

Atomic Structure

Chemistry, Zumdahl & Zumdahl – Chapter 7

Houssam El-Rassy, PhD

Assistant Professor

Department of Chemistry, Room 520

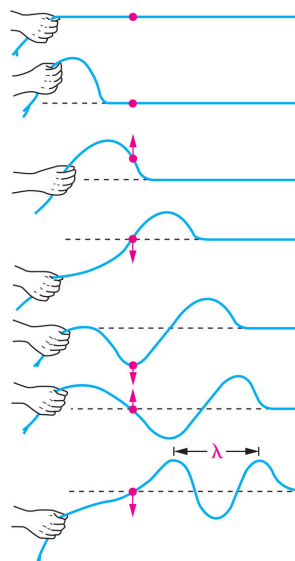
Ext. 4051 , E-mail: Houssam.Rassy@aub.edu.lb

June 22, 2011

American University of Beirut

Properties of Waves

- Electric and magnetic fields propagate as waves through empty space or through a medium.
- A wave transmits energy.



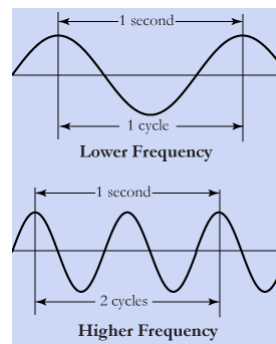
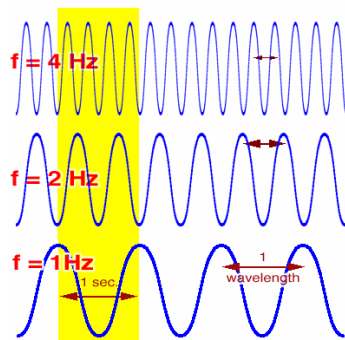
Copyright © 2007 Pearson Prentice Hall, Inc.

WAVELENGTH - The distance between identical points on successive waves. (λ)

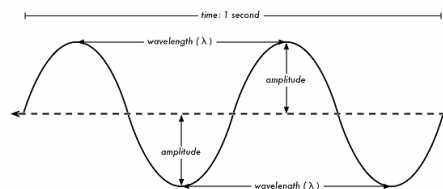
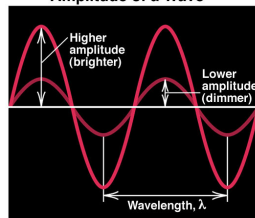
cm μm nm \AA pm
 (10^{-2} m) (10^{-6} m) (10^{-9} m) (10^{-10} m) (10^{-12} m)

FREQUENCY - The number of waves that pass through a particular point per second. (ν) – in Hz or s^{-1}

AMPLITUDE - The vertical distance from the midline to a peak, or trough in the wave.

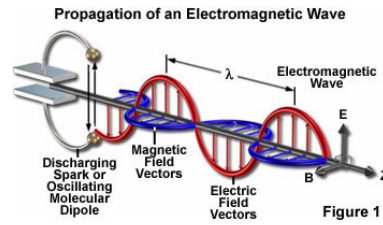
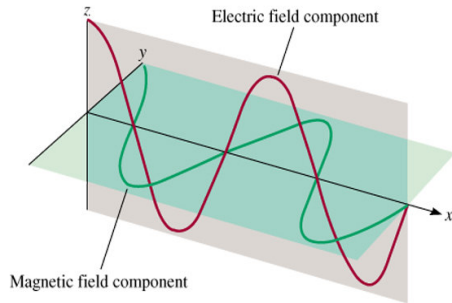


Amplitude of a Wave



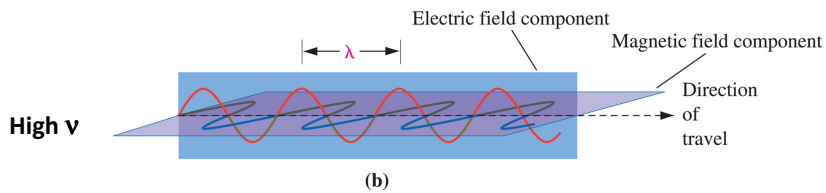
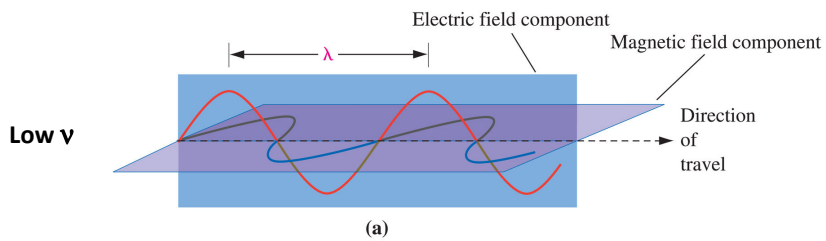
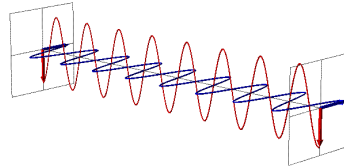
Maxwell (1873), proposed that **visible light consists of electromagnetic waves.**

Electromagnetic radiation is the emission and transmission of energy in the form of electromagnetic waves.

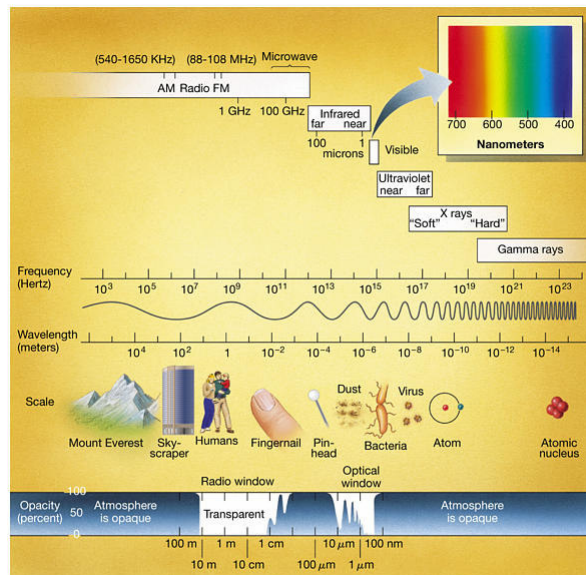
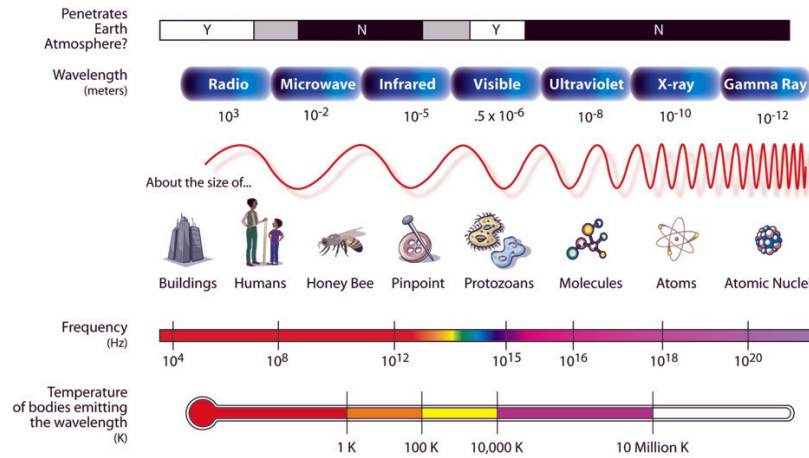


Speed of light (c) in vacuum = 3.00×10^8 m/s

All electromagnetic radiation
 $\lambda \times \nu = c$



THE ELECTROMAGNETIC SPECTRUM



EXAMPLE 8-1

Relating Frequency and Wavelength of Electromagnetic Radiation. Most of the light from a sodium vapor lamp has a wavelength of 589 nm. What is the frequency of this radiation?

Solution

We can first convert the wavelength of the light from nanometers to meters and then apply equation (8.1).

