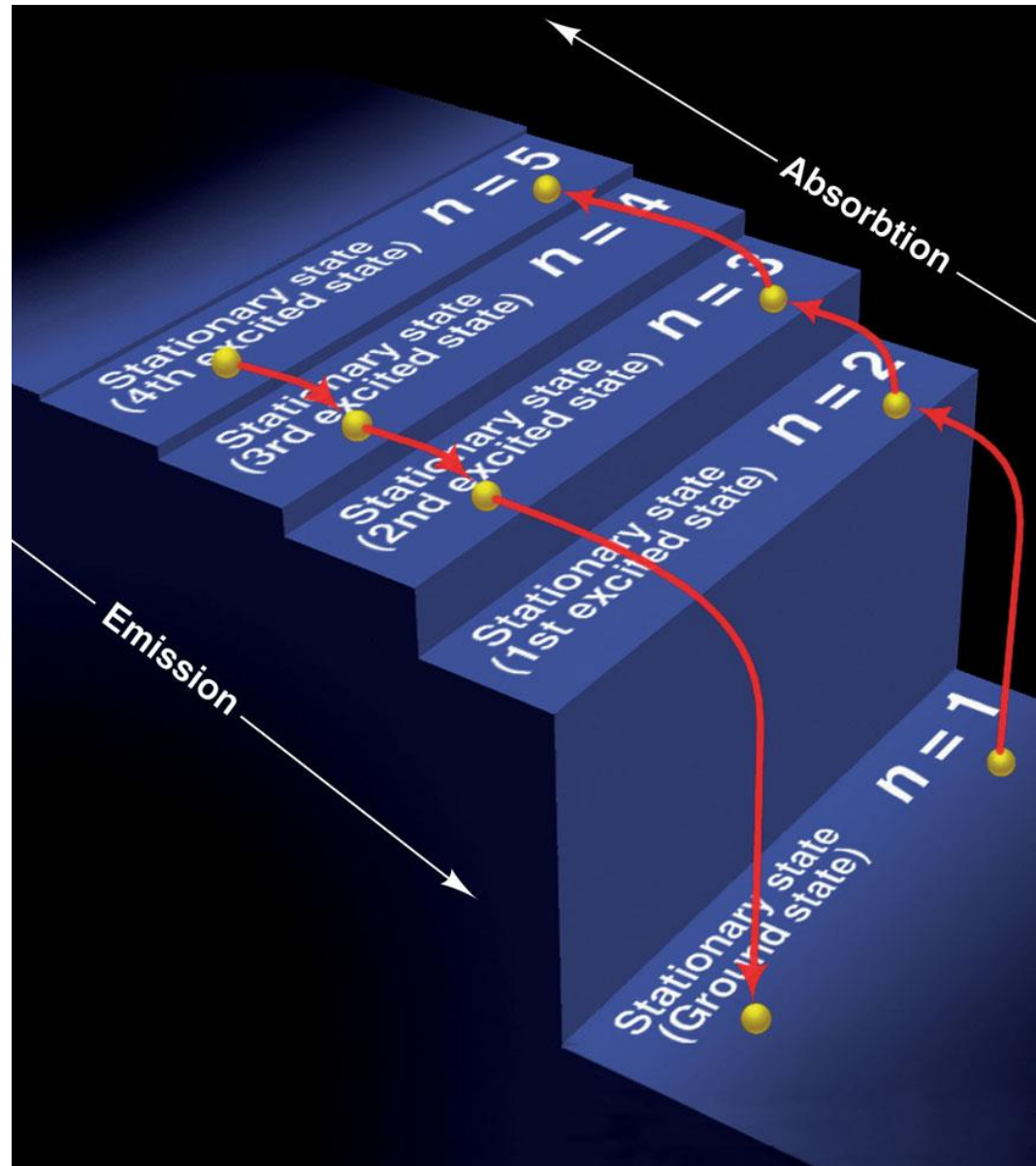
- In an atom, electrons revolve around the positively charged nucleus in a definite circular path called as orbits or shells. Electrons do not absorb or emit energy while rotating in a particular orbit.



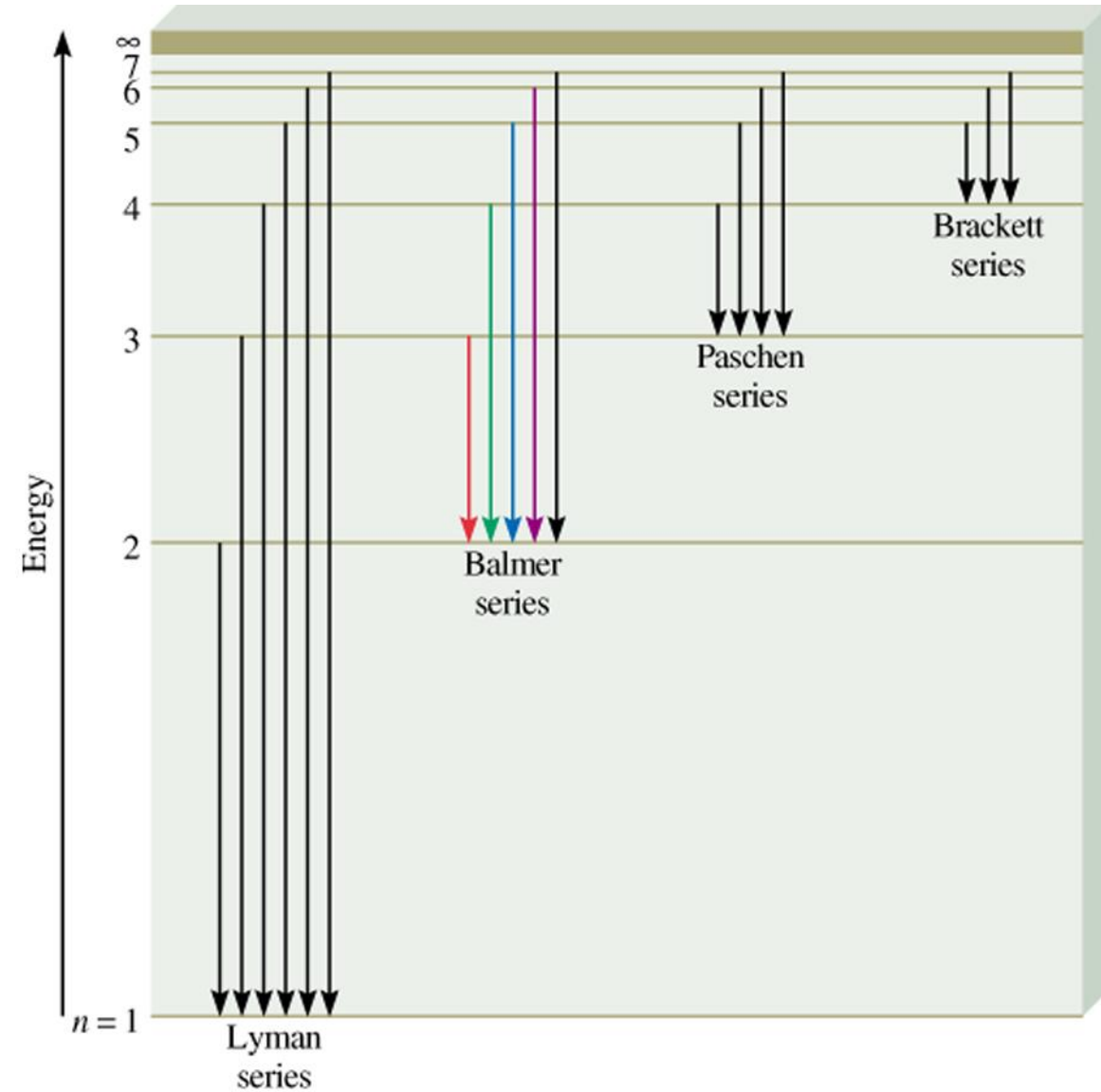
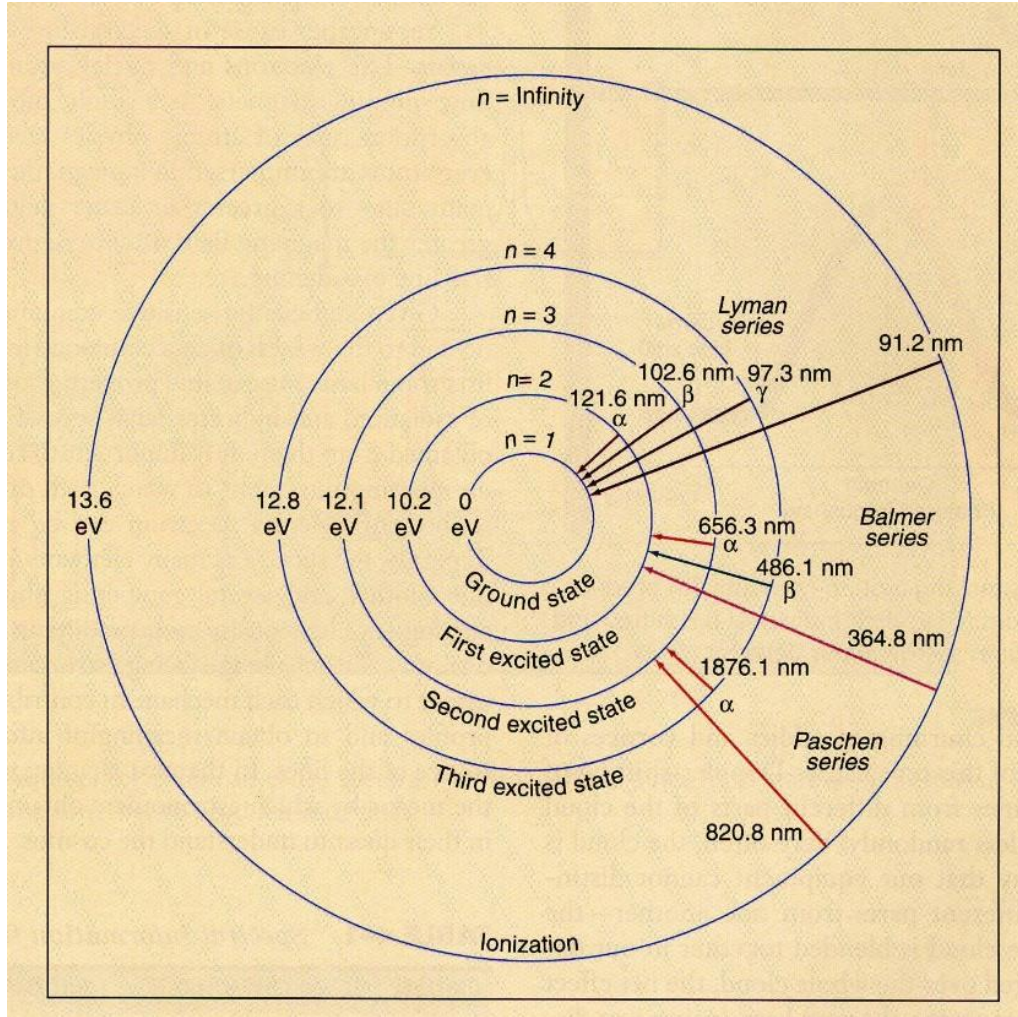
$$\Delta E = E_1 - E_2 = h\nu$$

- The electrons in an atom move from a lower energy level to a higher energy level by gaining the required energy and an electron moves from a higher energy level to lower energy level by losing energy.

Niels Bohr's Atomic Model



Niels Bohr's Atomic Model



Limitations of Bohr's Atomic Theory

- It could not explain the spectra obtained from larger atoms.
- It violates the Heisenberg Uncertainty Principle.
- Failed to explain the Zeeman Effect (effect of magnetic field on the spectra of atoms) and Stark effect (effect of electric field on the spectra of atoms).

Niels Bohr's Atomic Model – Calculating Energy

- An electron in a higher energy level (initial energy level, E_i) undergoes a transition to a lower energy level (final energy level, E_f). In this process, the electron loses energy, which is emitted as a photon.

Then, $E_i = -R_H/n_i^2$; $E_f = -R_H/n_f^2$;

R_H (Rydberg constant) = $2.178 \times 10^{-18} \text{ J}$

$$\Delta E = E_f - E_i = -R_H(1/n_f^2 - 1/n_i^2) = R_H(1/n_i^2 - 1/n_f^2)$$

To calculate the wavelength (λ) of the radiation,

$$E = h\nu = hc/\lambda \quad ; [h \text{ (Planck constant)} = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}]$$

$$\text{Or, } \lambda = hc/E$$

$$\text{Alternatively, } 1/\lambda = R_H(1/n_i^2 - 1/n_f^2) \quad [R_H = 1.096776 \times 10^7 \text{ m}^{-1}]$$

Calculating Energy and Wavelength of an Electron

Problem: A hydrogen atom absorbs a photon of UV light and its electron enters the $n = 4$ energy level. Calculate (a) the change in energy of the atom and (b) the wavelength (in nm) of the photon.