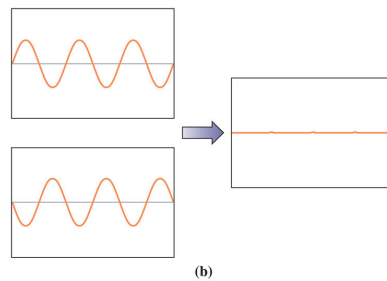
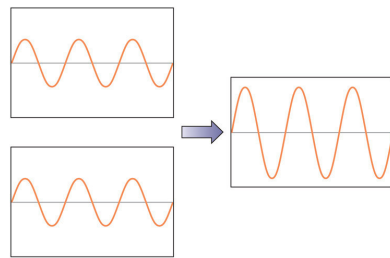
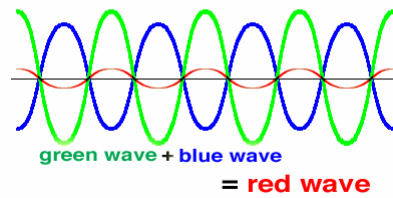
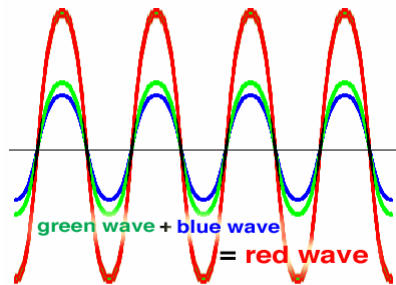
$$\lambda = 589 \text{ nm} \times \frac{1 \times 10^{-9} \text{ m}}{1 \text{ nm}} = 5.89 \times 10^{-7} \text{ m}$$

$$c = 2.998 \times 10^8 \text{ ms}^{-1}$$

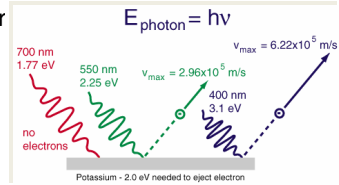
$$\nu = ?$$

Rearrange equation (8.1) to the form $\nu = c/\lambda$, and solve for ν .

$$\nu = \frac{c}{\lambda} = \frac{2.998 \times 10^8 \text{ m s}^{-1}}{5.89 \times 10^{-7} \text{ m}} = 5.09 \times 10^{14} \text{ s}^{-1} = 5.09 \times 10^{14} \text{ Hz}$$

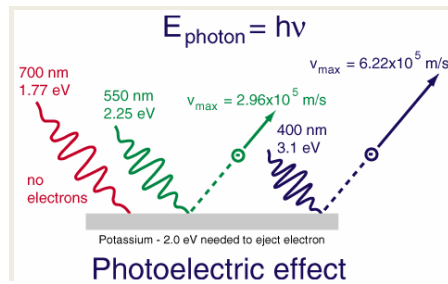


The photoelectron effect refers to the phenomenon in which electrons are emitted from the surface of a metal when light strikes it.



The following observations characterize the photoelectric effect:

- Studies in which the frequency of light is varied show that no electrons are emitted by a given metal below a specific threshold frequency ν_0 .
- For light with frequency lower than the threshold frequency, no electrons are emitted regardless of the intensity of the light.
- For light with frequency greater than the threshold frequency, the number of electrons emitted increases with the intensity of light.
- For light with frequency greater than the threshold frequency, the kinetic energy of the emitted electrons increases linearly with the frequency of the light.



Photoelectric effect

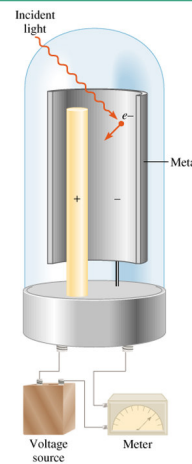
$$KE_{\text{electron}} = \frac{1}{2} mv^2 = hv - hv_0$$

Mass of electron

Velocity of electron

Energy of incident photon

Energy required to remove electron from metal's surface

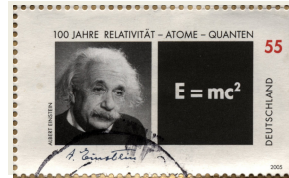


$h = 6.62607 \times 10^{-34} \text{ Js}$: Planck's constant

In a related development, Einstein derived the famous equation:

$$E = mc^2$$

Energy Mass Speed of light



$$E_{\text{photon}} = hc/\lambda$$

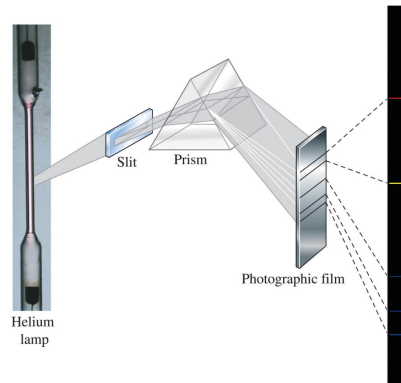
The apparent mass of a photon of light with wavelength λ is given by

$$m = E/c^2 = (hc/\lambda)/c^2 = h/\lambda c$$

$$m = h/\lambda v$$

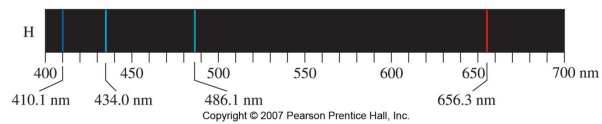
$$\lambda = h/mv \quad \text{de Broglie's equation}$$

Helium

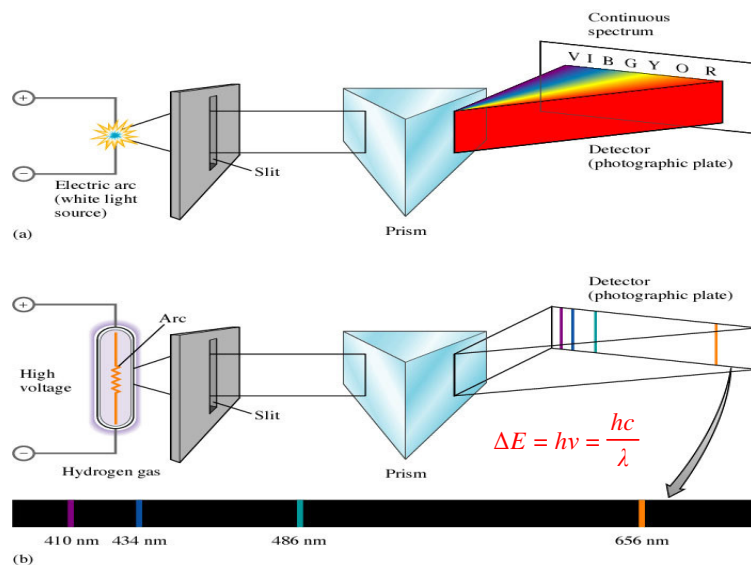


Copyright © 2007 Pearson Prentice Hall, Inc.

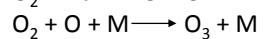
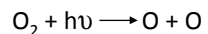
Hydrogen



Copyright © 2007 Pearson Prentice Hall, Inc.



Chemical reactions that are induced by light are called photochemical reactions.



M is a "third body" such as N_2

Photon can be treated like reactant.

$$\lambda = 242.4 \text{ nm}$$

EXAMPLE 8 - 2

Using Planck's Equation to Calculate the Energy of Photons of Light. For radiation of wavelength 242.4 nm, the longest wavelength that will bring about the photodissociation of O_2 , what is the energy of (a) one photon, and (b) a mole of photons of this light?

- (a) To use Planck's equation, we need the frequency of the radiation. This we can get from equation (8.1) after first expressing the wavelength in meters.

$$\nu = \frac{c}{\lambda} = \frac{2.998 \times 10^8 \text{ m s}^{-1}}{242.4 \times 10^{-9} \text{ m}} = 1.237 \times 10^{15} \text{ s}^{-1}$$

Planck's equation is written for *one* photon of light. We emphasize this by including the unit, photon^{-1} , in the value of h .

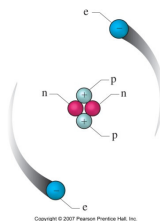
$$\begin{aligned} E &= h\nu = 6.626 \times 10^{-34} \times \frac{\text{J s}}{\text{photon}} \times 1.237 \times 10^{15} \text{ s}^{-1} \\ &= 8.196 \times 10^{-19} \text{ J/photon} \end{aligned}$$

- (b) Once we have the energy per photon, we can multiply it by the Avogadro constant to convert to a per-mole basis.

$$\begin{aligned} E &= 8.196 \times 10^{-19} \text{ J/photon} \times 6.022 \times 10^{23} \text{ photons/mol} \\ &= 4.936 \times 10^5 \text{ J/mol} \end{aligned}$$

(This quantity of energy is sufficient to raise the temperature of 10.0 L of water by 11.8 °C.)

- Rutherford assumed the electrons orbited the nucleus analogous to planets around the sun.

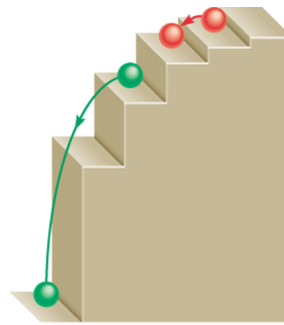


- However, a charged particle moving in a circular path should lose energy.
- This means that the atom should be unstable according to Rutherford's theory.
- Bohr noted the line spectra of certain elements and assumed the electrons were confined to specific energy states. These were called **orbits**.

- Since the energy states are quantized, the light emitted from excited atoms must be quantized and appear as line spectra.
- After lots of math, Bohr showed that:

$$E_n = -R_H \left(\frac{1}{n^2} \right)$$

where n is the **principal quantum number** (i.e., $n = 1, 2, 3, \dots$ and nothing else), and R_H is the Rydberg constant = 2.18×10^{-18} J.



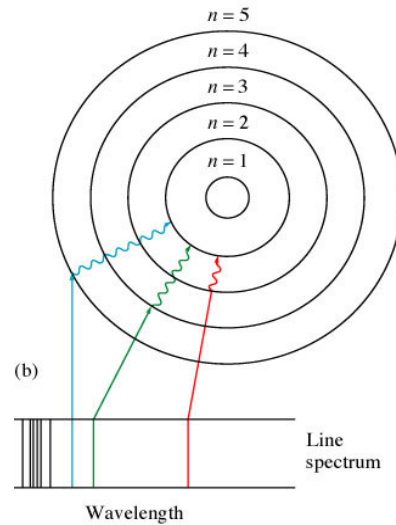
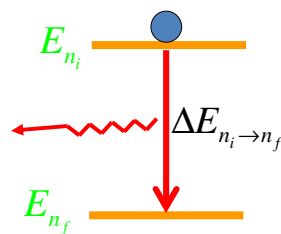
- The first orbit in the Bohr model has $n = 1$ (ground state) is closest to the nucleus, and has negative energy by convention.
- The furthest orbit in the Bohr model has n close to infinity and corresponds to zero energy.
- Electrons in the Bohr model can only move between orbits by absorbing and emitting energy in quanta ($h\nu$).
- The amount of energy absorbed or emitted on movement between states is given by:

$$\Delta E = E_f - E_i = h\nu$$

We have the resonance condition: $\Delta E = E_f - E_i = h\nu$

We can easily show that the frequency of emitted photon when the electron transits from n_i to n_f is:

$$\nu = \frac{\Delta E}{h} = \left(\frac{R_H}{h} \right) \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$



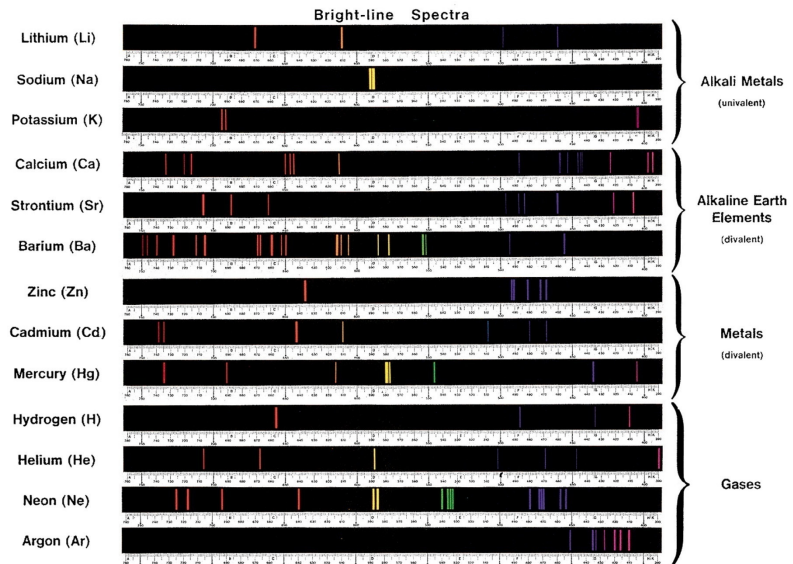
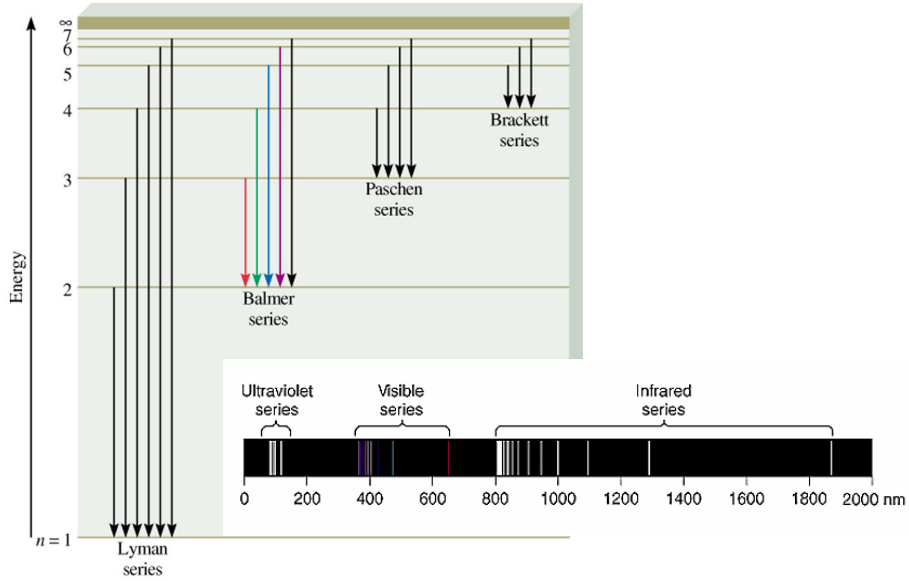
If we fix n_f and consider the transitions from $n_i > n_f$ then we obtain series of lines:

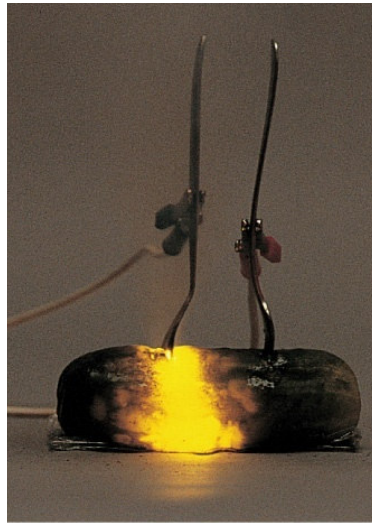
- When $n_f = 2$: this is the **Balmer** series of **VISIBLE** lines:

$$\Delta E_{n_i \rightarrow 2} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad n_i = 3, 4, 5, \dots$$

- When $n_f = 1$: this is the **Lyman** series of **UV** lines:

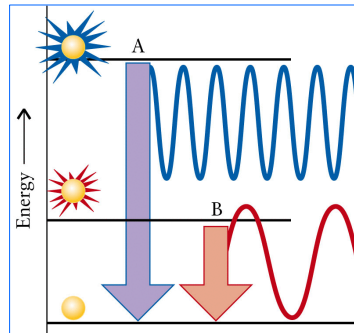
$$\Delta E_{n_i \rightarrow 1} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad n_i = 2, 3, 4, 5, \dots$$





When a high voltage is applied between the forks, some of the sodium ions in the pickle are converted to sodium atoms in the excited state.