SOLUTION:

$$\begin{aligned} \text{(a)} \quad \Delta E &= 2.18 \times 10^{-18} \text{ J} \left(\frac{1}{n_{\text{initial}}^2} - \frac{1}{n_{\text{final}}^2} \right) = 2.18 \times 10^{-18} \text{ J} \left(\frac{1}{1^2} - \frac{1}{4^2} \right) \\ &= 2.18 \times 10^{-18} \text{ J} \left(1 - \frac{1}{16} \right) = \boxed{2.05 \times 10^{-18} \text{ J}} \end{aligned}$$

$$\text{(b)} \quad \lambda = \frac{hc}{\Delta E} = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(3.00 \times 10^8 \text{ m/s})}{2.05 \times 10^{-18} \text{ J}} = \boxed{9.74 \times 10^{-8} \text{ m}}$$

$$9.74 \times 10^{-8} \text{ m} \times \frac{1 \text{ nm}}{10^{-9} \text{ m}} = \boxed{97.4 \text{ nm}}$$

Calculating Energy and Wavelength of an Electron

Problem: Calculate the wavelength (in nm) of a photon emitted by a hydrogen atom when its electron drops from the $n = 5$ state to the $n = 3$ state.

SOLUTION:

$$E_{\text{photon}} = \Delta E = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$E_{\text{photon}} = 2.18 \times 10^{-18} \text{ J} \times (1/25 - 1/9)$$

$$E_{\text{photon}} = \Delta E = -1.55 \times 10^{-19} \text{ J}$$

$$E_{\text{photon}} = h \times c / \lambda$$

$$\lambda = h \times c / E_{\text{photon}}$$

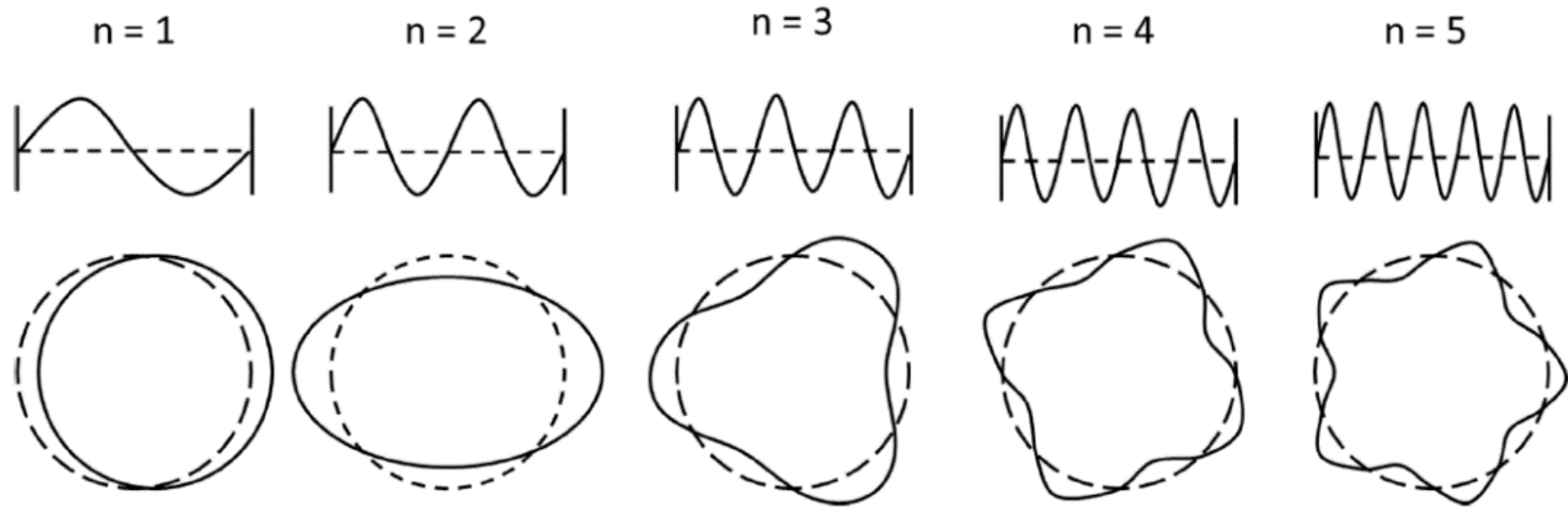
$$\lambda = 6.63 \times 10^{-34} \text{ (J}\cdot\text{s)} \times 3.00 \times 10^8 \text{ (m/s)} / 1.55 \times 10^{-19} \text{ J}$$

$$\lambda = 1280 \text{ nm}$$

Calculating Energy and Wavelength of an Electron

Problem: Calculate the shortest and longest wavelengths of Balmer series of hydrogen atom. Given $R = 1.097 \times 10^7 \text{ m}^{-1}$.

Dual nature of electrons



According to Planck's equation,
 $E = h\nu$;
 h is Planck's constant, ν is frequency

Using Einstein's equation,
 $E = mc^2$; m is the mass, c is velocity

Therefore, $mc^2 = h\nu$;

or, $mc = h\nu/c = h/\lambda$

or, $\lambda = h/mc$

or, $\lambda = h/mu$

For electron, velocity $c = u$

Dual nature of electrons

Problem: Find the wavelength of an electron with a speed of $1.00 \times 10^6 \text{ m/s}$ (electron mass = $9.11 \times 10^{-31} \text{ kg}$; $h = 6.626 \times 10^{-34} \text{ kg} \cdot \text{m}^2/\text{s}$).

SOLUTION: $\lambda = \frac{h}{mu}$

$$\lambda = \frac{6.626 \times 10^{-34} \text{ kg} \cdot \text{m}^2/\text{s}}{9.11 \times 10^{-31} \text{ kg} \times 1.00 \times 10^6 \text{ m/s}} \quad \boxed{= 7.27 \times 10^{-10} \text{ m}}$$

Dual nature of electrons

Calculate the wavelength of the “particle” in the following two cases: (a) The fastest serve in tennis is about 150 miles per hour, or 68 m/s. Calculate the wavelength associated with a 6.0×10^{-2} -kg tennis ball traveling at this speed. (b) Calculate the wavelength associated with an electron (9.1094×10^{-31} kg) moving at 68 m/s.

Solution:

$$\begin{aligned}\lambda &= \frac{h}{mu} \\ &= \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(6.0 \times 10^{-2} \text{ kg}) \times 68 \text{ m/s}} \\ &= 1.6 \times 10^{-34} \text{ m}\end{aligned}$$

(b) In this case,

$$\begin{aligned}\lambda &= \frac{h}{mu} \\ &= \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(9.1094 \times 10^{-31} \text{ kg}) \times 68 \text{ m/s}} \\ &= 1.1 \times 10^{-5} \text{ m}\end{aligned}$$

Heisenberg Uncertainty Principle

'It is impossible to know simultaneously both the momentum p (defined as mass times velocity) and the position of a particle with certainty'.

The diagram illustrates the Heisenberg Uncertainty Principle equation: $\Delta p \Delta x \geq \frac{h}{4\pi}$. The symbols are color-coded: Δp is green, Δx is blue, h is red, and 4π is purple. Three arrows point to the symbols: a green arrow from the text 'uncertainty in position' points to Δx ; a blue arrow from the text 'uncertainty of momentum' points to Δp ; and a red arrow from the text 'Planck's constant' points to h .

$$\Delta p \Delta x \geq \frac{h}{4\pi}$$

Planck's constant

uncertainty in position

uncertainty of momentum

Quantum Mechanical Model - Schrödinger Wave Equation

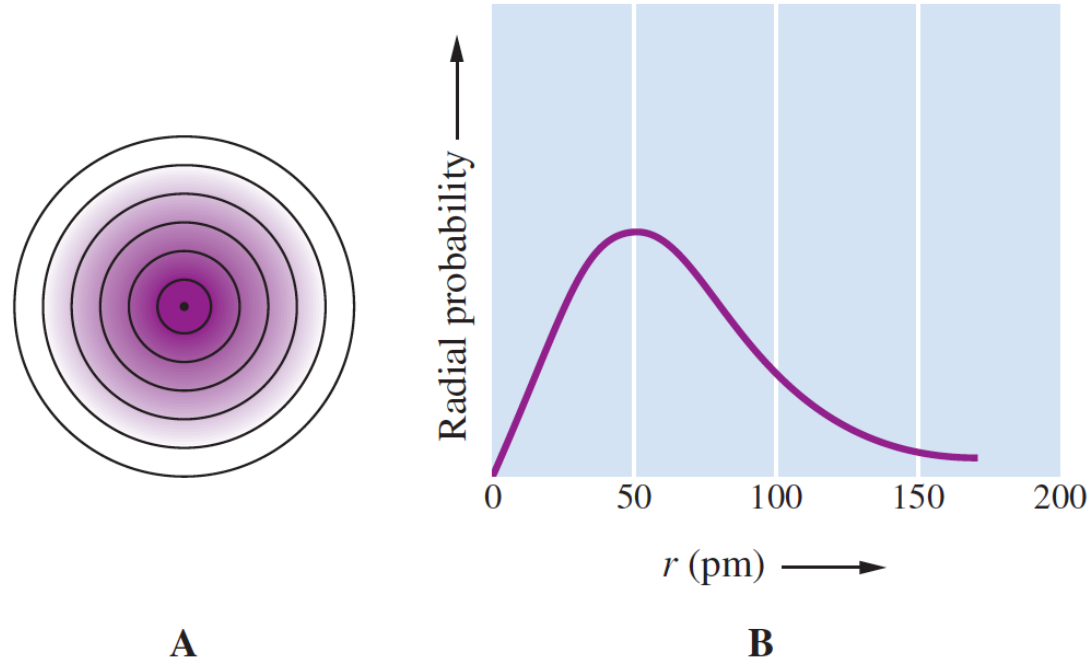
- In 1926 Schrodinger wrote an equation that described both the particle and wave nature of the e^- .

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2m}{h^2} (E - V)\psi = 0$$

$$\nabla^2\psi + \frac{8\pi^2m}{h^2} (E - V)\psi = 0$$

- Ψ (psi) is a wave function, obtained by solving Schrödinger wave equation; provides information about an electron in an atom.
- Ψ^2 , gives the probability of finding the electron within a region of space.

Quantum Mechanical Model - Schrödinger Wave Equation

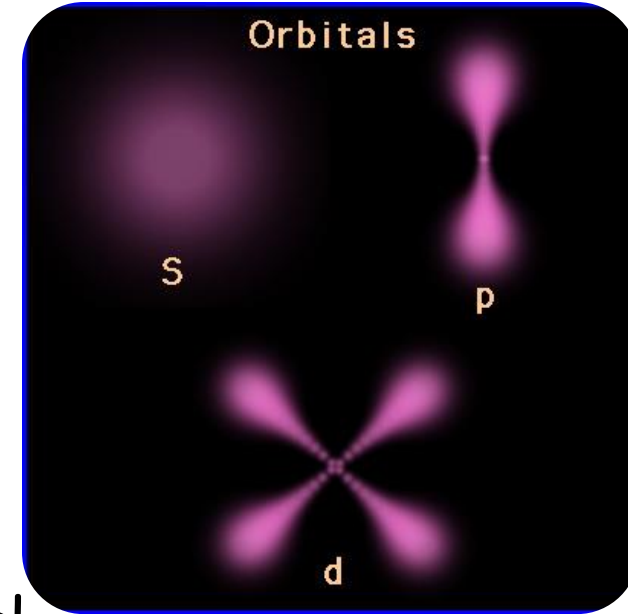


- (A) The diagram shows the probability density for an electron in a hydrogen atom. The region is marked off in shells about the nucleus.
- (B) The graph shows the probability of finding the electron within shells at various distances from the nucleus (radial probability).