These atoms emit the characteristic yellow light as they relax to the ground state.



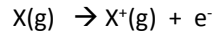
What is the energy gap between the first and second electronic orbit of H?

$$\begin{aligned}
 E_2 & \text{ --- } \\
 & \updownarrow \Delta E \\
 E_1 & \text{ --- }
 \end{aligned}
 \quad
 \begin{aligned}
 \Delta E = E_2 - E_1 &= \left(\frac{-R_H}{n_2^2} \right) - \left(\frac{-R_H}{n_1^2} \right) \\
 &= \left(\frac{-R_H}{2^2} \right) - \left(\frac{-R_H}{1^2} \right) \\
 &= R_H \left(\frac{1}{1^2} - \frac{1}{2^2} \right) = \frac{3}{4} R_H = 1.64 \times 10^{-18} \text{ J}
 \end{aligned}$$

If an electron transits from $n = 2$ to $n = 1$, then the frequency of the photon emitted is:

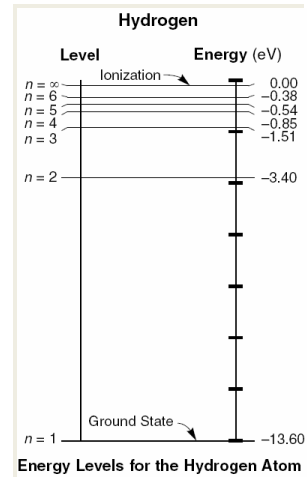
$$\begin{aligned}
 \nu &= \frac{|\Delta E|}{h} = \frac{1.64 \times 10^{-18} \text{ J}}{6.626 \times 10^{-34} \text{ J} \cdot \text{s}} \\
 &= 2.475 \times 10^{15} \text{ s}^{-1} \text{ (Hz)}
 \end{aligned}$$

The ionization energy is the energy required to remove an electron from a gaseous atom or ion:



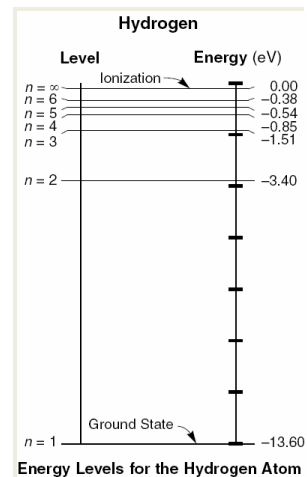
What is the ionization energy of Hydrogen ?

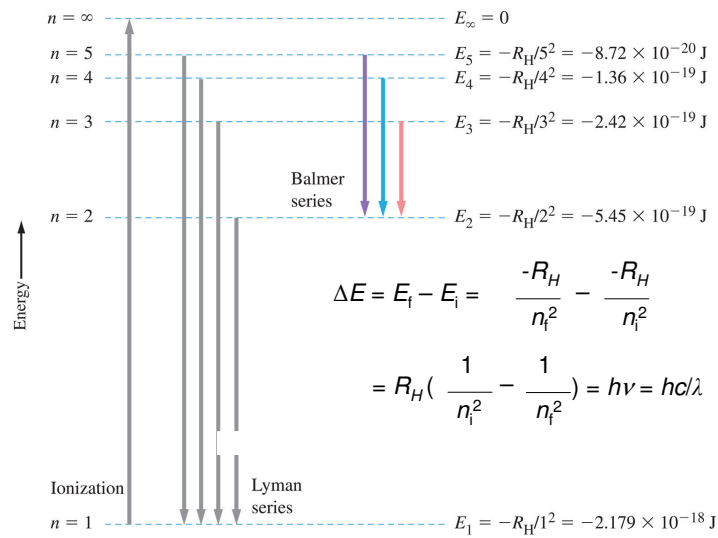
$$\begin{aligned} \Delta E_{\text{ionization}} &= E_f - E_i = \left(\frac{-R_H}{n_f^2} \right) - \left(\frac{-R_H}{n_i^2} \right) \\ &= \left(\frac{-R_H}{\infty^2} \right) - \left(\frac{-R_H}{1^2} \right) \\ &= 0 - \left(\frac{-R_H}{1^2} \right) = +R_H = 2.18 \times 10^{-18} \text{ J} \end{aligned}$$



What is the ionization energy of Hydrogen from $n=2$?

$$\begin{aligned} \Delta E'_{\text{ionization}} &= E_f - E_i = \left(\frac{-R_H}{n_f^2} \right) - \left(\frac{-R_H}{n_i^2} \right) \\ &= \left(\frac{-R_H}{\infty^2} \right) - \left(\frac{-R_H}{2^2} \right) \\ &= 0 - \left(\frac{-R_H}{2^2} \right) = \frac{+R_H}{4} = 5.45 \times 10^{-19} \text{ J} \end{aligned}$$





A transition to $n = 4$ results in emission of a photon of frequency $1.141 \times 10^{14} \text{ Hz}$. What is the initial energy level of the electron?

$$\Delta E = h\nu = (6.626 \times 10^{-34} \text{ J}\cdot\text{s}) (1.141 \times 10^{14} \text{ s}^{-1}) = 7.560 \times 10^{-20} \text{ J}$$

$$\Delta E = -7.560 \times 10^{-20} \text{ J} \quad \text{since light is emitted.}$$

$$\Delta E = E_4 - E_n = -7.560 \times 10^{-20} \text{ J} \Rightarrow$$

$$-7.560 \times 10^{-20} \text{ J} = -(2.178 \times 10^{-18} \text{ J}) \left(\frac{1}{4^2} - \frac{1}{n^2} \right) \Rightarrow$$

$$3.71 \times 10^{-2} = 6.250 \times 10^{-2} - \frac{1}{n^2} \Rightarrow n^2 = 35.98$$

$$\Rightarrow n = 6$$

For Hydrogen-like ions, the Bohr's energy Formula becomes:

$$E_{\text{hydrogenlike}} = -R_H \left(\frac{Z^2}{n^2} \right)$$

Z is the nuclear charge.

For He^+ , $Z = 2$

For Li^{2+} , $Z = 3$

For Be^{3+} , $Z = 4$

EXAMPLE 8-5

Using the Bohr Model. Determine the kinetic energy of the electron ionized from a Li^{2+} ion in its ground state, using a photon of frequency $5.000 \times 10^{16} \text{ s}^{-1}$.

Solution

The energy of the electron in the Li^{2+} ion is calculated using equation (8.9).

$$E_1 = \frac{-3^2 \times 2.179 \times 10^{-18} \text{ J}}{1^2} = -1.961 \times 10^{-17} \text{ J} \quad \text{Should be positive}$$

The energy of a photon of frequency $5.000 \times 10^{16} \text{ s}^{-1}$ is

$$E = h\nu = 6.626 \times 10^{-34} \times \frac{\text{J s}}{\text{photon}} \times 5.000 \times 10^{16} \text{ s}^{-1} = 3.313 \times 10^{-17} \text{ J photon}^{-1}$$

The ionization energy, the energy required to remove the electron, is $E_i = E_1 = 1.961 \times 10^{-17} \text{ J}$. The extra energy from the photon is transferred as kinetic energy to the electron. Thus, the kinetic energy of the electron is

$$\text{kinetic energy} = 3.313 \times 10^{-17} \text{ J} - 1.961 \times 10^{-17} \text{ J} = 1.352 \times 10^{-17} \text{ J}$$

- Can't explain emission spectra of atoms and ions with multiple electrons
- Can't explain the effect of magnetic fields on emission spectra
- Mixture of classical and non-classical physics
- Modern quantum mechanics replaced the Bohr theory in 1926.

- Wave-Particle Duality
 - Einstein suggested particle-like properties of light could explain the photoelectric effect.
 - Dispersion of light into a spectrum by a prism suggests photons are wave-like.
- de Broglie, 1924
 - Small particles of matter may at times display wavelike properties.