Schrödinger's Quantum mechanical model

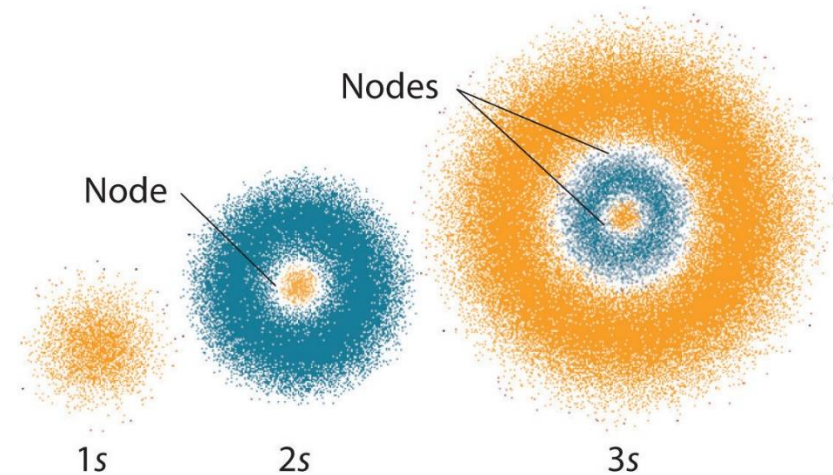
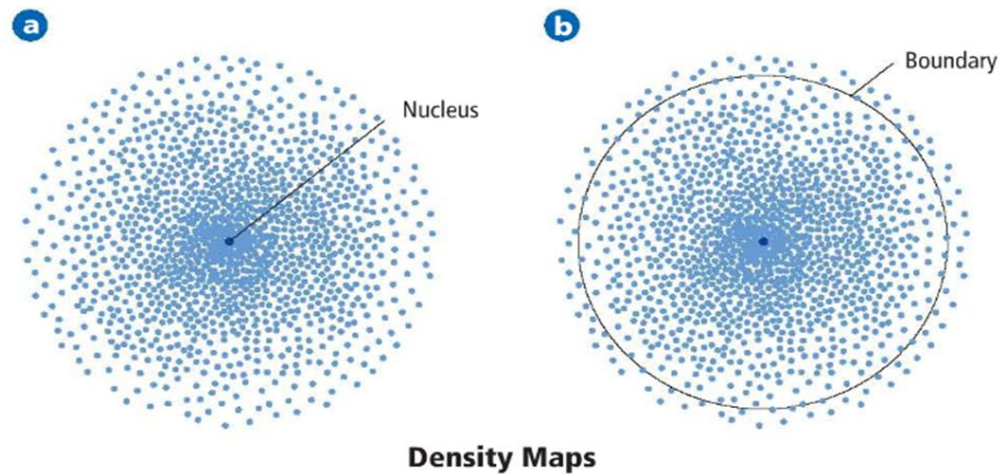
Key points:

- Electrons do not follow fixed paths
- They move randomly in areas of probability (orbitals)
- There are specific energies associated with each orbital



Quantum mechanical model

- The only quantity that can be known is the probability for an electron to occupy a certain region around the nucleus.
- Schrödinger's equation applied equally well to elements other than hydrogen (unlike Bohr's model).
- Bohr orbits were replaced with quantum-mechanical orbitals.



Quantum mechanical model

- Each electron is described by Four Quantum numbers (QN)
 - ✓ Principal QN (n)
 - ✓ Azimuthal QN / Subsidiary QN (l)
 - ✓ Magnetic QN (m)
 - ✓ Spin QN (s)

Quantum mechanical model

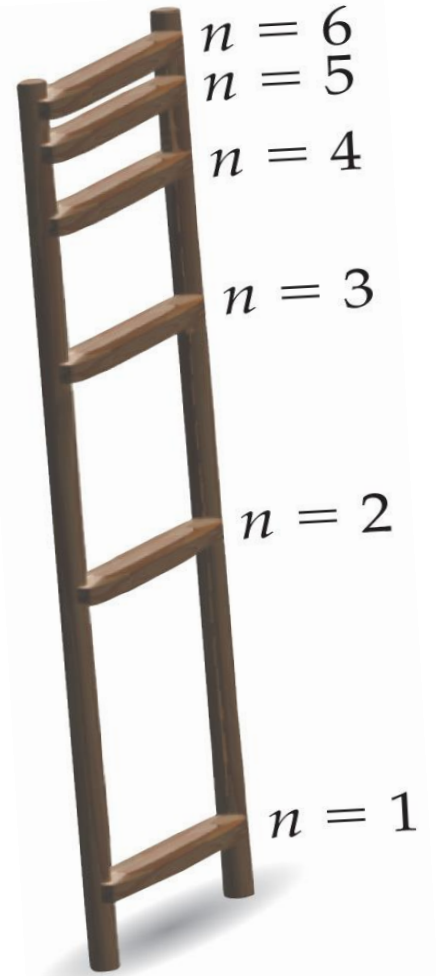
➤ Each electron is described by Four Quantum numbers (QM)

□ Principal QM (n) :

- indicates the relative size and energy of atomic orbitals.
 - $n = 1, 2, 3, \dots$
- ✓ This quantum number is the one on which the energy of an electron in an atom primarily depends.
- ✓ The smaller the value of n , the lower the energy and the smaller the orbital.

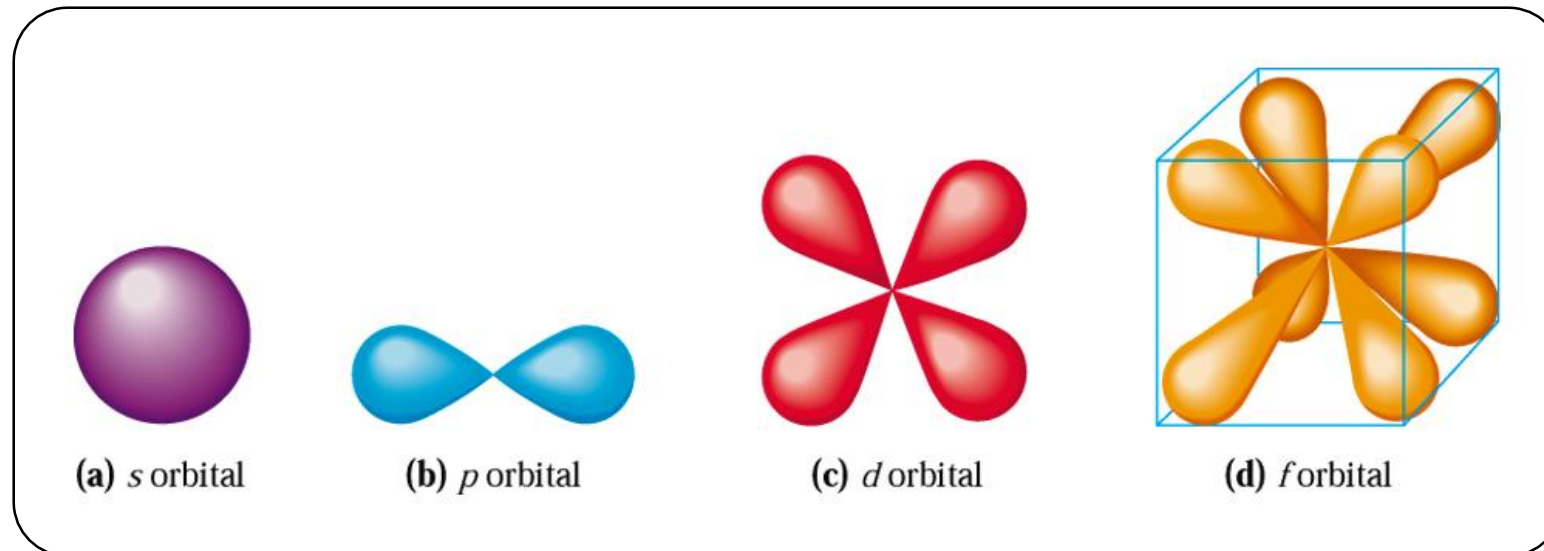
❖ Shells are sometimes designated by uppercase letters:

Letter	K	L	M	N	...
n	1	2	3	4	



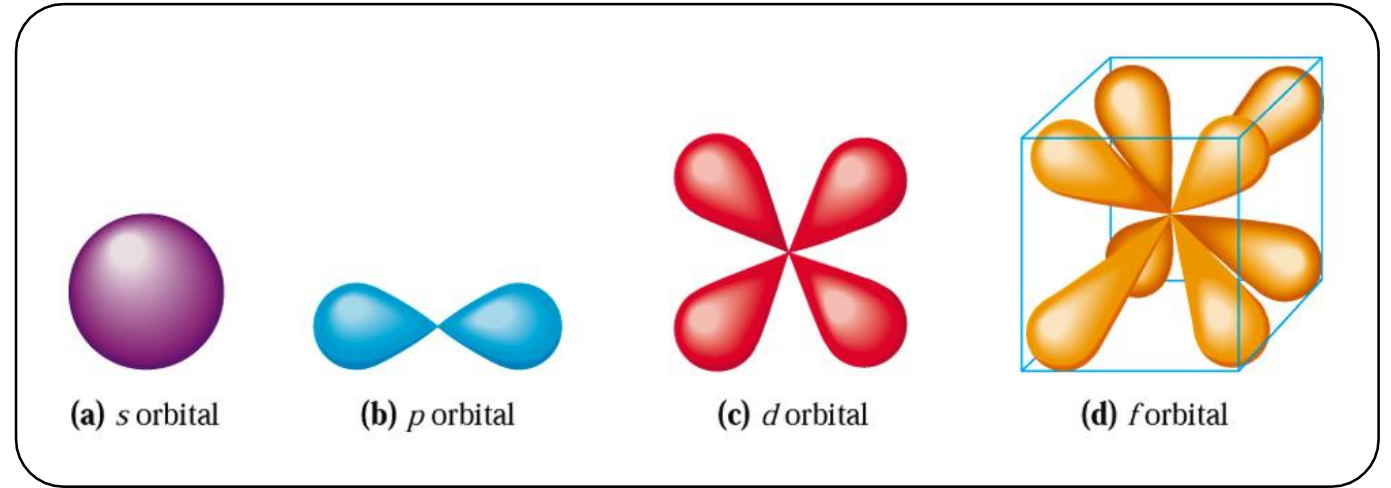
□ Azimuthal QM/Subsidiary QM/Angular momentum QM (l)

- ✓ This quantum number distinguishes orbitals of a given n (shell) having different shapes.
- ✓ It can have values from 0, 1, 2, 3, ... to a maximum of $(n - 1)$.
- ✓ For a given n , there will be n different values of l , or n types of subshells (denoted by s , p , d or f).



□ Azimuthal QM/Subsidiary QM/Angular momentum QM (l)

- ✓ s orbital has spherical shape
- ✓ p orbital has two lobes
- ✓ d orbital has four lobes and
- ✓ f orbital has eight lobes.



n	1	2	3	4
l	0	1	2	3
Letter	s	p	d	f

□ Azimuthal QM/Subsidiary QM/Angular momentum QM (l)

❖ *Not every subshell type exists in every shell!*

- 2p exists but 1p does not exist - why?

We know, $l = 0$ to $(n-1)$; the value of l cannot be equal to or greater than n

For 2p: $n = 2$, $l = 1$; which is valid

But for 1p: $n = 1$, $l = 1$; which is not valid.

□ Azimuthal QM/Subsidiary QM/Angular momentum QM (l)

❖ *Not every subshell type exists in every shell!*

- 3d exists but 2d does not exist - why?

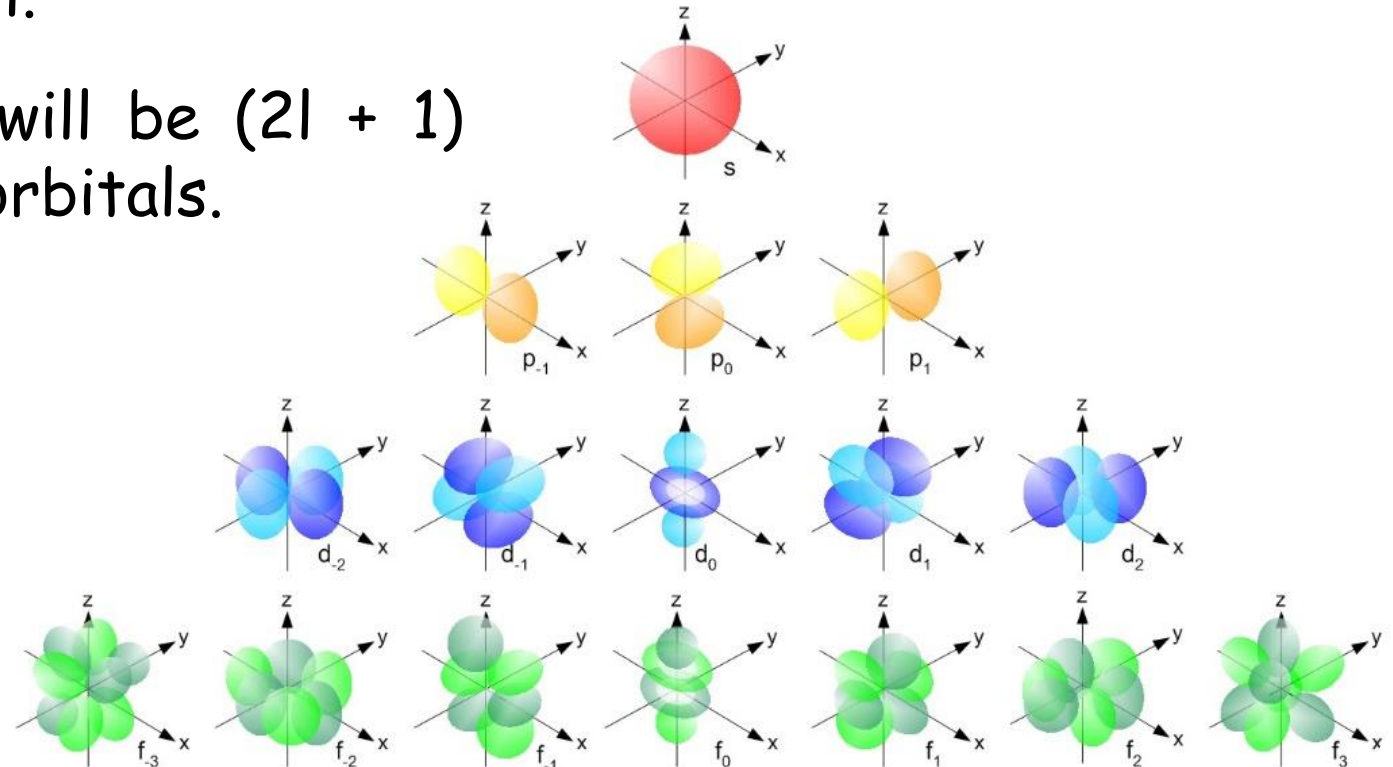
We know, $l = 0$ to $(n-1)$; the value of l cannot be equal to or greater than n

For 2d: $n = 2$, $l = 2$; which is not valid

But for 3d: $n = 3$, $l = 2$; which is valid.

□ Magnetic Quantum Number, m

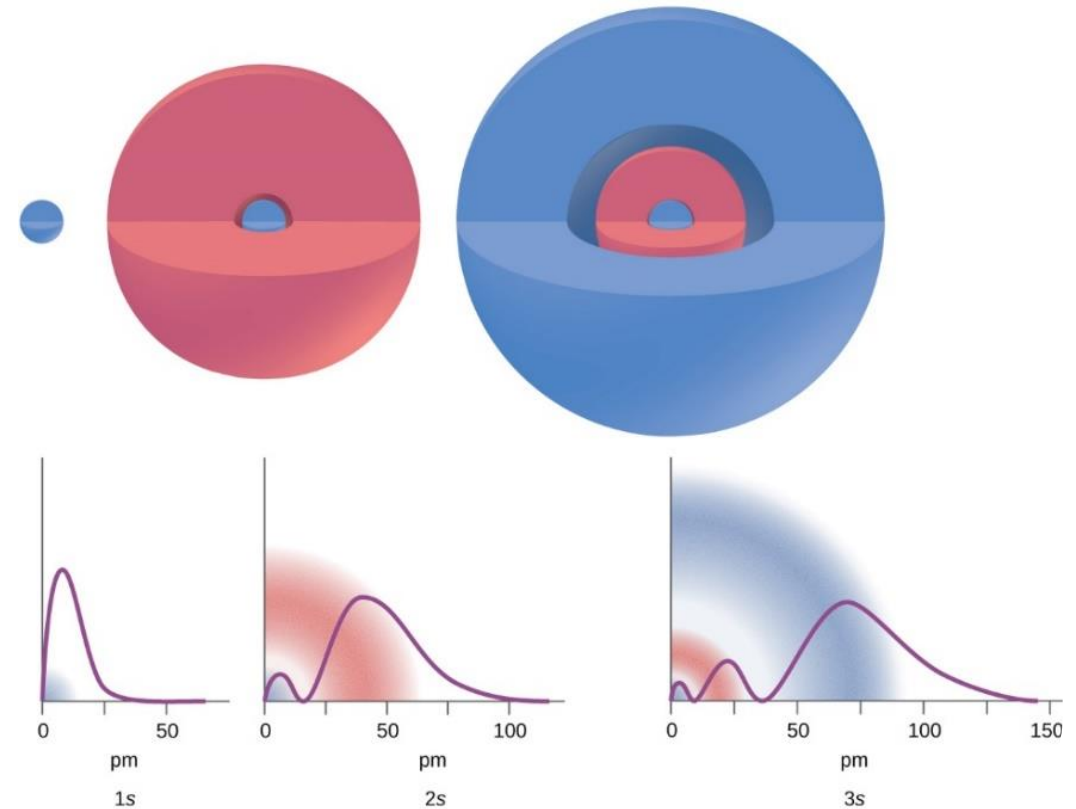
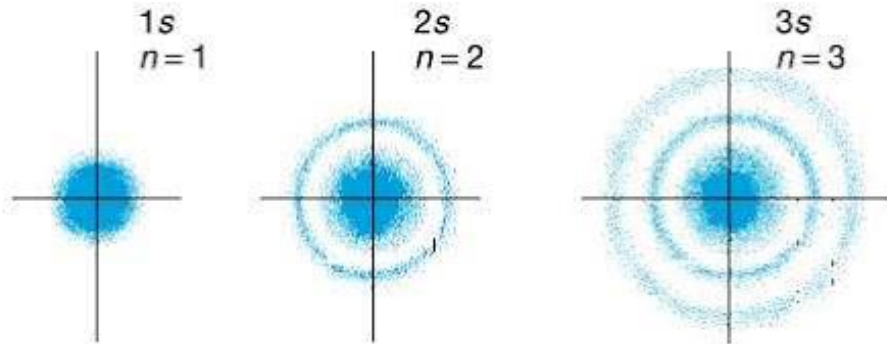
- This quantum number distinguishes orbitals of a given n and l - that is, of a given energy and shape but having different orientations.
- The magnetic quantum number depends on the value of l and can have any integer value from $-l$ to 0 to $+l$.
- For a given subshell, there will be $(2l + 1)$ values and therefore $(2l + 1)$ orbitals.



□ Magnetic Quantum Number, m

When $n = 1$, l has only one value, 0; therefore, m has only one value, 0.

So, the first shell ($n = 1$) has one subshell, an s-subshell, 1s. That subshell, in turn, has one orbital.

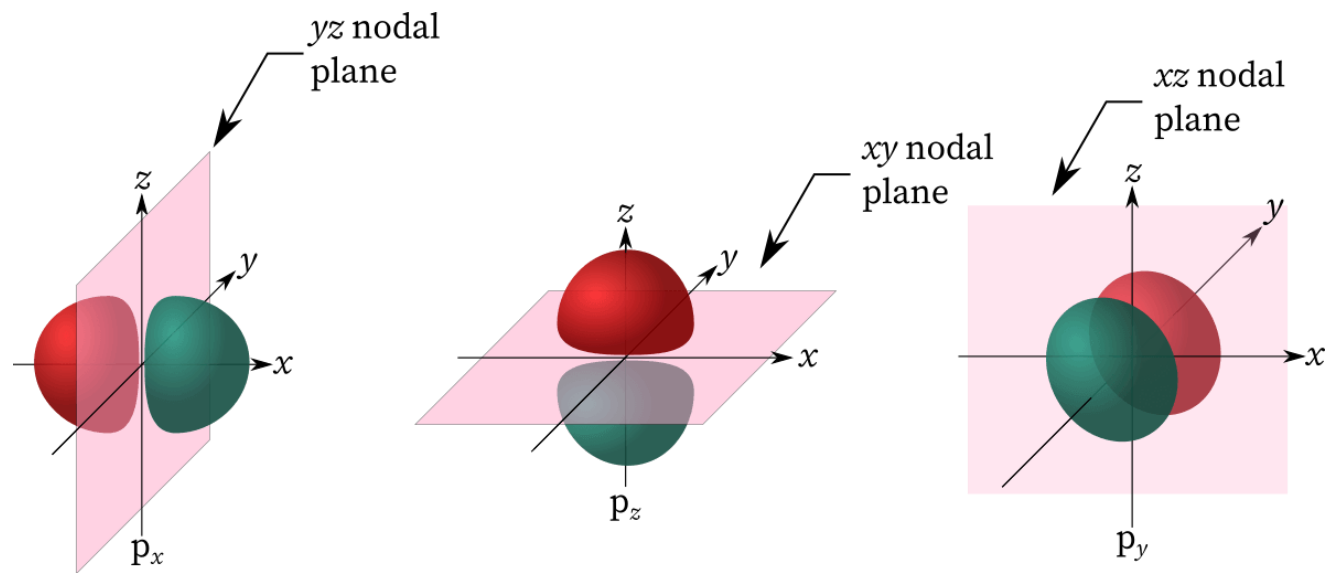


□ Magnetic Quantum Number, m

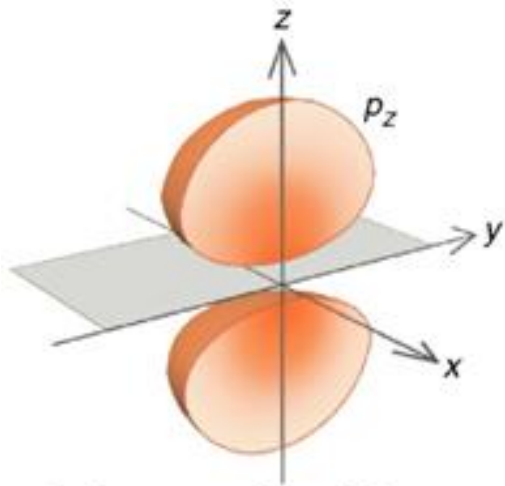
When $n = 2$, l has two values, 0 and 1.

When $l = 0$, m_l has only one value, 0. So there is a 2s subshell with one orbital.

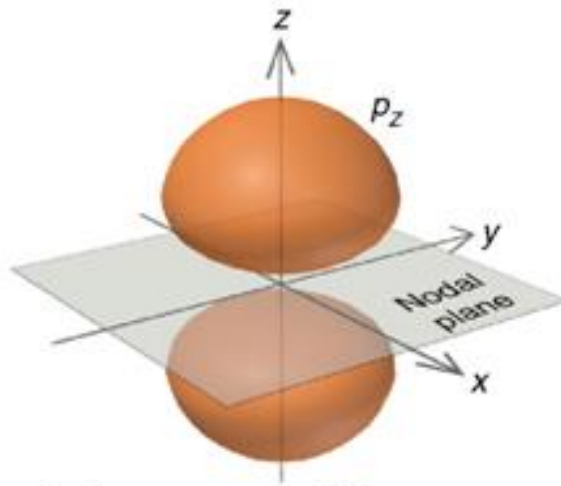
When $l = 1$, m_l has only three values, -1, 0, 1. So there is a 2p subshell with three orbitals.