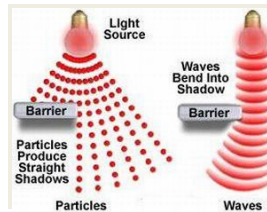
$$E = mc^2$$

$$h\nu = mc^2$$

$$h\nu/c = mc = p$$

$$p = h/\lambda$$

$$\lambda = h/p = h/mv$$



Louis de Broglie
(1892 - 1987)
Nobel Prize 1929

EXAMPLE 8-6

Calculating the Wavelength Associated with a Beam of Particles. What is the wavelength associated with electrons traveling at one-tenth the speed of light?

Solution

The electron mass, expressed in kilograms, is 9.109×10^{-31} kg (recall Table 2.1). The electron velocity is $u = 0.100 \times c = 0.100 \times 3.00 \times 10^8 \text{ m s}^{-1} = 3.00 \times 10^7 \text{ m s}^{-1}$. Planck's constant $h = 6.626 \times 10^{-34} \text{ J s} = 6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-2} \text{ s} = 6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}$. Substituting these data into equation (8.10), we obtain

$$\lambda = \frac{6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{(9.109 \times 10^{-31} \text{ kg})(3.00 \times 10^7 \text{ m s}^{-1})}$$

$$= 2.42 \times 10^{-11} \text{ m} = 24.2 \text{ pm}$$

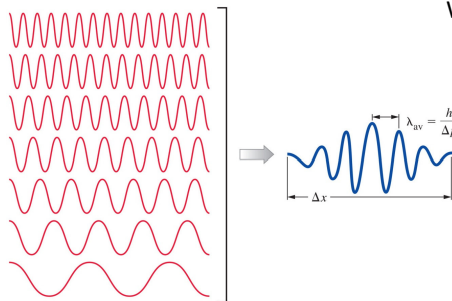
Only when wavelengths are comparable to atomic or nuclear dimensions that wave-particle duality is important.

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



Werner Heisenberg
(1901 - 1976)
Nobel Prize 1932

De Broglie law: $p = h/\lambda$
Knowing λ can precisely know p .
But where is the particle position on the wave?



EXAMPLE 8-7

Calculating the Uncertainty of the Position of an Electron. A 12-eV electron can be shown to have a speed of 2.05×10^6 m/s. Assuming that the precision (uncertainty) of this value is 1.5%, with what precision can we simultaneously measure the position of the electron?

Solution

The uncertainty in the electron speed is

$$\Delta u = 0.015 \times 2.05 \times 10^6 \text{ m s}^{-1} = 3.1 \times 10^4 \text{ m s}^{-1}$$

The electron mass, 9.109×10^{-31} kg (recall Table 2.1), is known much more precisely than the electron speed, which means that

$$\begin{aligned} \Delta p &= m\Delta u = 9.109 \times 10^{-31} \text{ kg} \times 3.1 \times 10^4 \text{ m s}^{-1} \\ &= 2.8 \times 10^{-26} \text{ kg m s}^{-1} \end{aligned}$$

From equation (8.11), the uncertainty in the electron's position is

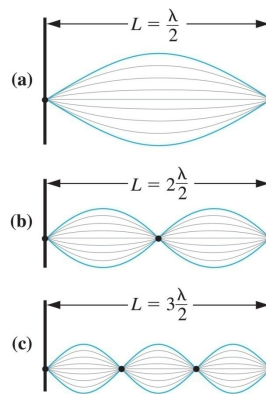
$$\Delta x = \frac{h}{4\pi\Delta p} = \frac{6.63 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{4 \times 3.14 \times 2.8 \times 10^{-26} \text{ kg m s}^{-1}} = 1.9 \times 10^{-9} \text{ m} = 1.9 \times 10^3 \text{ pm}$$

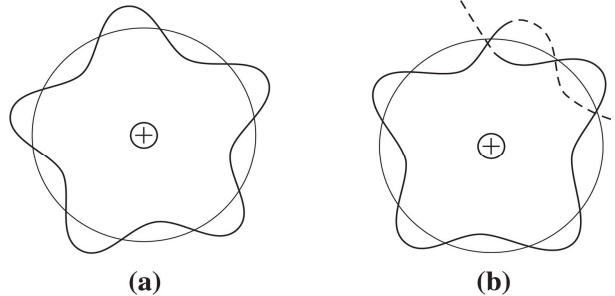
which is about 10 atomic diameters. Given the uncertainty in its speed, there is simply no way to pin down the electron's position with any greater precision than that.

- Standing waves.
 - The permitted wavelength of standing waves are quantized.
 - Nodes do not undergo displacement.

$$\lambda = \frac{2L}{n}, \quad n = 1, 2, 3, \dots$$

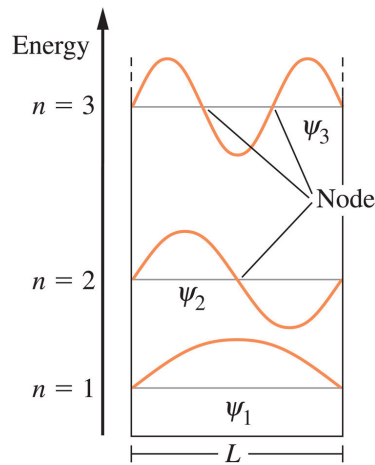
$$\text{Total number of nodes} = n + 1$$





Copyright © 2007 Pearson Prentice Hall, Inc.

These patterns are two-dimensional cross-sections of a much more complicated three-dimensional wave. The wave pattern in (a), a standing wave, is an acceptable representation. It has an integral number of wavelengths (five) about the nucleus; successive waves reinforce one another. The pattern in (b) is unacceptable. The number of wavelengths is nonintegral, and successive waves tend to cancel each other; that is, the crest in one part of the wave overlaps a trough in another part of the wave, and there is no resultant wave at all.



- ψ , psi, the wave function.
 - Should correspond to a standing wave within the boundary of the system being described.

- Particle in a box.

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

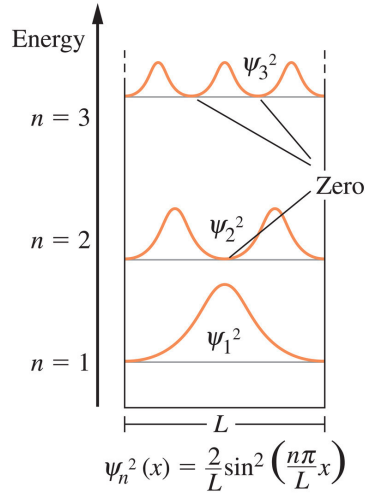
x is the distance traveled by a particle.

The first three wave functions and their energies are shown in relation to the position of the particle within the box. The wave function changes sign at the nodes.

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

The wave functions

Copyright © 2007 Pearson Prentice Hall, Inc.



The probabilities of a particle in a one-dimensional box.

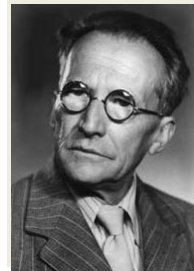
The squares of the first three wave functions and their energies are shown in relation to the position of the particle within the box. There is no chance of finding the particle at the points where $\Psi^2 = 0$.

The probabilities

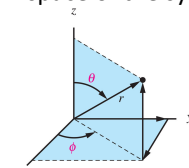
Copyright © 2007 Pearson Prentice Hall, Inc.

In 1926, Schrodinger, using a complicated mathematical technique, formulated an equation that describes the behavior and energies of submicroscopic particles in general, an equation analogous to Newton's laws of motion for macroscopic objects.

The **Schrodinger equation** incorporates both particle behavior, in term of mass m , and wave behavior, in terms of a wave function ψ (psi), which depends on the location in space of the system (such as electron in an atom).



Erwin Schrödinger
(1887 - 1961)
Nobel Prize 1933



$$E\psi = H \psi$$

$$H(x,y,z) \text{ or } H(r,\theta,\phi) \quad \psi(r,\theta,\phi) = R(r) Y(\theta,\phi)$$

$R(r)$ is the radial wave function.