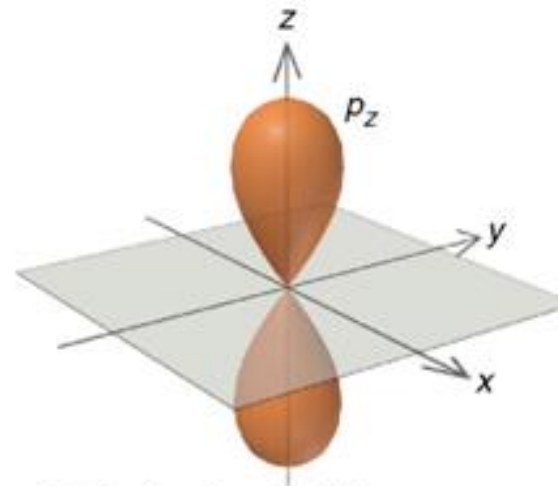
□ Magnetic Quantum Number, m



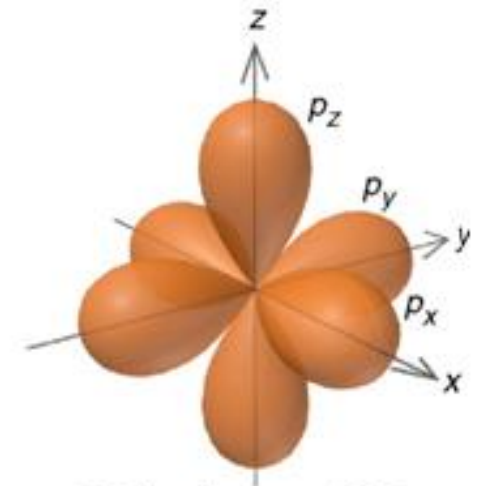
B Cross section of electron cloud depiction



C Accurate probability contour



D Stylized probability contour



E The three p orbitals

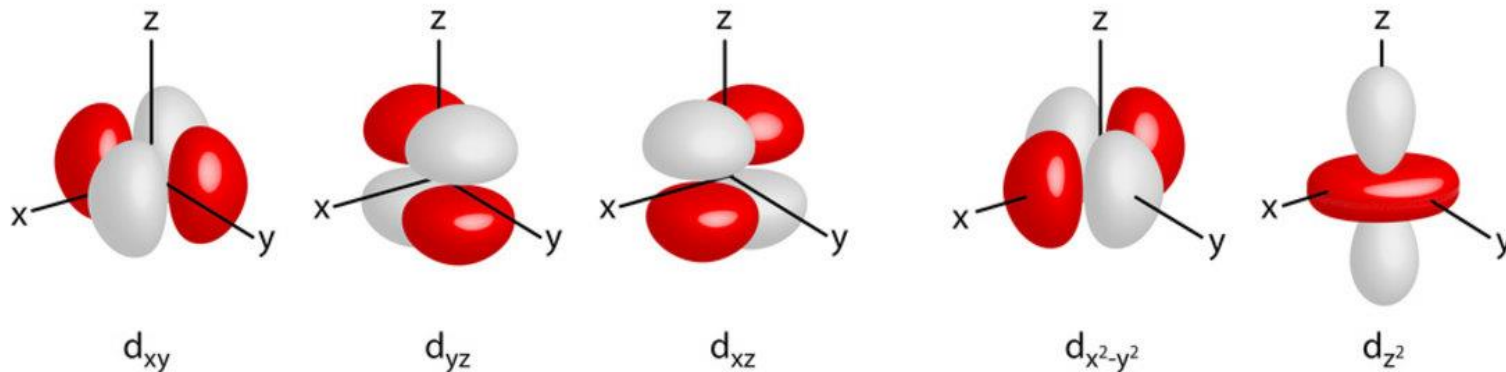
□ Magnetic Quantum Number, m

When $n = 3$, l has three values, 0, 1, and 2.

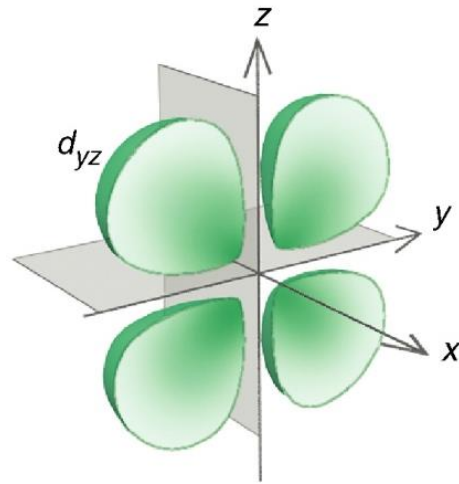
When $l = 0$, m_l has only one value, 0. So there is a 3s subshell with one orbital.

When $l = 1$, m_l has only three values, -1, 0, 1. So there is a 3p subshell with three orbitals.

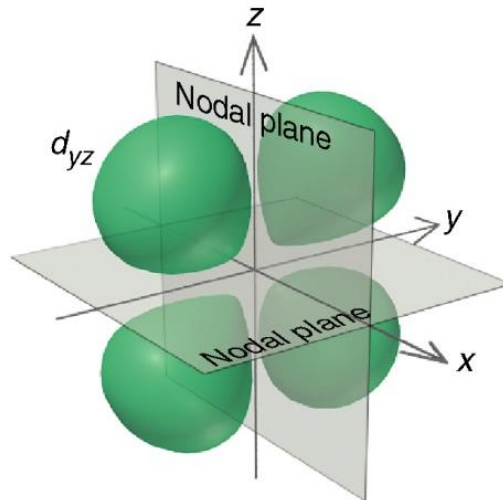
When $l = 2$, m_l has only five values, -2, -1, 0, 1, 2. So there is a 3d subshell with five orbitals



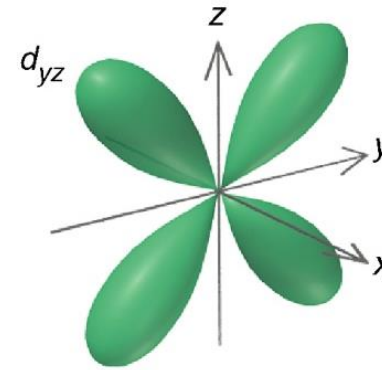
□ Magnetic Quantum Number, m



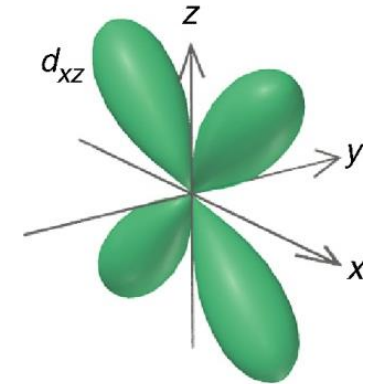
B Cross section of electron cloud depiction



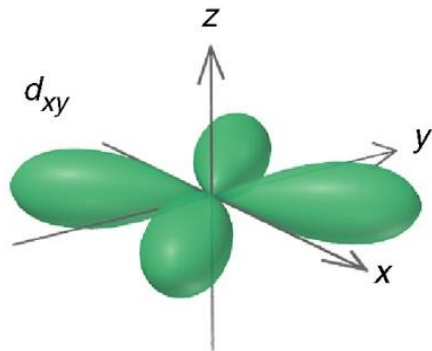
C Accurate probability contour



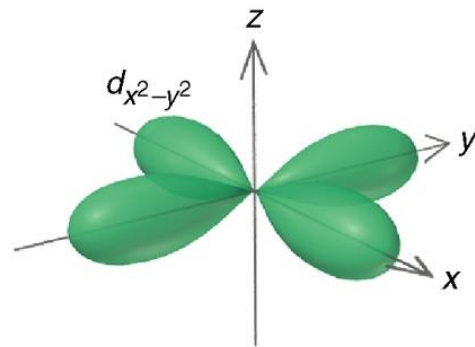
D Stylized probability contour



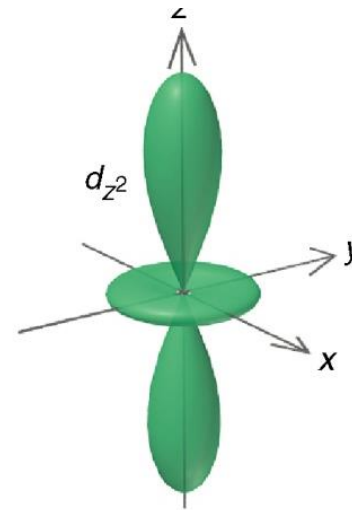
E



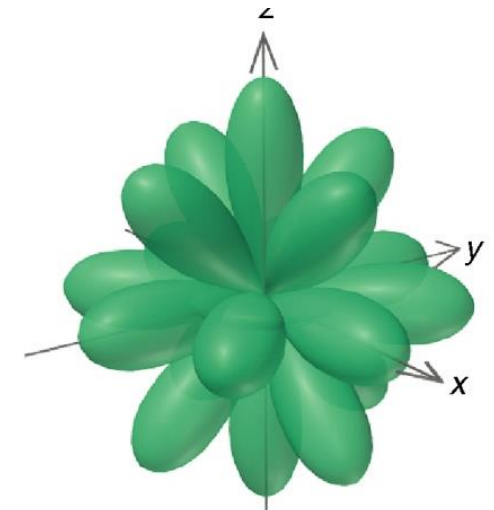
F



G



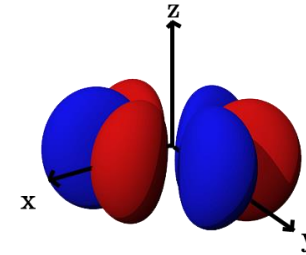
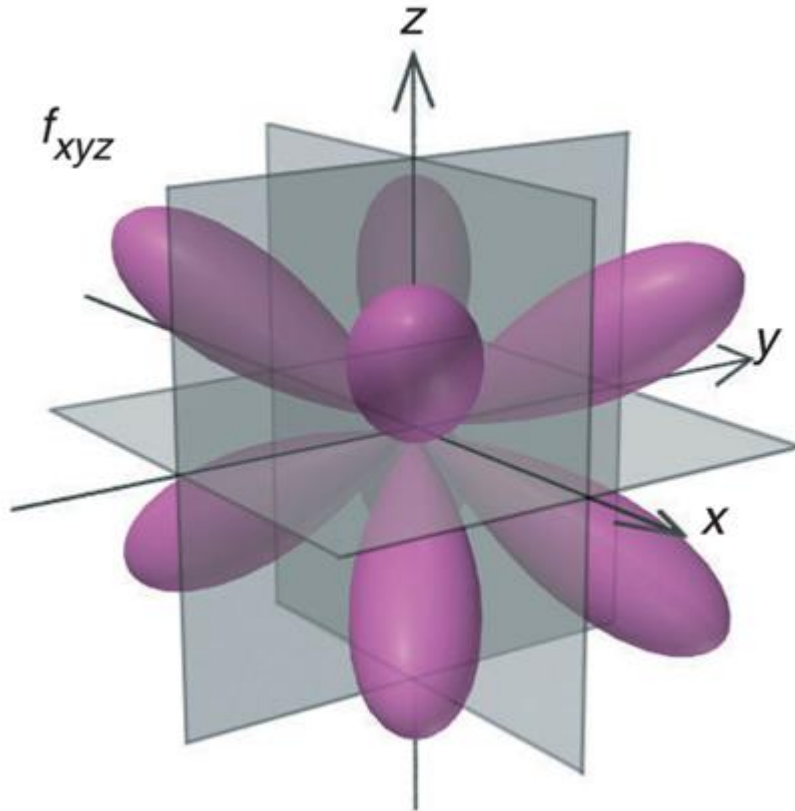
H



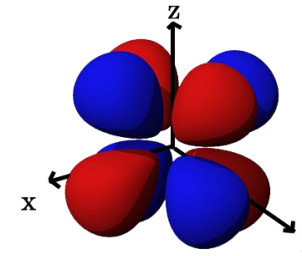
I The five d orbitals

□ Magnetic Quantum Number, m

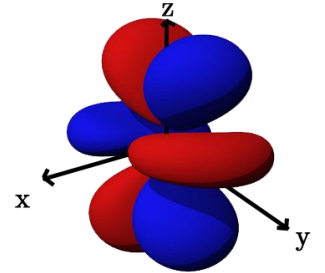
f orbitals



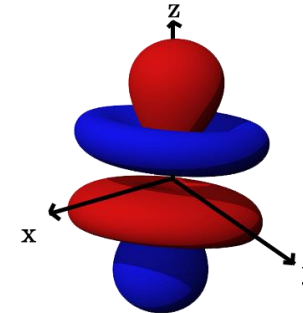
$f_{y(3x^2-y^2)}$



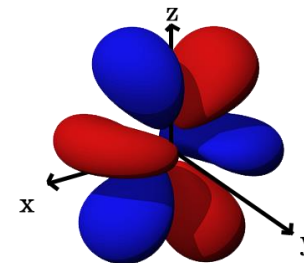
$f_{z(x^2-y^2)}$



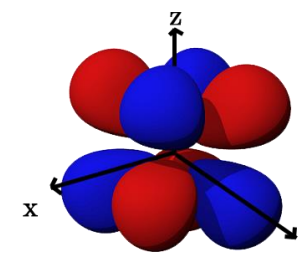
f_{yz^2}



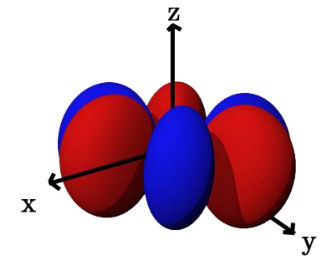
f_{z^3}



f_{xz^2}



f_{xyz}



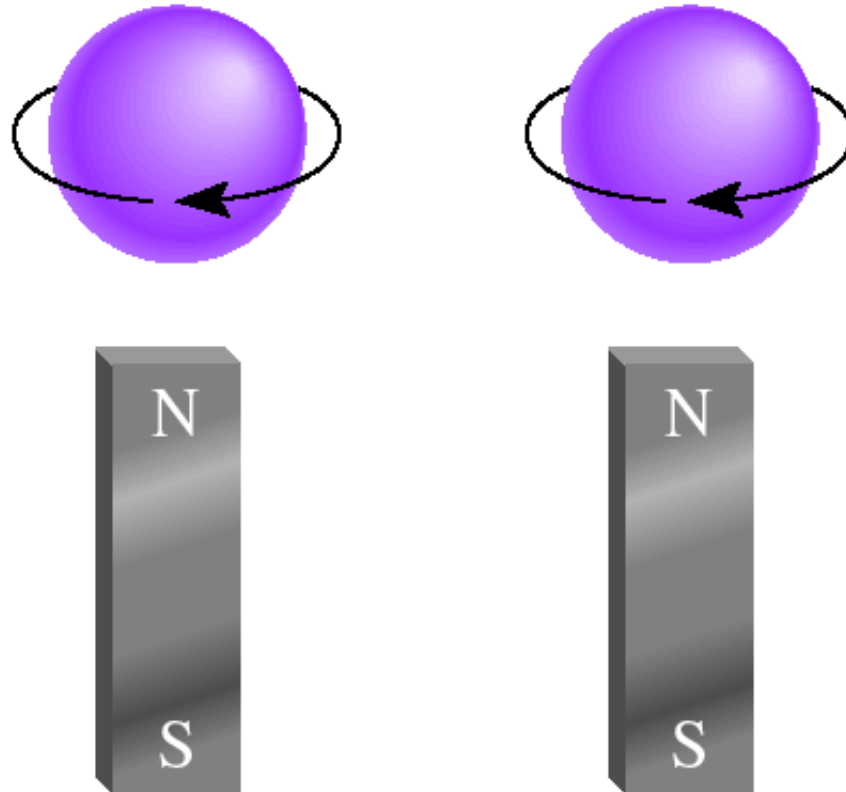
$f_{x(x^2-3y^2)}$

□ Spin Quantum Number (s):

- defines the direction of spin on an axis of each electron (one axis, therefore 2 spins possible)

Clockwise (+1/2)

Counterclockwise (-1/2)



Determining Quantum Numbers

Problem: What values of the angular momentum (l) and magnetic (m) quantum numbers are allowed for a principal quantum number (n) of 3? How many orbitals are allowed for $n = 3$?

SOLUTION: For $n = 3$, allowed values of l are $= 0, 1$, and 2

For $l = 0$ $m_l = 0$

For $l = 1$ $m_l = -1, 0$, or $+1$

For $l = 2$ $m_l = -2, -1, 0, +1$, or $+2$

There are 9 m_l values and therefore 9 orbitals with $n = 3$.

Determining Quantum Numbers

Problem: Give the name, magnetic quantum numbers, and number of orbitals for each sublevel with the following quantum numbers:

(a) $n = 3, l = 2$ (b) $n = 2, l = 0$ (c) $n = 5, l = 1$ (d) $n = 4, l = 3$

SOLUTION:

	n	l	sublevel name	possible m_l values	# of orbitals
(a)	3	2	3d	-2, -1, 0, 1, 2	5
(b)	2	0	2s	0	1
(c)	5	1	5p	-1, 0, 1	3
(d)	4	3	4f	-3, -2, -1, 0, 1, 2, 3	7

Determining Quantum Numbers

Problem: What is wrong with each of the following quantum numbers designations and/or sublevel names?

	n	l	m_l	Name
(a)	1	1	0	1p
(b)	4	3	+1	4d
(c)	3	1	-2	3p

SOLUTION:

- (a) A sublevel with $n = 1$ can only have $l = 0$, not $l = 1$. The only possible sublevel name is 1s.
- (b) A sublevel with $l = 3$ is an f sublevel, not a d . The name should be 4f.
- (c) A sublevel with $l = 1$ can only have m_l values of -1, 0, or +1, not -2.

Quantum Numbers and Atomic Orbitals

n	l	m_l^*	Subshell Notation	Number of Orbitals in the Subshell
1	0	0	1s	1
2	0	0	2s	1
2	1	-1, 0, +1	2p	3
3	0	0	3s	1
3	1	-1, 0, +1	3p	3
3	2	-2, -1, 0, +1, +2	3d	5
4	0	0	4s	1
4	1	-1, 0, +1	4p	3
4	2	-2, -1, 0, +1, +2	4d	5
4	3	-3, -2, -1, 0, +1, +2, +3	4f	7

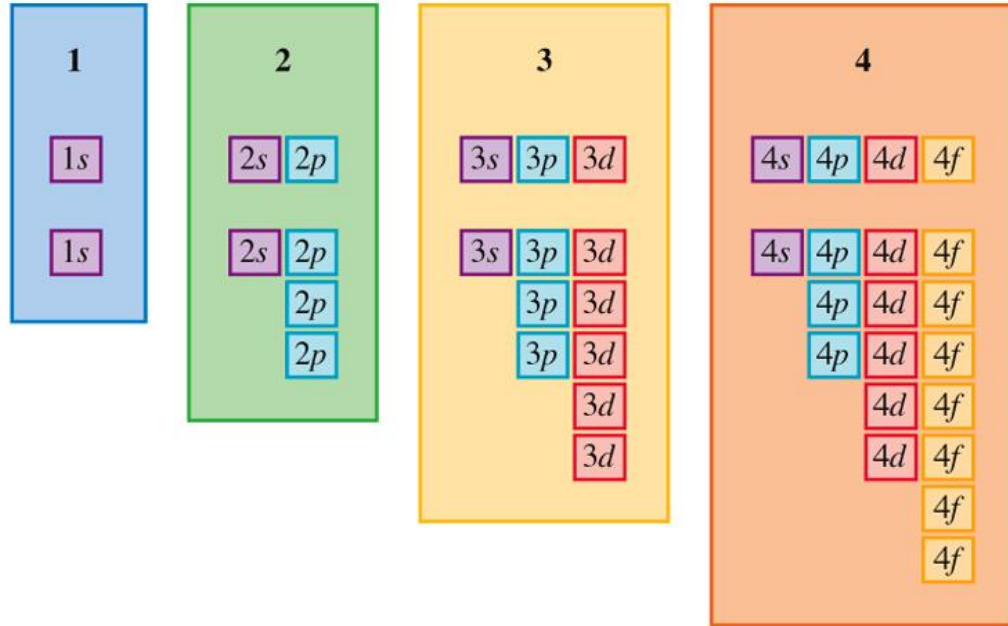
*Any one of the m_l quantum numbers may be associated with the n and l quantum numbers on the same line

Subshell arrangement

SHELLS

SUBSHELLS

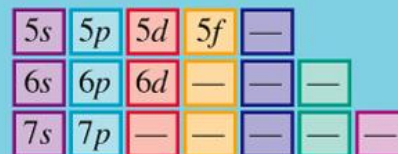
ORBITALS



IMPORTANT NUMERICAL RELATIONSHIPS

- Subshells within a shell = shell number
- Orbitals within a subshell depends on shell type:
1 for s 3 for p 5 for d 7 for f
- Electrons within an orbital = 2

Beginning with shell 5, not all subshells are needed to accommodate electrons. Those needed are



SHELL 4

4 subshells

$4f$ (14 electrons)
 $4d$ (10 electrons)
 $4p$ (6 electrons)
 $4s$ (2 electrons)

SHELL 3

3 subshells

$3d$ (10 electrons)
 $3p$ (6 electrons)
 $3s$ (2 electrons)

SHELL 2

2 subshells

$2p$ (6 electrons)
 $2s$ (2 electrons)

SHELL 1

1 subshell

$1s$ (2 electrons)

□ Aufbau Principle

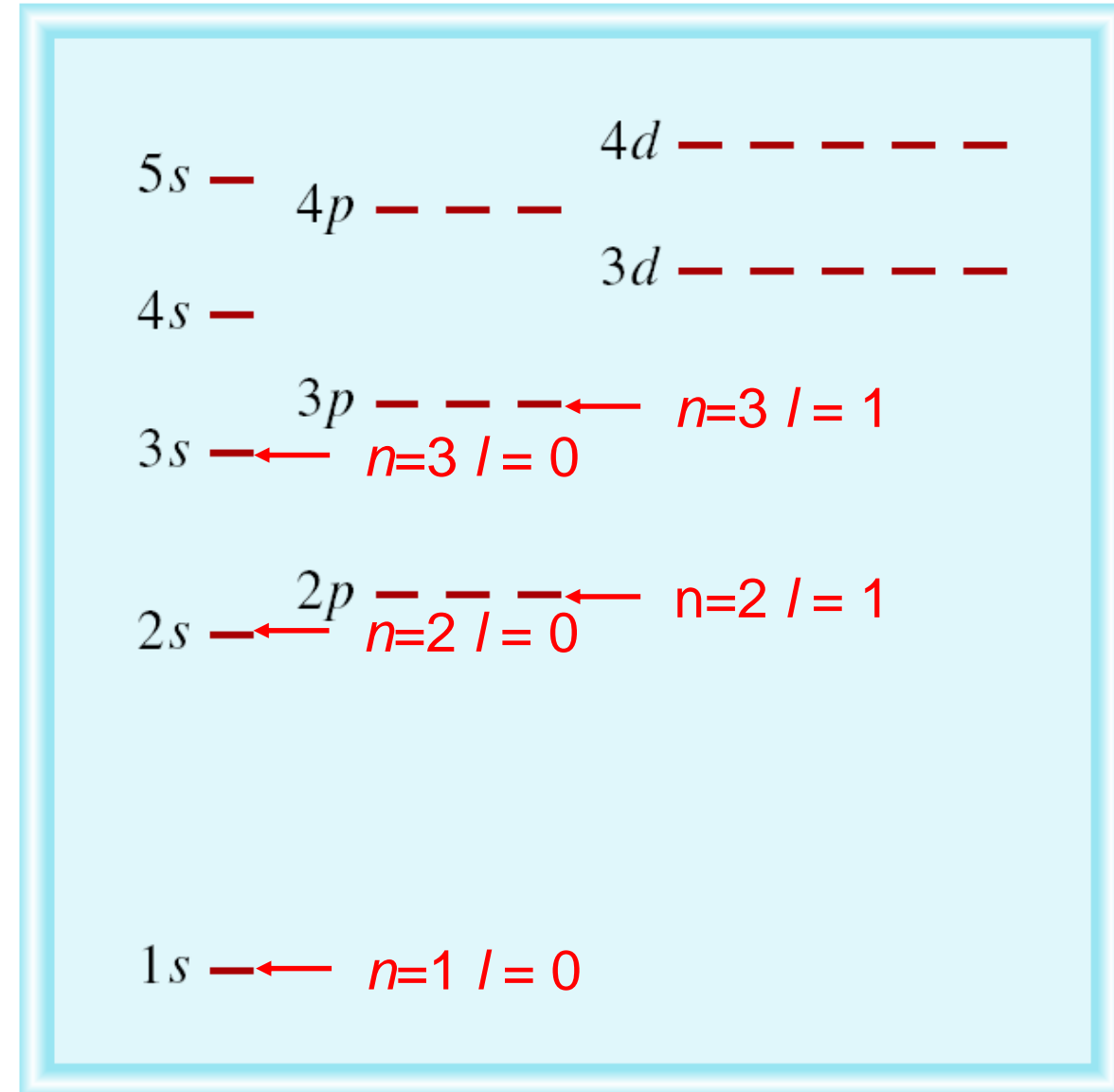
- In an atom, electrons fill up the orbitals with lowest energy first, and gradually fill up the orbitals in increasing order of energy.
- Energy of an orbital is the sum of n and l .