$Y(\theta,\phi)$ is the angular wave function.

Spherical polar coordinates
 $x^2 + y^2 + z^2 = r^2$
 $x = r \sin \theta \cos \phi$
 $y = r \sin \theta \sin \phi$
 $z = r \cos \theta$

Copyright © 2007 Pearson Prentice Hall, Inc.

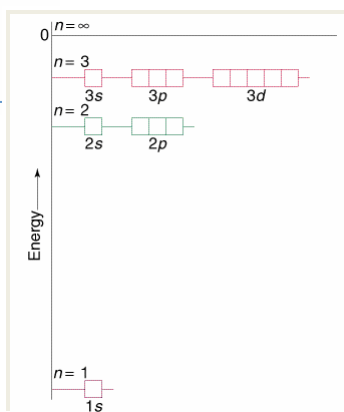
When solving the Shrodinger equation for the hydrogen atom, we find many wave functions (orbitals) that satisfy it. Each of these orbitals is characterized by a series of numbers called **quantum numbers**, which describe various properties of the orbital:

- The **principal quantum number** (n) has integral values: 1, 2, 3, ... The principal quantum number is related to the size and energy of the orbital.
- The **angular momentum quantum number** (l) has integral values from 0 to $n-1$ for each value of n . This quantum number is related to the shape of atomic orbitals.
 - $l = 0 \rightarrow s$ orbital
 - $l = 1 \rightarrow p$ orbital
 - $l = 2 \rightarrow d$ orbital
 - $l = 3 \rightarrow f$ orbital
- The **magnetic quantum number** (m_l) has integral values between $-l$ and $+l$, including zero. The value of m_l is related to the orientation of the orbital in space relative to the other orbitals in the atom.

Relationship Among Values of n , l , and m_l Through $n = 4$

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2	0	2s	0	1	4
	1	2p	1, 0, -1	3	
3	0	3s	0	1	9
	1	3p	1, 0, -1	3	
	2	3d	2, 1, 0, -1, -2	5	
4	0	4s	0	1	16
	1	4p	1, 0, -1	3	
	2	4d	2, 1, 0, -1, -2	5	
	3	4f	3, 2, 1, 0, -1, -2, -3	7	

Orbitals at the same energy level are said to be degenerate.



EXAMPLE 8-8

Applying Relationships Among Quantum Numbers. Can an orbital have the quantum numbers $n = 2$, $\ell = 2$, and $m_\ell = 2$?

Solution

No. The ℓ quantum number cannot be greater than $n - 1$. Thus, if $n = 2$, ℓ can be only 0 or 1. And if ℓ can be only 0 or 1, m_ℓ cannot be 2; m_ℓ must be 0 if $\ell = 0$ and may be $-1, 0$, or $+1$ if $\ell = 1$.

◀ Chemists often refer to the three quantum numbers simply as the “ n ,” “ ℓ ” and “ m_ℓ ” quantum numbers rather than designating them by name.

EXAMPLE 8-9

Relating Orbital Designations and Quantum Numbers. Write an orbital designation corresponding to the quantum numbers $n = 4$, $\ell = 2$, $m_\ell = 0$.

Solution

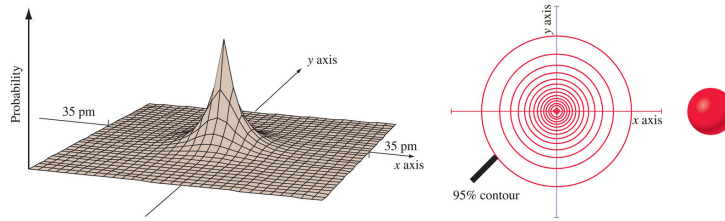
The magnetic quantum number, m_ℓ , is not reflected in the orbital designation. The type of orbital is determined by the ℓ quantum number. Because $\ell = 2$, the orbital is of the d type. Because $n = 4$, the orbital designation is $4d$.

- Represent the probability densities of the orbitals of the hydrogen atom as three dimensional surfaces.
- Each orbital has a distinctive shape.
- Acquire a broad *qualitative* understanding.

TABLE 8.1 The Angular and Radial Wave Functions of a Hydrogen-like Atom

Angular Part $Y(\theta, \phi)$	Radial Part $R_{n, \ell}(r)$
$Y(s) = \left(\frac{1}{4\pi}\right)^{1/2}$	$R(1s) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma/2}$
	$R(2s) = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2} (2 - \sigma)e^{-\sigma/2}$
	$R(3s) = \frac{1}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2} (6 - 6\sigma + \sigma^2)e^{-\sigma/2}$
$Y(p_x) = \left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \cos \phi$	$R(2p) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}$
$Y(p_y) = \left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \sin \phi$	$R(3p) = \frac{1}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} (4 - \sigma)\sigma e^{-\sigma/2}$
$Y(p_z) = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$	
$Y(d_{z^2}) = \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$	$R(3d) = \frac{1}{9\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/2}$
$Y(d_{x^2-y^2}) = \left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \cos 2\phi$	
$Y(d_{xy}) = \left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \sin 2\phi$	$\sigma = \frac{2Zr}{na_0}$
$Y(d_{xz}) = \left(\frac{15}{4\pi}\right)^{1/2} \sin \theta \cos \theta \cos \phi$	
$Y(d_{yz}) = \left(\frac{15}{4\pi}\right)^{1/2} \sin \theta \cos \theta \sin \phi$	

Copyright © 2007 Pearson Prentice Hall, Inc.



Copyright © 2007 Pearson Prentice Hall, Inc.

$$\psi(1s) = R(r) \times Y(\theta, \phi) = \frac{2e^{-r/a_0}}{a_0^{3/2}} \times \frac{1}{\sqrt{4\pi}} = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}}$$

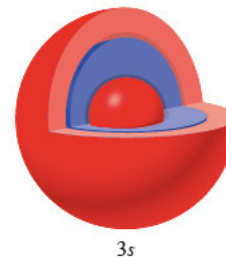
Copyright © 2007 Pearson Prentice Hall, Inc.

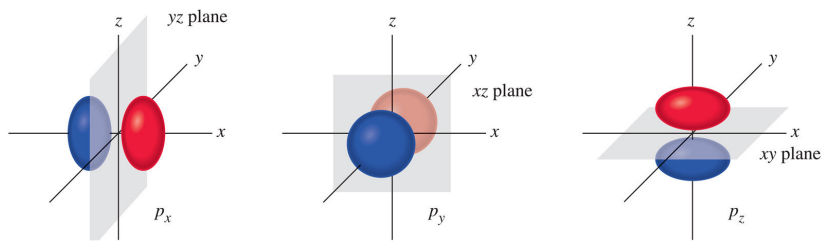
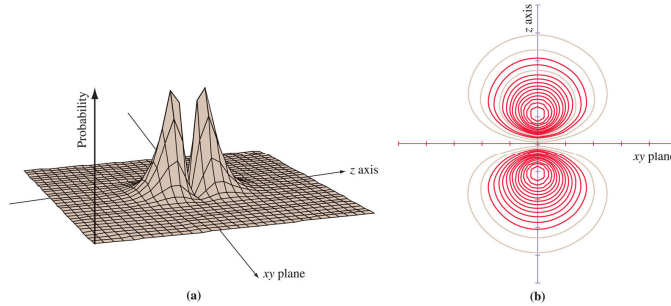
a_0 : Bohr radius = 53 pm

$$\psi(2s) = R(r) \times Y(\theta, \phi) = \frac{1}{2\sqrt{2}} \frac{1}{a_0^{3/2}} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0} \times \frac{1}{\sqrt{4\pi}} = \frac{1}{4} \left(\frac{1}{2\pi a_0^3} \right)^{1/2} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

Copyright © 2007 Pearson Prentice Hall, Inc.

$$\psi(2s) = R(r) \times Y(\theta, \phi) = \frac{1}{2\sqrt{2}} \frac{1}{a_0^{3/2}} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0} \times \frac{1}{\sqrt{4\pi}} = \frac{1}{4} \left(\frac{1}{2\pi a_0^3} \right)^{1/2} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$



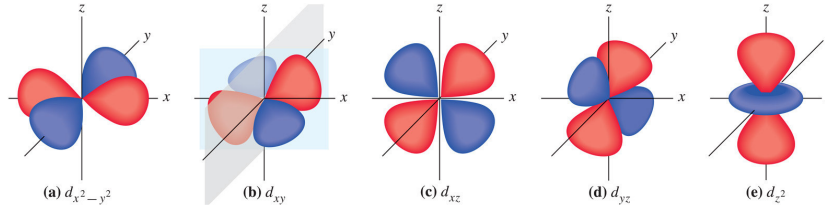


Copyright © 2007 Pearson Prentice Hall, Inc.