- For example:

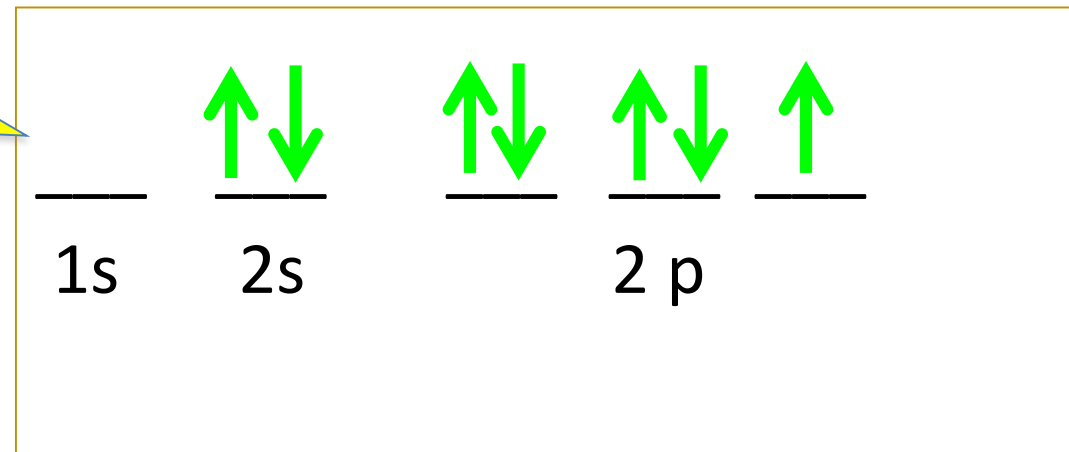
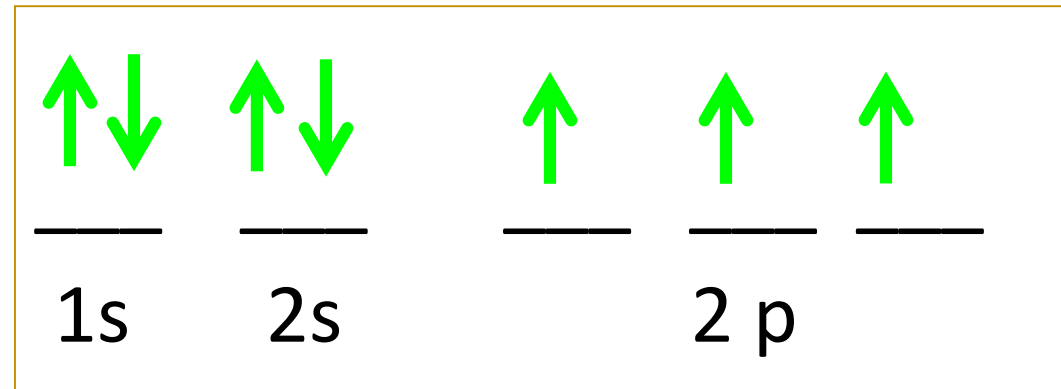
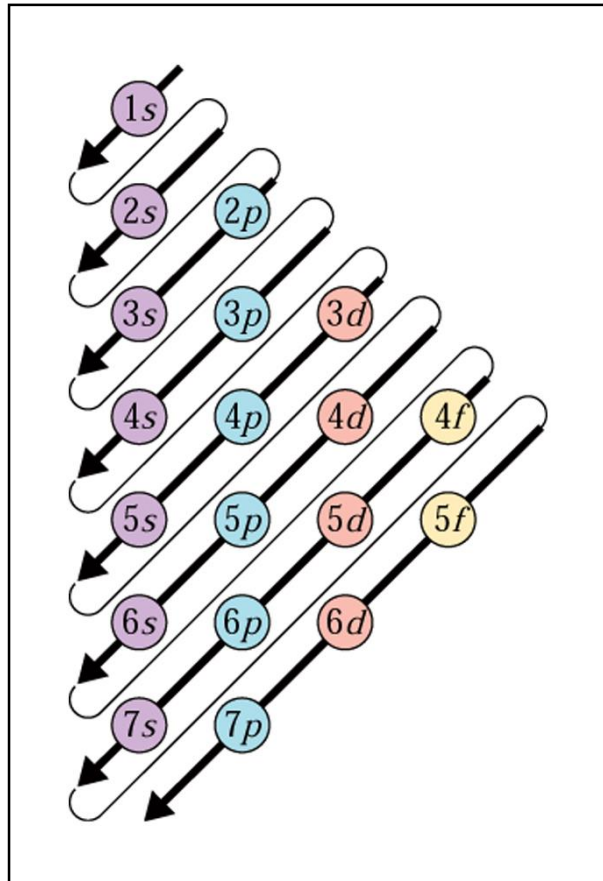
Energy of $3d$ is $(3+2) = 5$

Energy of $4s$ is $(4+0) = 4$

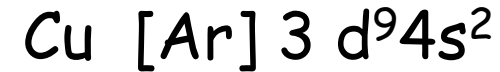
Energy ↑



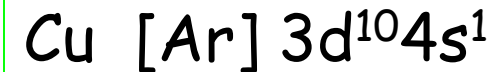
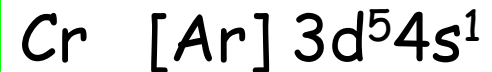
□ Aufbau Principle



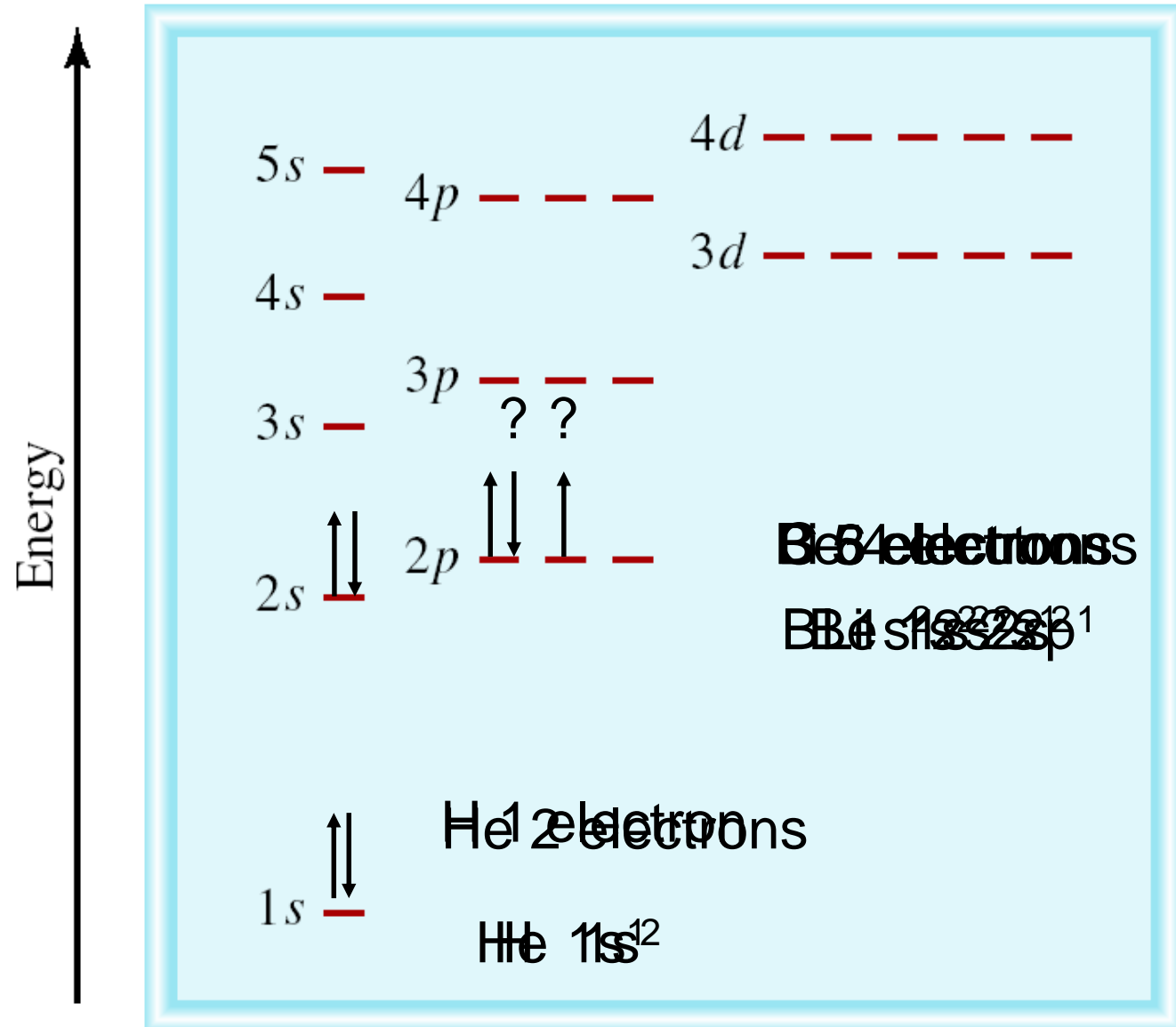
Exceptions to the Aufbau Rule



However, the actual electron configuration, determined experimentally, are:

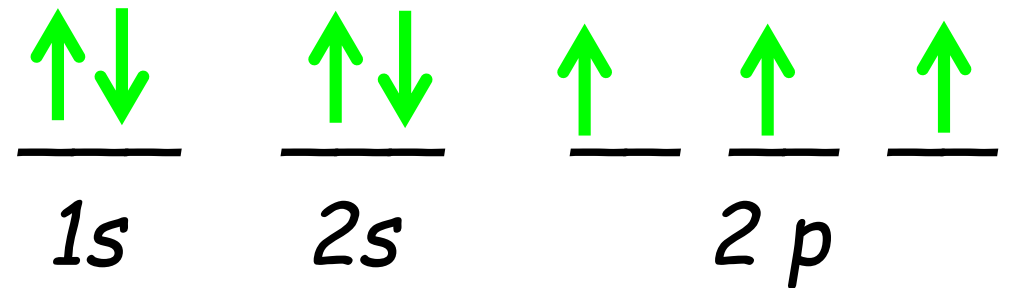
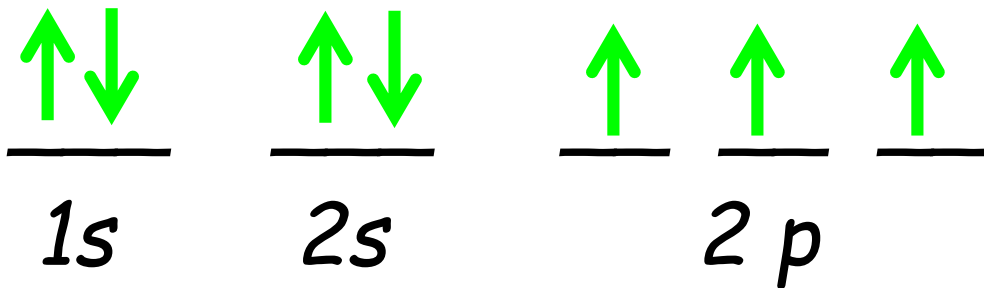
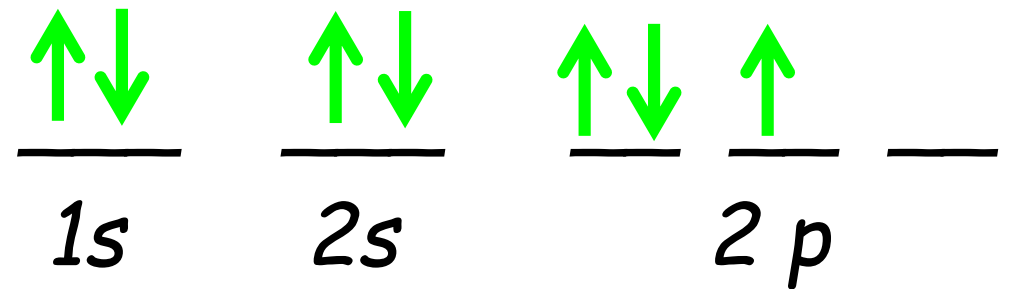
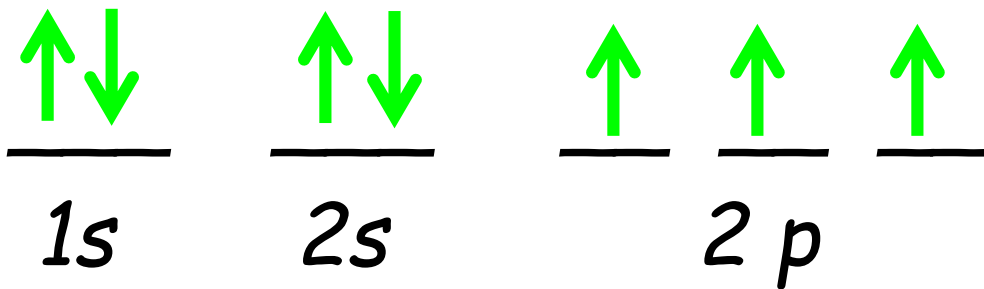


□ Hund's Rule



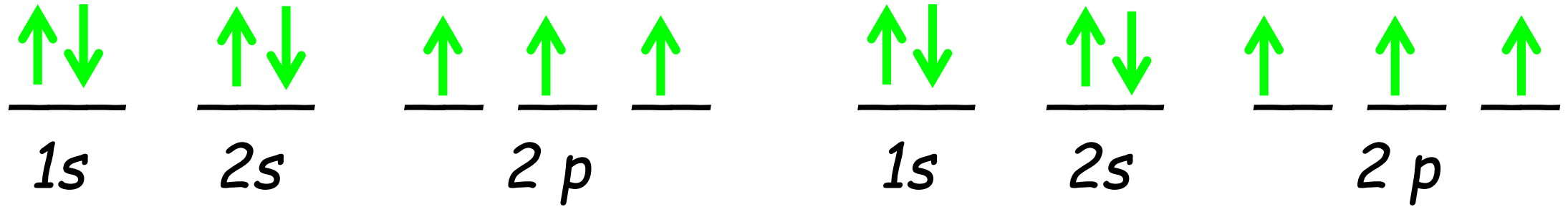
□ Hund's Rule

- Every orbital in a subshell is singly occupied with one electron before any an orbital is doubly occupied, and all electrons in singly occupied orbitals have the same spin.