TABLE 8.1 The Angular and Radial Wave Functions of a Hydrogen-like Atom

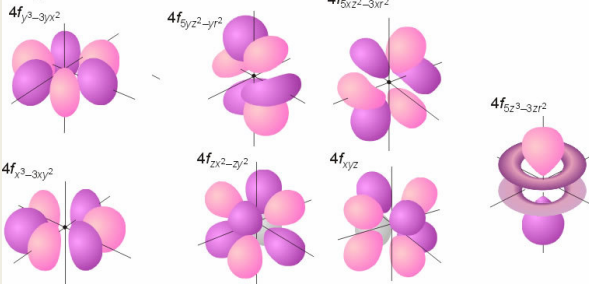
Angular Part $Y(\theta, \phi)$	Radial Part $R_n, \ell(r)$
$Y(s) = \left(\frac{1}{4\pi}\right)^{1/2}$	$R(1s) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma/2}$
	$R(2s) = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2} (2 - \sigma)e^{-\sigma/2}$
	$R(3s) = \frac{1}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2} (6 - 6\sigma + \sigma^2)e^{-\sigma/2}$
$Y(p_x) = \left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \cos \phi$	$R(2p) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}$
$Y(p_y) = \left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \sin \phi$	$R(3p) = \frac{1}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} (4 - \sigma)\sigma e^{-\sigma/2}$
$Y(p_z) = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$	
$Y(d_{z^2}) = \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$	$R(3d) = \frac{1}{9\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/2}$
$Y(d_{x^2-y^2}) = \left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \cos 2\phi$	
$Y(d_{xy}) = \left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \sin 2\phi$	$\sigma = \frac{2Zr}{na_0}$
$Y(d_{xz}) = \left(\frac{15}{4\pi}\right)^{1/2} \sin \theta \cos \theta \cos \phi$	
$Y(d_{yz}) = \left(\frac{15}{4\pi}\right)^{1/2} \sin \theta \cos \theta \sin \phi$	

Copyright © 2007 Pearson Prentice Hall, Inc.

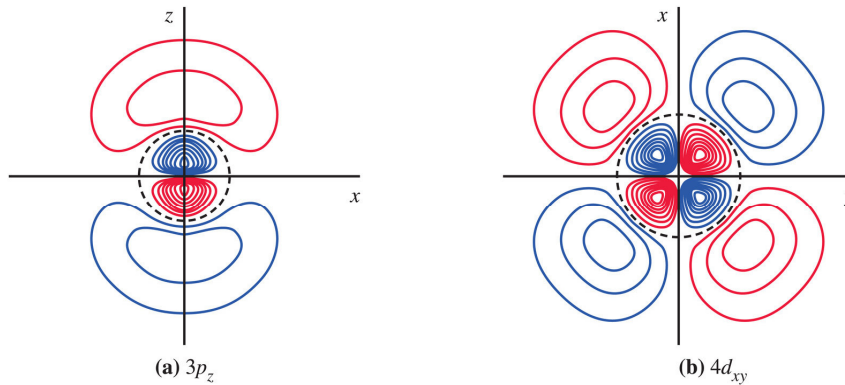


Copyright © 2007 Pearson Prentice Hall, Inc.

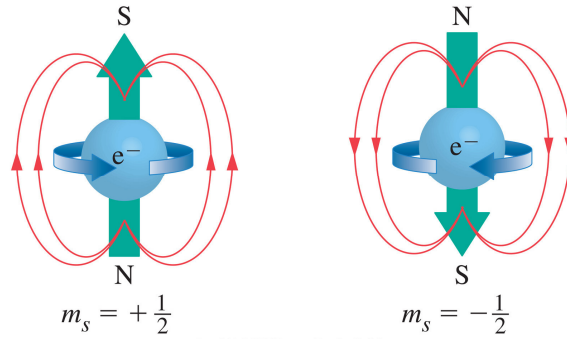
Shapes of 4f Orbitals



7 f-orbitals
14 electrons

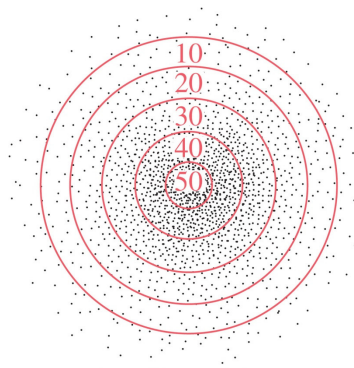


Copyright © 2007 Pearson Prentice Hall, Inc.



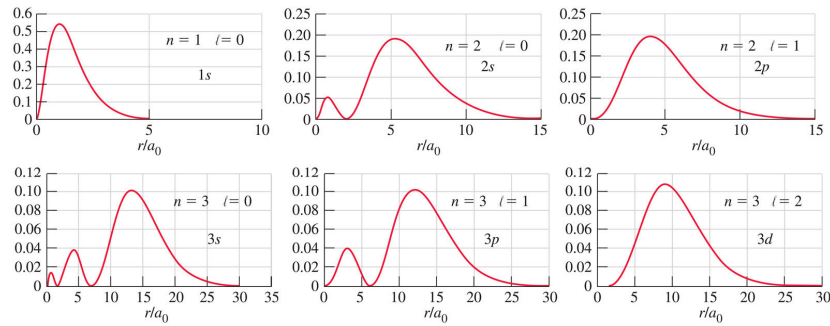
Two possibilities for electron spin are shown with their associated magnetic fields. Two electrons with opposing spins have opposing magnetic fields that cancel, leaving no net magnetic field for the pair.

- Schrödinger equation was for only one e^- .
- Electron-electron repulsion in multi-electron atoms.
- Hydrogen-like orbitals (by approximation).



s electrons are more effective screening the nucleus from outer electrons than are electrons in p or d orbitals.

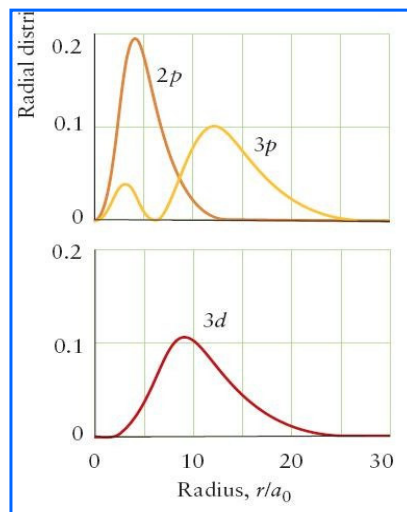
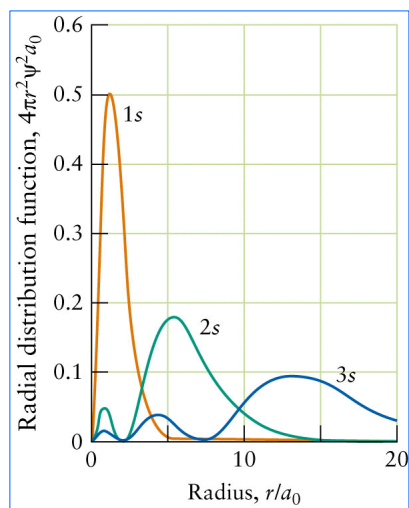
Radial probability distribution: $4\pi r^2 R^2(r)$