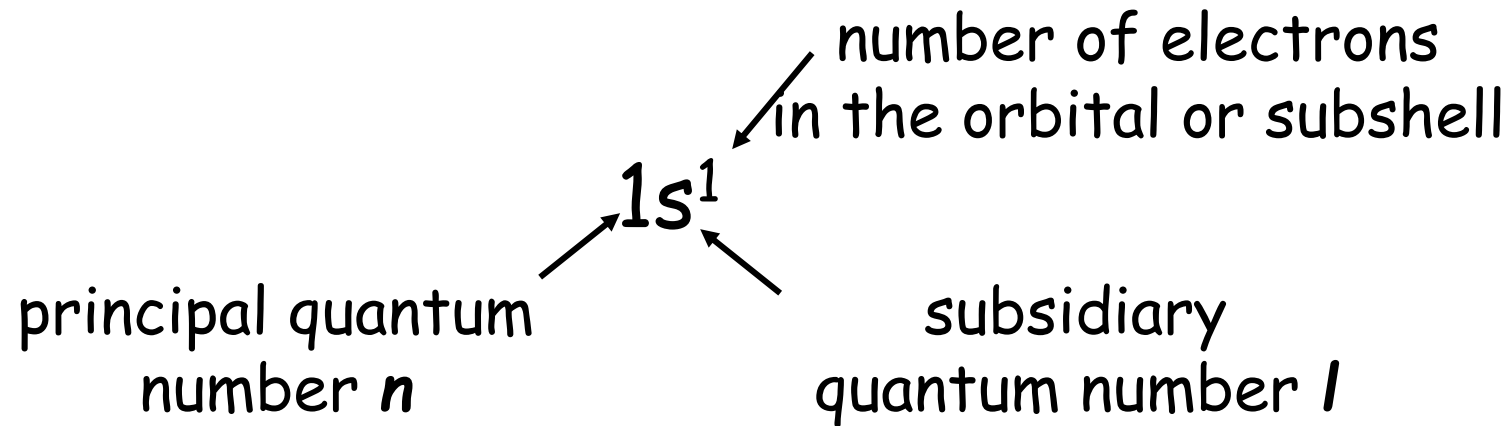
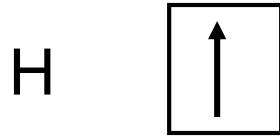
□ Pauli's exclusion Principle

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



Electron Configurations of Atoms

- Electron configuration is how the electrons are distributed among the various atomic orbitals in an atom.



Electron Configurations of Atoms

- What is the electron configuration of Mg?

Mg 12 electrons

$1s < 2s < 2p < 3s < 3p < 4s$

$1s^2 2s^2 2p^6 3s^2$ $2 + 2 + 6 + 2 = 12$ electrons

$[\text{Ne}] 1s^2 2s^2 2p^6$ Therefore, Mg is sometimes abbreviated as $[\text{Ne}] 3s^2$

Electron Configurations of Atoms

- What are the possible quantum numbers for the last (outermost) electron in Cl?

Cl 17 electrons $1s < 2s < 2p < 3s < 3p < 4s$

$1s^2 2s^2 2p^6 3s^2 3p^5$ $2 + 2 + 6 + 2 + 5 = 17$ electrons

Last electron added to 3p orbital

$n = 3$ $l = 1$ $m_l = -1, 0, \text{ or } +1$ $m_s = \frac{1}{2} \text{ or } -\frac{1}{2}$

Electron Configurations of Atoms

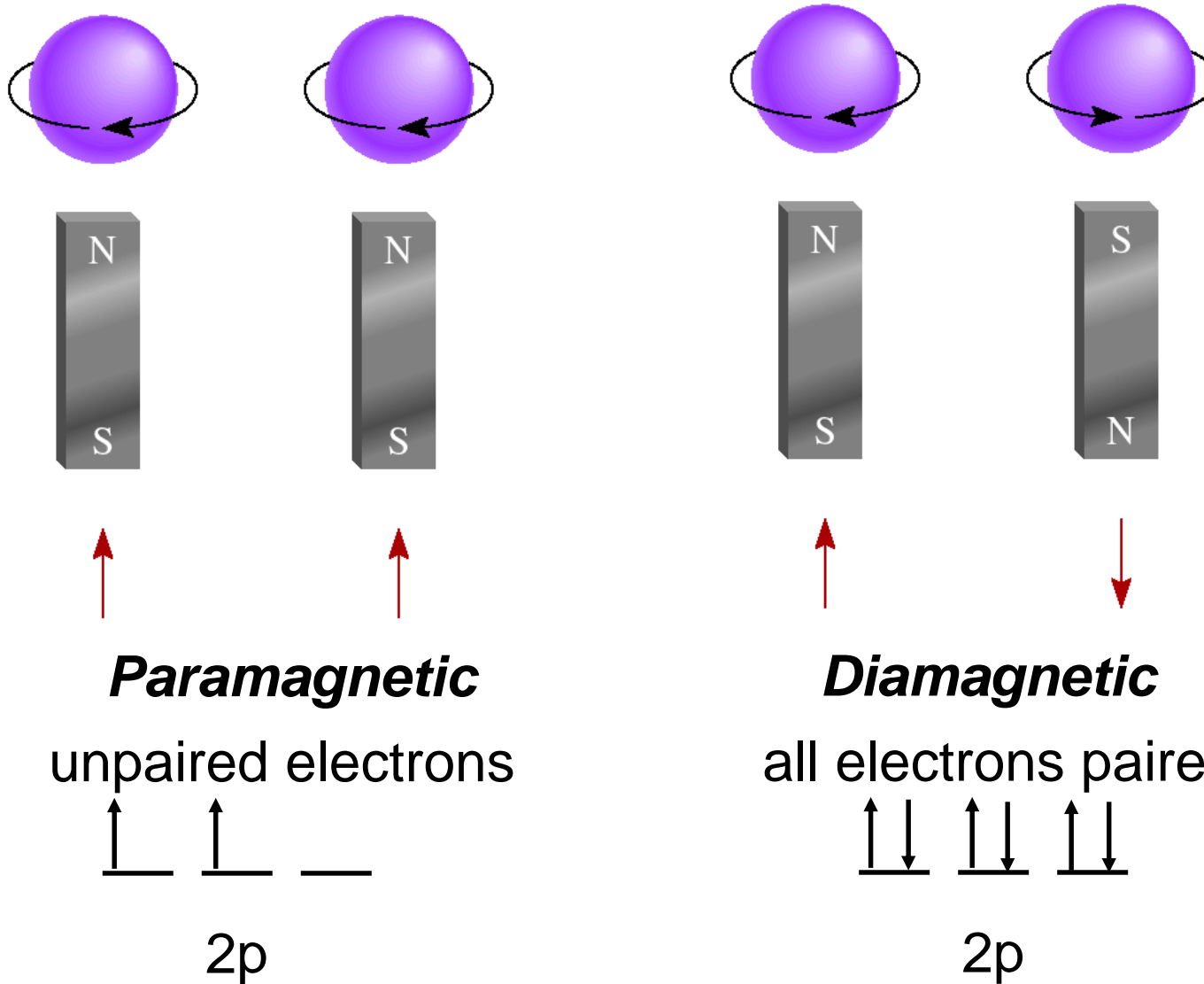
Atomic Number	Symbol	Electron Configuration	Atomic Number	Symbol	Electron Configuration	Atomic Number	Symbol	Electron Configuration
1	H	$1s^1$	38	Sr	$[\text{Kr}]5s^2$	75	Re	$[\text{Xe}]6s^24f^{14}5d^5$
2	He	$1s^2$	39	Y	$[\text{Kr}]5s^24d^1$	76	Os	$[\text{Xe}]6s^24f^{14}5d^6$
3	Li	$[\text{He}]2s^1$	40	Zr	$[\text{Kr}]5s^24d^2$	77	Ir	$[\text{Xe}]6s^24f^{14}5d^7$
4	Be	$[\text{He}]2s^2$	41	Nb	$[\text{Kr}]5s^14d^4$	78	Pt	$[\text{Xe}]6s^14f^{14}5d^9$
5	B	$[\text{He}]2s^22p^1$	42	Mo	$[\text{Kr}]5s^14d^5$	79	Au	$[\text{Xe}]6s^14f^{14}5d^{10}$
6	C	$[\text{He}]2s^22p^2$	43	Tc	$[\text{Kr}]5s^24d^5$	80	Hg	$[\text{Xe}]6s^24f^{14}5d^{10}$
7	N	$[\text{He}]2s^22p^3$	44	Ru	$[\text{Kr}]5s^14d^7$	81	Tl	$[\text{Xe}]6s^24f^{14}5d^{10}6p^1$
8	O	$[\text{He}]2s^22p^4$	45	Rh	$[\text{Kr}]5s^14d^8$	82	Pb	$[\text{Xe}]6s^24f^{14}5d^{10}6p^2$
9	F	$[\text{He}]2s^22p^5$	46	Pd	$[\text{Kr}]4d^{10}$	83	Bi	$[\text{Xe}]6s^24f^{14}5d^{10}6p^3$
10	Ne	$[\text{He}]2s^22p^6$	47	Ag	$[\text{Kr}]5s^14d^{10}$	84	Po	$[\text{Xe}]6s^24f^{14}5d^{10}6p^4$
11	Na	$[\text{Ne}]3s^1$	48	Cd	$[\text{Kr}]5s^24d^{10}$	85	At	$[\text{Xe}]6s^24f^{14}5d^{10}6p^5$
12	Mg	$[\text{Ne}]3s^2$	49	In	$[\text{Kr}]5s^24d^{10}5p^1$	86	Rn	$[\text{Xe}]6s^24f^{14}5d^{10}6p^6$
13	Al	$[\text{Ne}]3s^23p^1$	50	Sn	$[\text{Kr}]5s^24d^{10}5p^2$	87	Fr	$[\text{Rn}]7s^1$
14	Si	$[\text{Ne}]3s^23p^2$	51	Sb	$[\text{Kr}]5s^24d^{10}5p^3$	88	Ra	$[\text{Rn}]7s^2$
15	P	$[\text{Ne}]3s^23p^3$	52	Te	$[\text{Kr}]5s^24d^{10}5p^4$	89	Ac	$[\text{Rn}]7s^26d^1$
16	S	$[\text{Ne}]3s^23p^4$	53	I	$[\text{Kr}]5s^24d^{10}5p^5$	90	Th	$[\text{Rn}]7s^26d^2$
17	Cl	$[\text{Ne}]3s^23p^5$	54	Xe	$[\text{Kr}]5s^24d^{10}5p^6$	91	Pa	$[\text{Rn}]7s^25f^26d^1$
18	Ar	$[\text{Ne}]3s^23p^6$	55	Cs	$[\text{Xe}]6s^1$	92	U	$[\text{Rn}]7s^25f^36d^1$
19	K	$[\text{Ar}]4s^1$	56	Ba	$[\text{Xe}]6s^2$	93	Np	$[\text{Rn}]7s^25f^46d^1$

Electron Configurations of Atoms

1s		1s
2s		2p
3s		3p
4s	3d	4p
5s	4d	5p
6s	5d	6p
7s	6d	7p

4f
5f

Electron Configurations and Magnetic Properties



Thank You