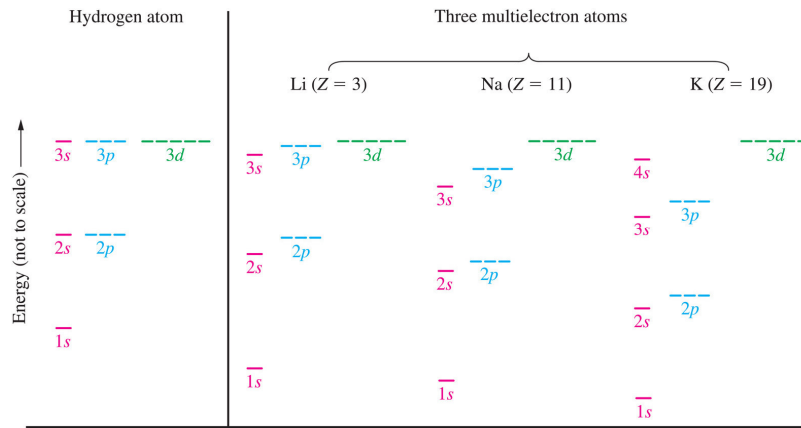


Copyright © 2007 Pearson Prentice Hall, Inc.

Z_{eff} is the effective nuclear charge.

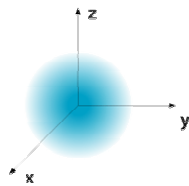
s electron experiences a higher Z_{eff} and is held more tightly than p electron in the same principle shell.





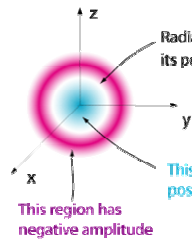
Copyright © 2007 Pearson Prentice Hall, Inc.

1s orbital
 $n = 1, \ell = 0, m_\ell = 0$



The 1s standing wave function (orbital) is all positive (i.e., no negative lobes) and has no nodal surfaces. It is spherically symmetric.

2s orbital
 $n = 2, \ell = 0, m_\ell = 0$

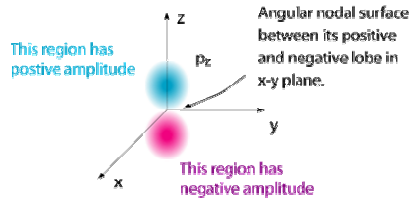


Radial nodal surface between its positive and negative lobe.

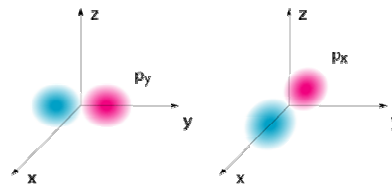
This region has positive amplitude

This region has negative amplitude

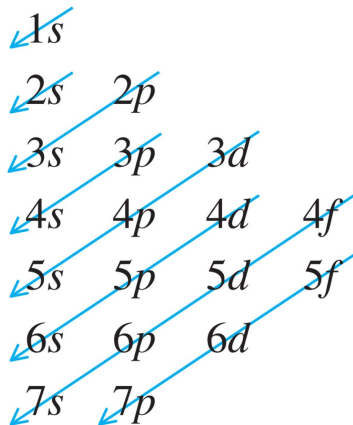
2p orbitals
 $n = 2, \ell = 1, m_\ell = -1, 0, +1$



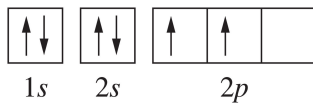
Angular nodal surface between its positive and negative lobe in x-y plane.



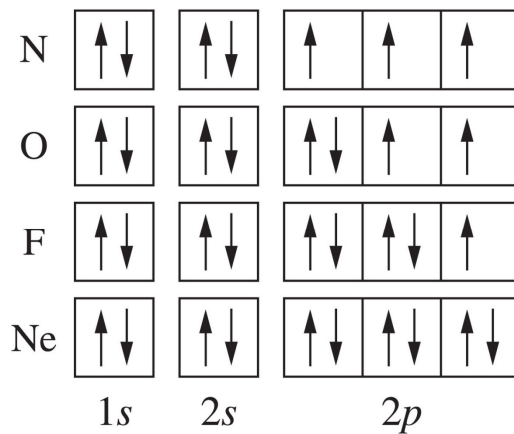
- A designation of how electrons are distributed among various orbitals in principle shells and subshells.
- Aufbau process.
 - Build up and minimize energy.
- Pauli exclusion principle.
 - No two electrons can have all four quantum numbers alike.
- Hund's rule.
 - Degenerate orbitals are occupied singly first.



Copyright © 2007 Pearson Prentice Hall, Inc.



Copyright © 2007 Pearson Prentice Hall, Inc.



Copyright © 2007 Pearson Prentice Hall, Inc.

Sc:	[Ar]	\uparrow \square \square \square \square	$\uparrow\downarrow$	[Ar] $3d^14s^2$
Ti:	[Ar]	\uparrow \uparrow \square \square \square	$\uparrow\downarrow$	[Ar] $3d^24s^2$
V:	[Ar]	\uparrow \uparrow \uparrow \square \square	$\uparrow\downarrow$	[Ar] $3d^34s^2$
Cr:	[Ar]	\uparrow \uparrow \uparrow \uparrow \uparrow	\uparrow	[Ar] $3d^54s^1$
Mn:	[Ar]	\uparrow \uparrow \uparrow \uparrow \uparrow	$\uparrow\downarrow$	[Ar] $3d^54s^2$
Fe:	[Ar]	$\uparrow\downarrow$ \uparrow \uparrow \uparrow \uparrow	$\uparrow\downarrow$	[Ar] $3d^64s^2$
Co:	[Ar]	$\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow \uparrow \uparrow	$\uparrow\downarrow$	[Ar] $3d^74s^2$
Ni:	[Ar]	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow \uparrow	$\uparrow\downarrow$	[Ar] $3d^84s^2$
Cu:	[Ar]	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	\uparrow	[Ar] $3d^{10}4s^1$
Zn:	[Ar]	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	$\uparrow\downarrow$	[Ar] $3d^{10}4s^2$

$\begin{matrix} 3d & & 4s \end{matrix}$
 Copyright © 2007 Pearson Prentice Hall, Inc.

TABLE 8.2 Electron Configurations of Some Groups of Elements

Group	Element	Configuration
1	H	$1s^1$
	Li	[He] $2s^1$
	Na	[Ne] $3s^1$
	K	[Ar] $4s^1$
	Rb	[Kr] $5s^1$
	Cs	[Xe] $6s^1$
	Fr	[Rn] $7s^1$
17	F	[He] $2s^22p^5$
	Cl	[Ne] $3s^23p^5$
	Br	[Ar] $3d^{10}4s^24p^5$
	I	[Kr] $4d^{10}5s^25p^5$
	At	[Xe] $4f^{14}5d^{10}6s^26p^5$
18	He	$1s^2$
	Ne	[He] $2s^22p^6$
	Ar	[Ne] $3s^23p^6$
	Kr	[Ar] $3d^{10}4s^24p^6$
	Xe	[Kr] $4d^{10}5s^25p^6$
	Rn	[Xe] $4f^{14}5d^{10}6s^26p^6$

Copyright © 2007 Pearson Prentice Hall, Inc.

Main-group elements

s block												p block							
1	2											13	14	15	16	17	18		
1	2											5	6	7	8	9	10		
H	He											B	C	N	O	F	Ne		
3												Transition elements							
3	4																		
Li	Be																		
11																			
Na	Mg																		
19																			
K	Ca	3	4	5	6	d block				10	11	12	13	14	15	16	17	18	
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	57	58
87	88	89	104	105	106	107	108	109	110	111	112	81	82	83	84	85	86	89	90
Fr	Ra	Ac†	Rf	Db	Sg	Bh	Hs	Mt				Tl	Pb	Bi	Po	At	Rn		

Inner-transition elements

														f block													
														58	59	60	61	62	63	64	65	66	67	68	69	70	71
														Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
														90	91	92	93	94	95	96	97	98	99	100	101	102	103
														Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr