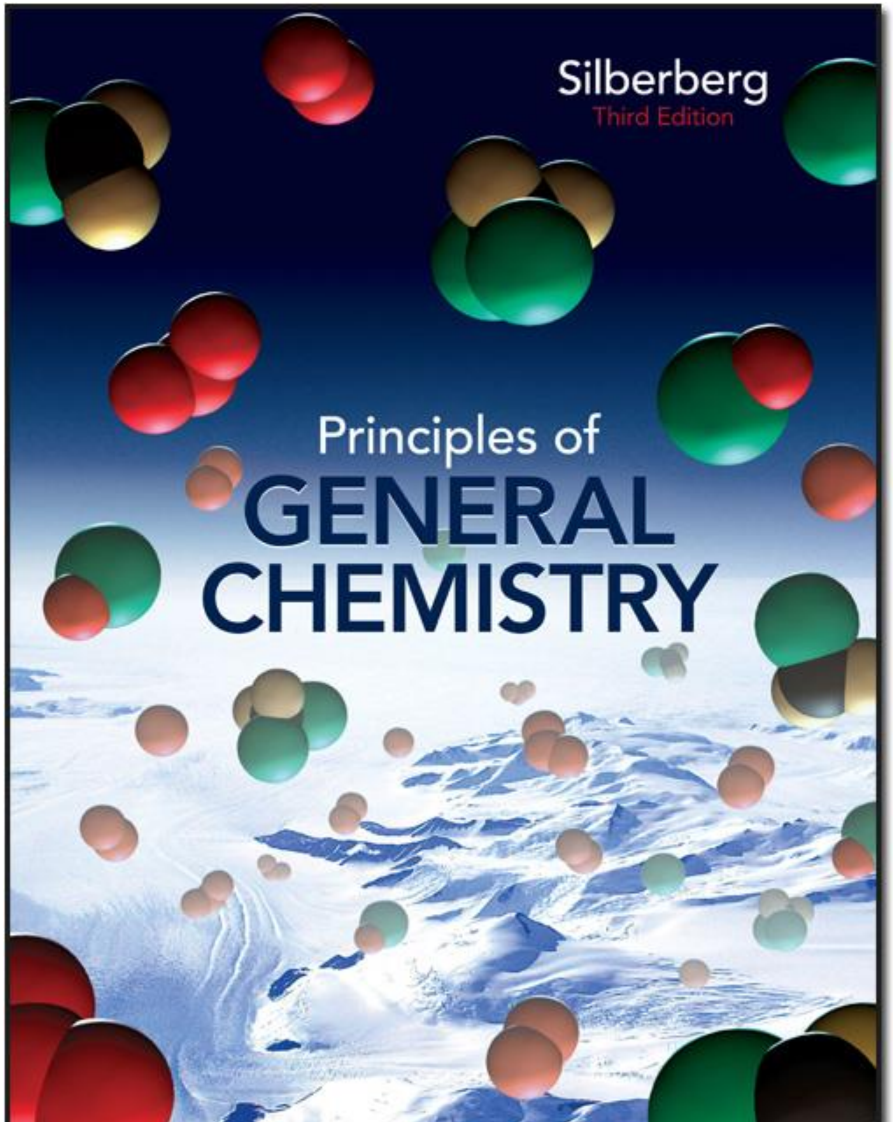

Dr. Diab Qadah

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CHEM 141

Chapter 7

Chapter 7

Quantum Theory and Atomic Structure

Quantum Theory and Atomic Structure

7.1 The Nature of Light

7.2 Atomic Spectra

7.3 The Wave-Particle Duality of Matter and Energy

7.4 The Quantum-Mechanical Model of the Atom

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 (ν)**, cycles per second
- **wavelength (λ)**, the distance a wave travels in one cycle
- **amplitude**, the height of a wave crest or depth of a trough.

The ***speed of light*** is a constant:

$$\boldsymbol{c = \nu \times \lambda}$$

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

Figure 7.1 The reciprocal relationship of frequency and wavelength.

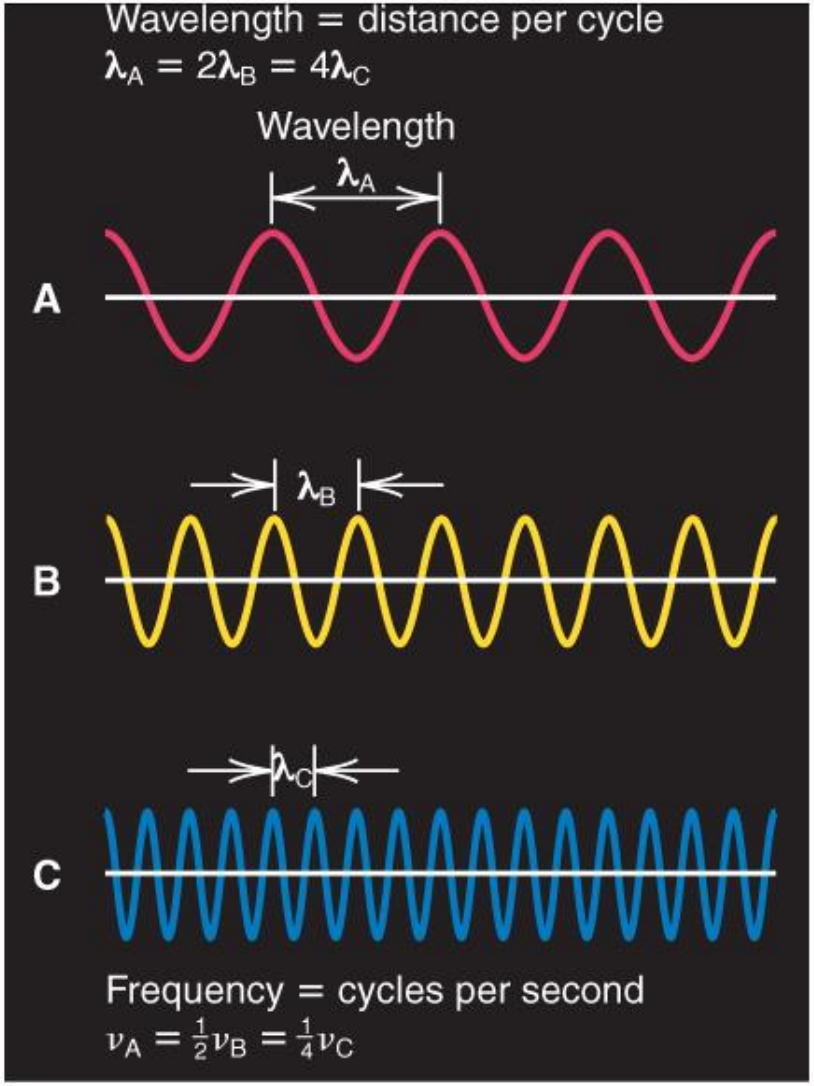


Figure 7.2 **Differing amplitude (brightness, or intensity) of a wave.**

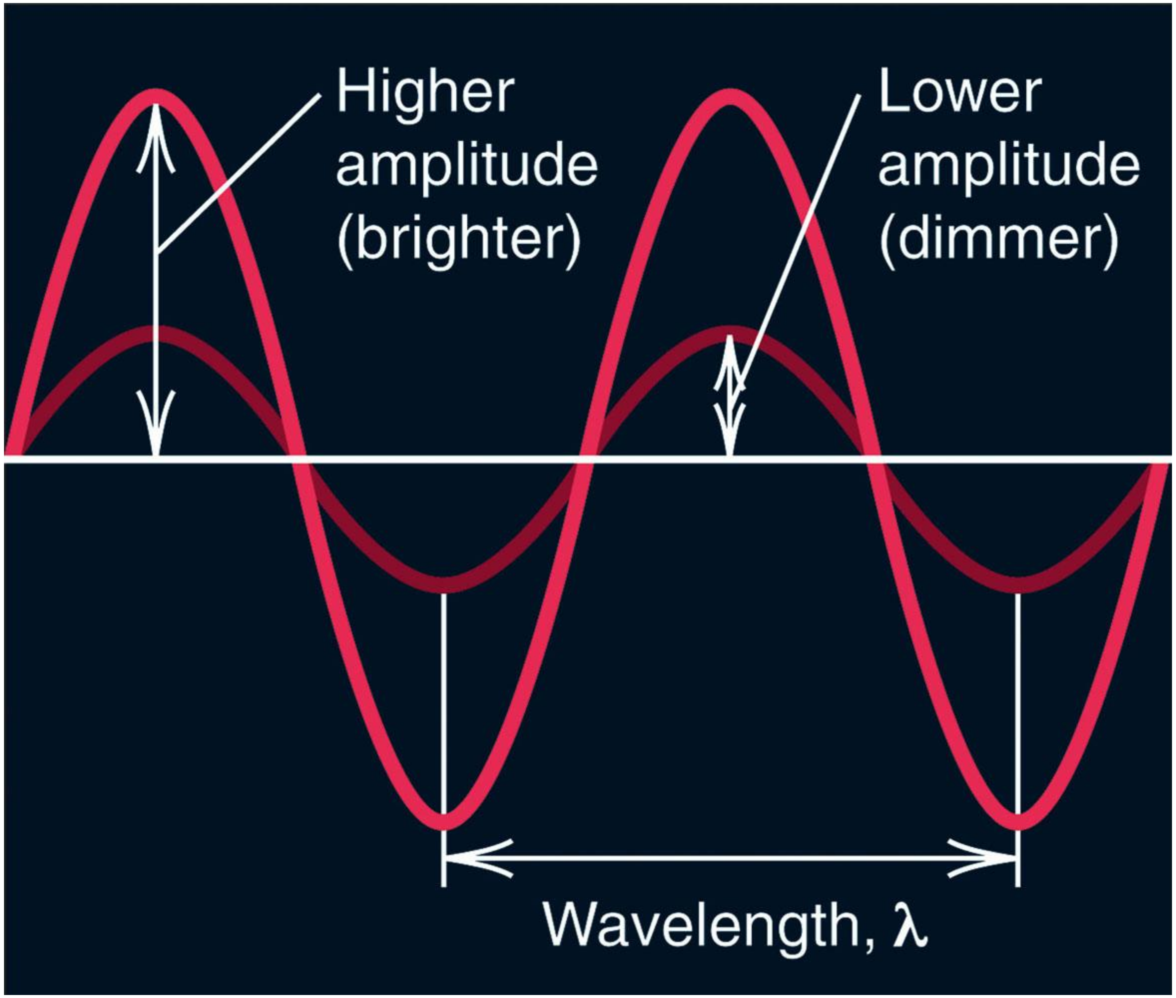
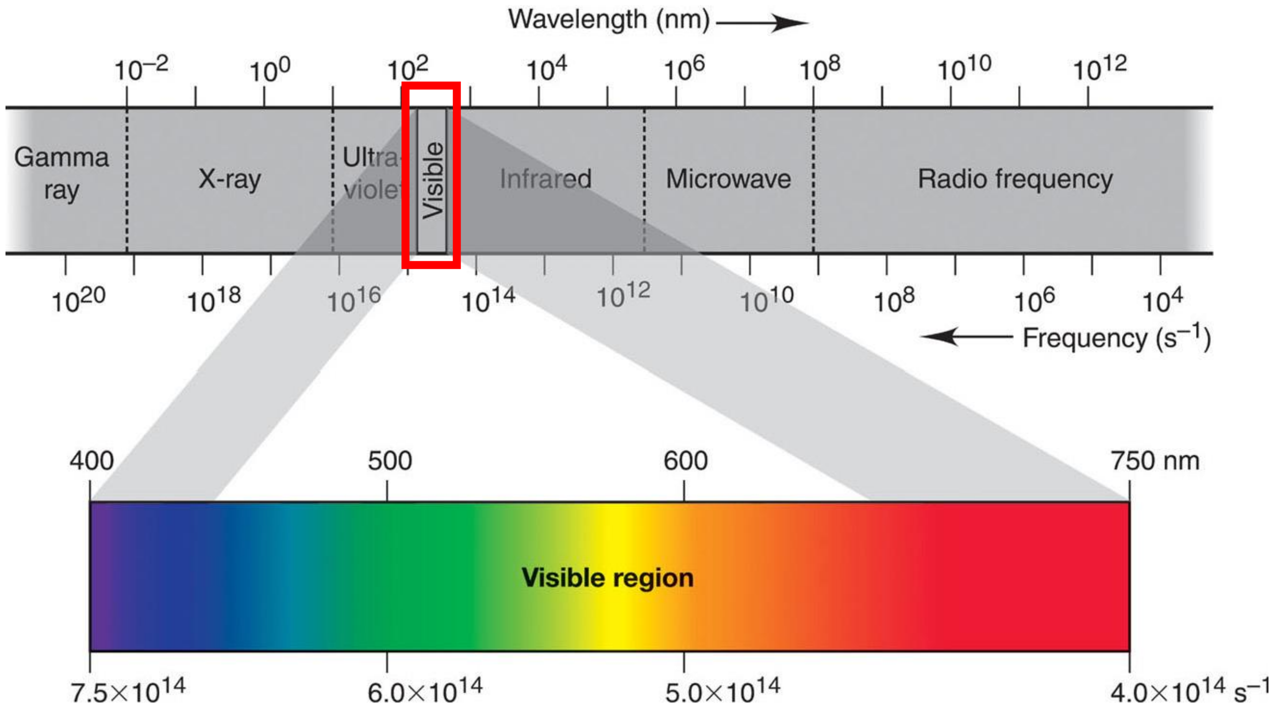


Figure 7.3 Regions of the electromagnetic spectrum.



Sample Problem 7.1 — Interconverting Wavelength and Frequency

PROBLEM: A dental hygienist uses x-rays (λ= 1.00Å) to take a series of dental radiographs while the patient listens to a radio station (λ = 325 cm) and looks out the window at the blue sky (λ= 473 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, 3.00×10^{8} m/s.)

PLAN: Use the equation $c = \nu\lambda$ to convert wavelength to frequency. Wavelengths need to be in meters because *c* has units of m/s.

wavelength in units given

↓ **use conversion factors**
1 Å = 10^{-10} m

wavelength in m

↓ $\nu = \dfrac{c}{\lambda}$

frequency (s^{-1} or Hz)

Sample Problem 7.1

SOLUTION:

Figure 7.4 Different behaviors of waves and particles.

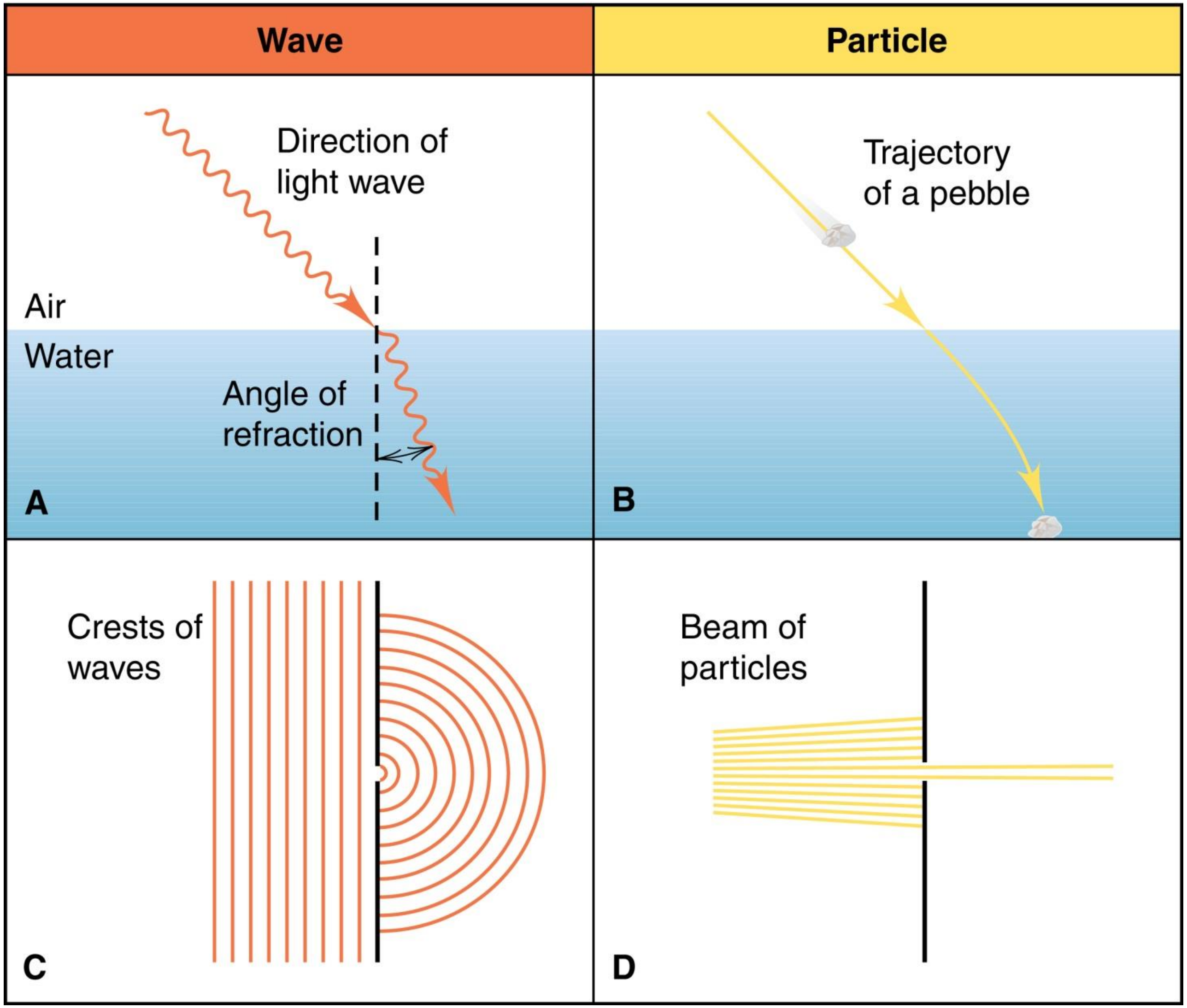
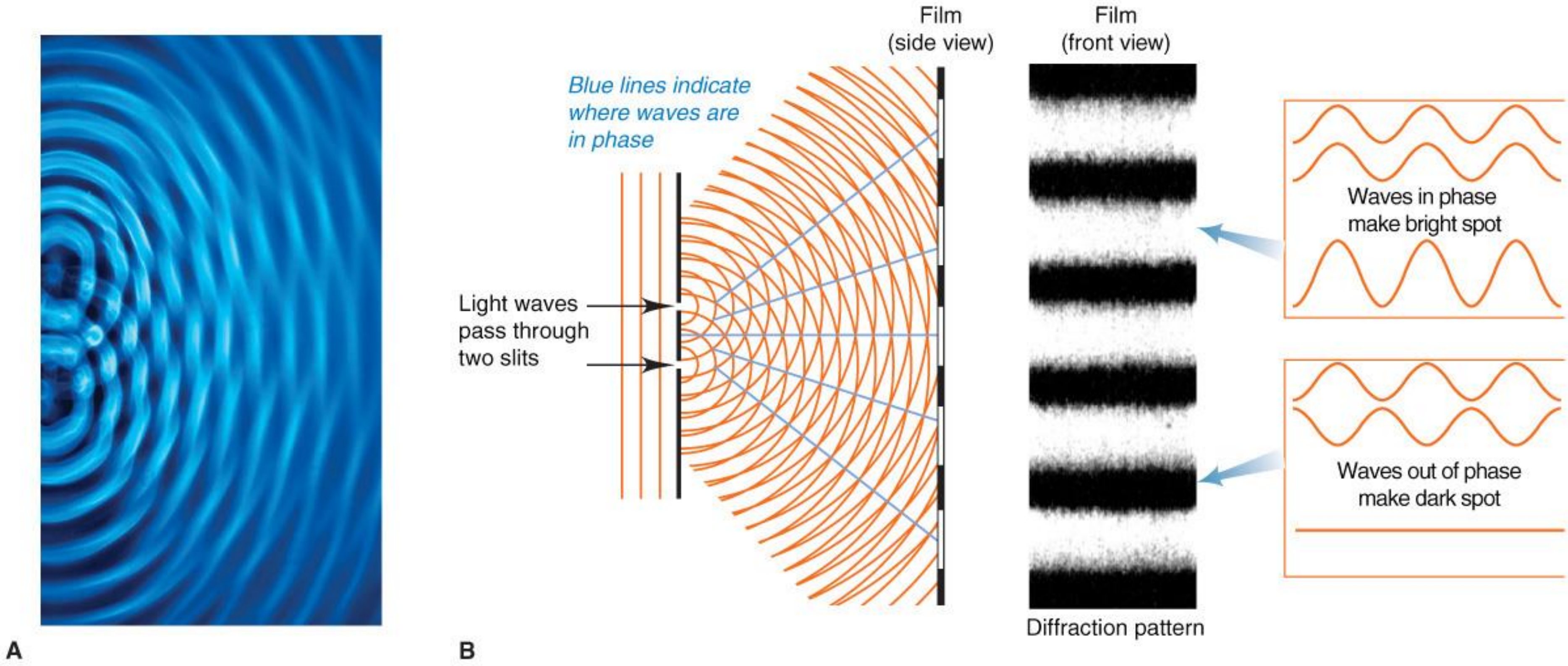


Figure 7.5 Formation of a diffraction pattern.



Energy and frequency

A solid object emits visible light when it is heated to about 1000 K. This is called ***blackbody radiation***.

The *color* (and the intensity) of the light changes as the temperature changes. Color is related to ***wavelength*** and ***frequency***, while temperature is related to ***energy***.

Energy is therefore related to frequency and wavelength:

$$\boxed{E = nh\nu}$$

E = energy
n is a positive integer
h is Planck's constant

The Quantum Theory of Energy

Any object (including atoms) can emit or absorb only ***certain quantities*** of energy.

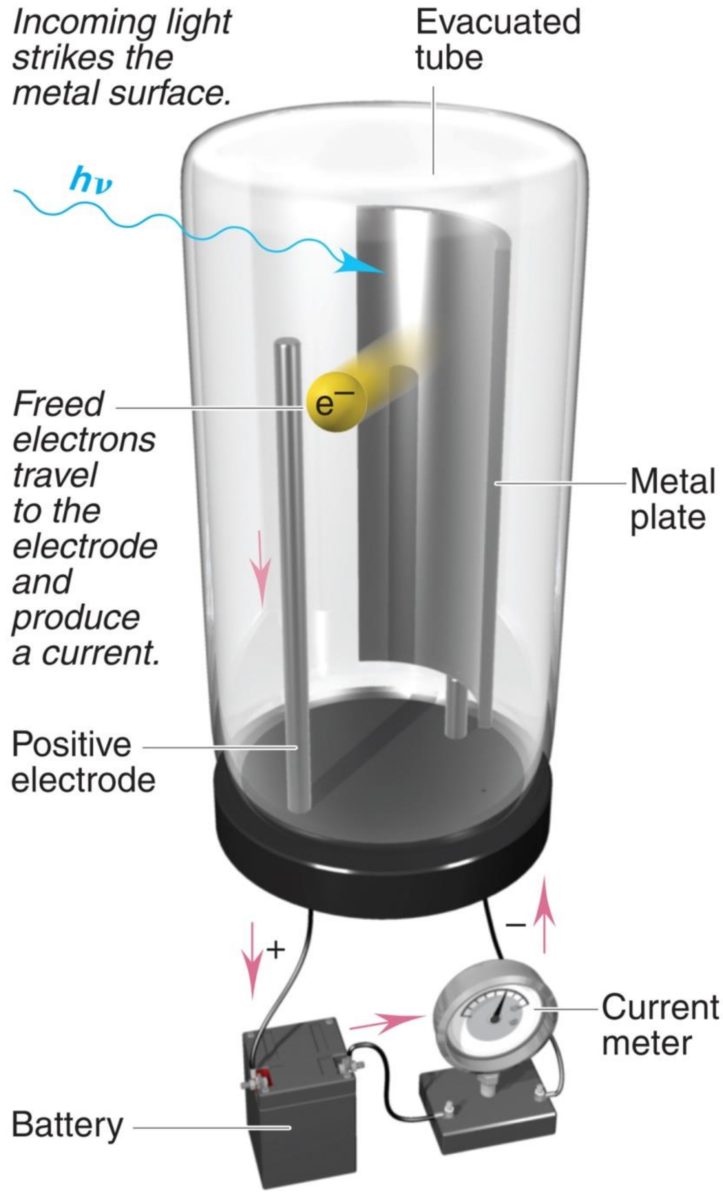
Energy is ***quantized***; it occurs in fixed quantities, rather than being continuous. Each fixed quantity of energy is called a ***quantum***.

An atom changes its energy state by emitting or absorbing one or more ***quanta*** of energy.

$$\Delta E = E_{\text{emitted or absorbed}} = \Delta nh\nu$$

where n can only be a whole number.

Figure 7.6 The photoelectric effect.



Sample Problem 7.2 **Calculating the Energy of Radiation from Its Wavelength**

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?

Figure 7.7A The line spectrum of hydrogen.

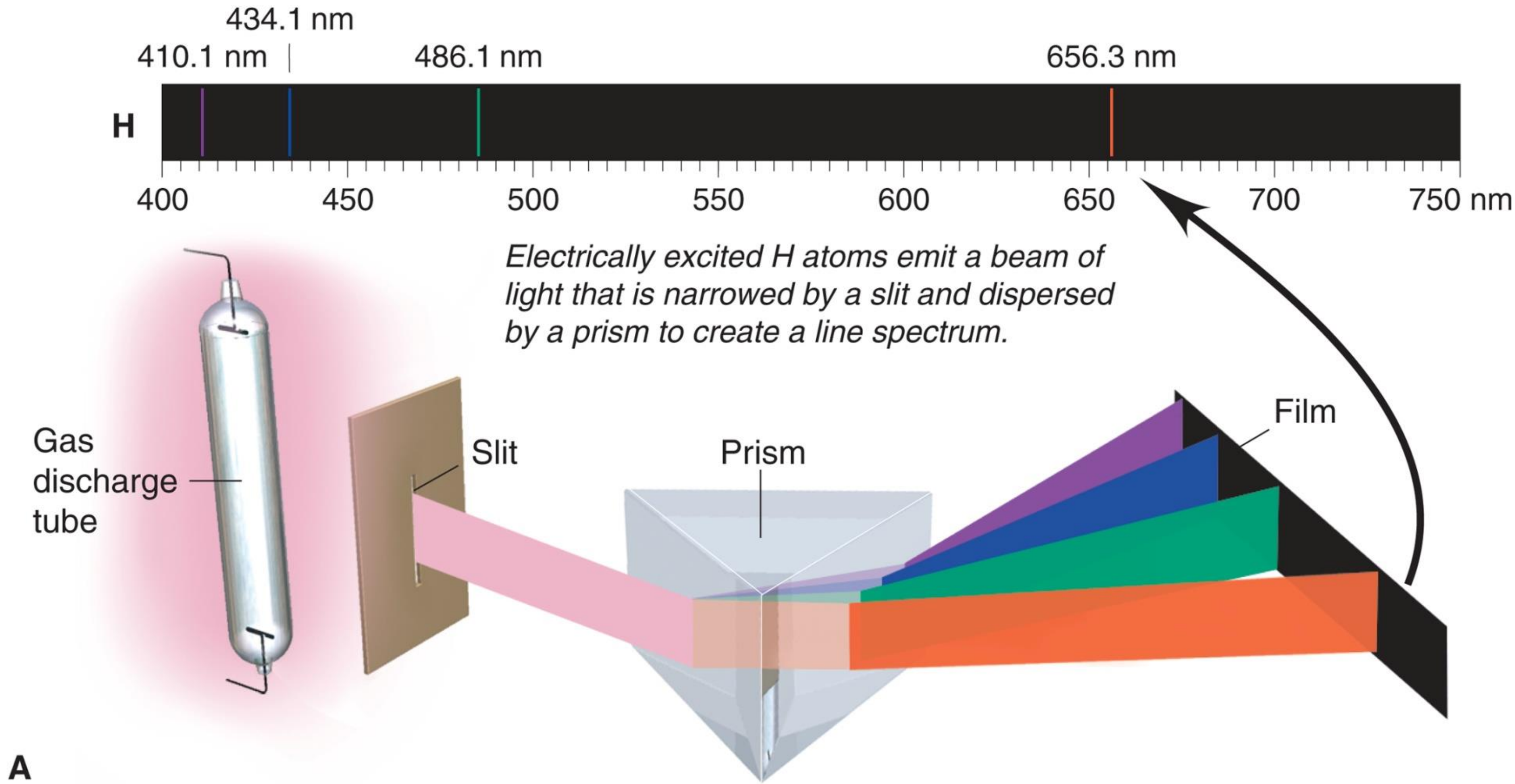


Figure 7.7B The line spectra of Hg and Sr.

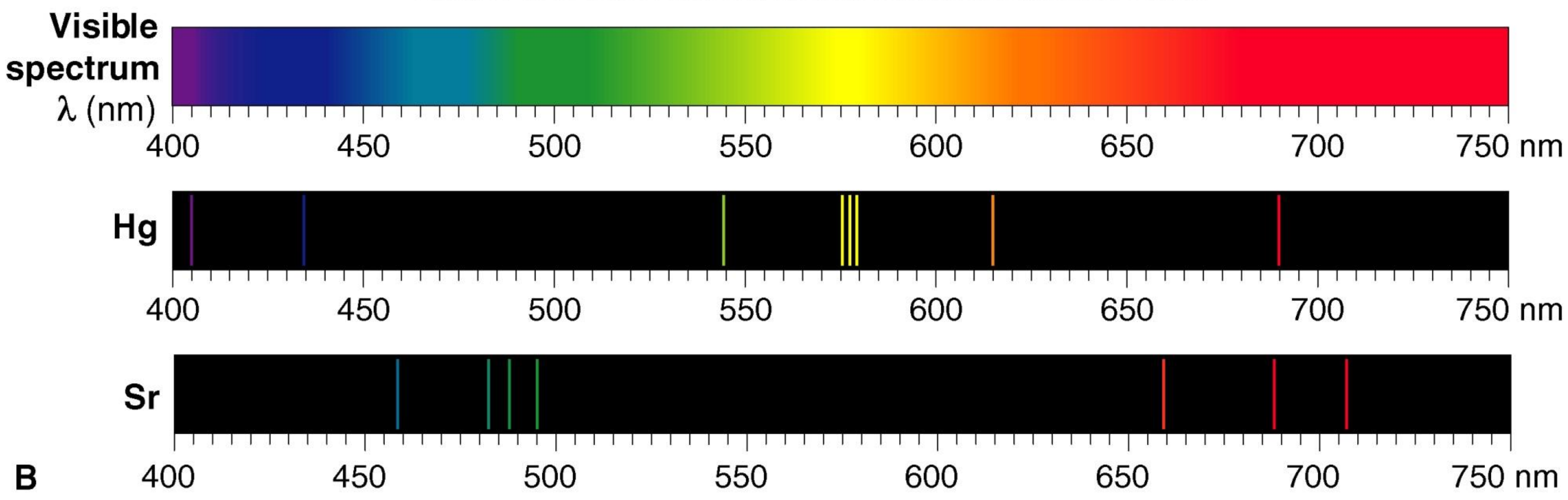
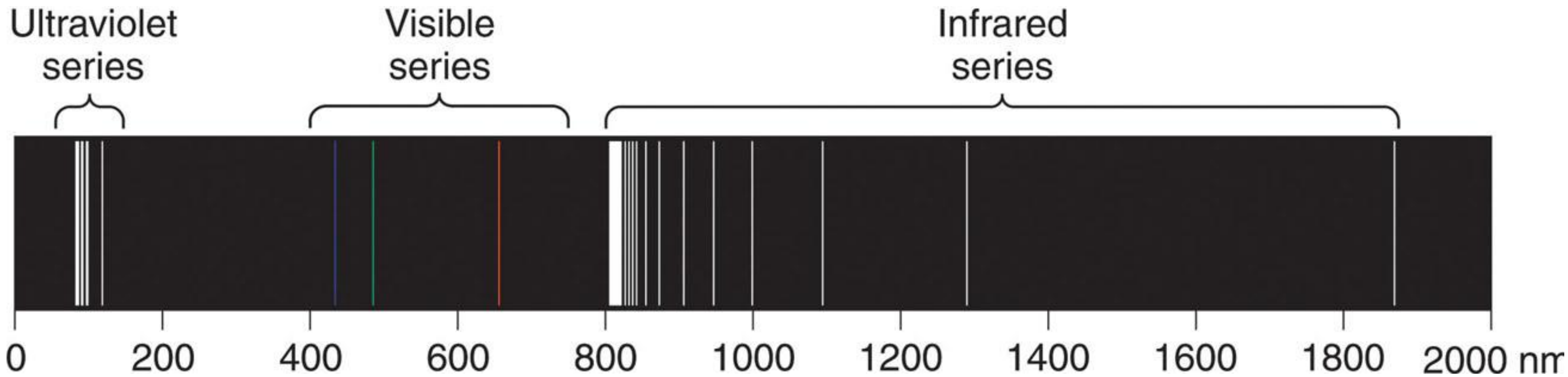


Figure 7.8 Three series of spectral lines of atomic hydrogen.



Rydberg equation

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

R is the Rydberg constant = 1.096776x10^{7} m^{-1}

for the visible series, $n_1 = 2$ and $n_2 = 3, 4, 5, ...$

The Bohr Model of the Hydrogen Atom

Bohr's atomic model postulated the following:

- The H atom has only certain energy levels, which Bohr called ***stationary states***.
  - Each state is associated with a fixed circular orbit of the electron around the nucleus.
  - The higher the energy level, the farther the orbit is from the nucleus.
  - When the H electron is in the first orbit, the atom is in its lowest energy state, called the ***ground state***.

- The atom does not radiate energy while in one of its stationary states.
- The atom changes to another stationary state only by absorbing or emitting a photon.
  - The energy of the photon ($h\nu$) equals the difference between the energies of the two energy states.
  - When the E electron is in any orbit higher than $n = 1$, the atom is in an ***excited state***.

Figure 7.9 **A quantum "staircase" as an analogy for atomic energy levels.**

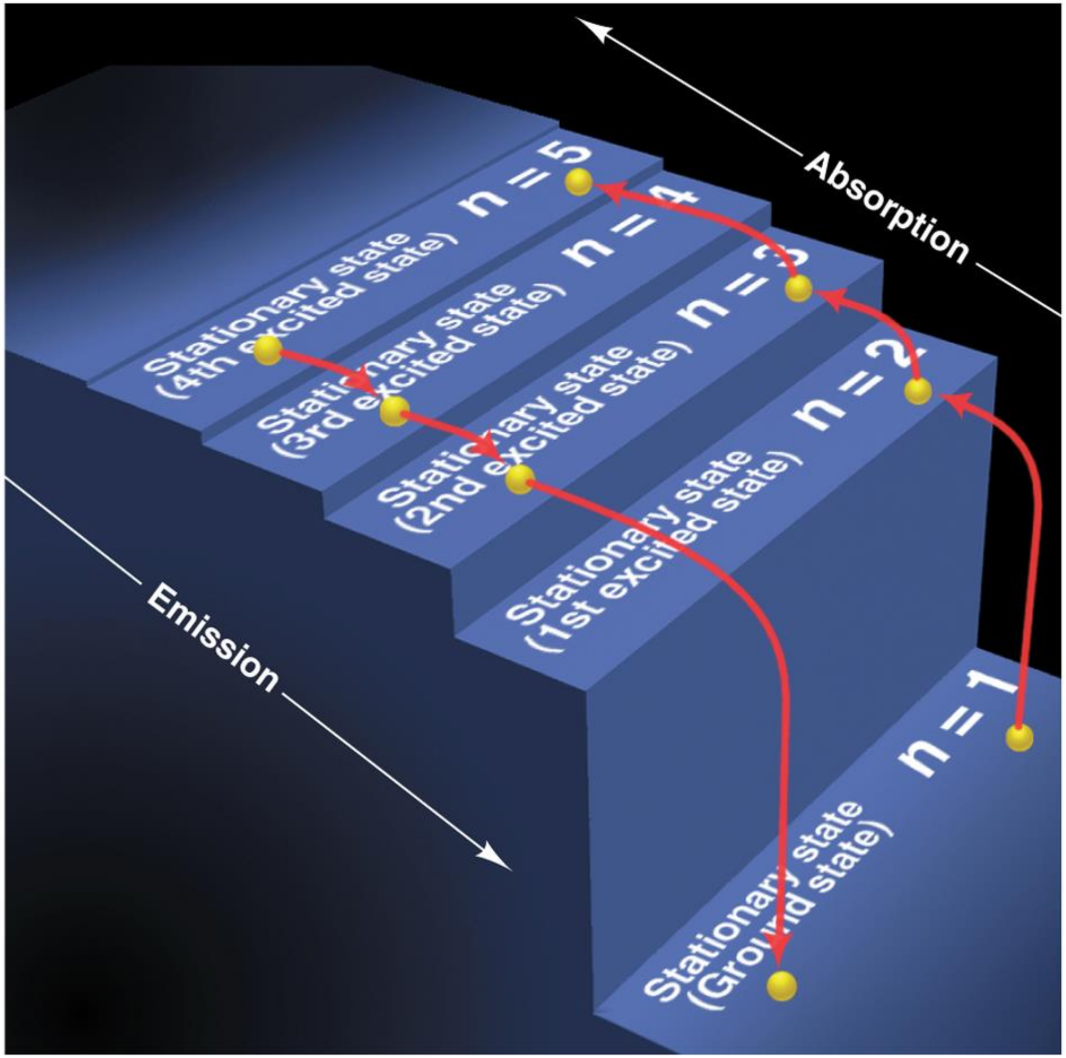
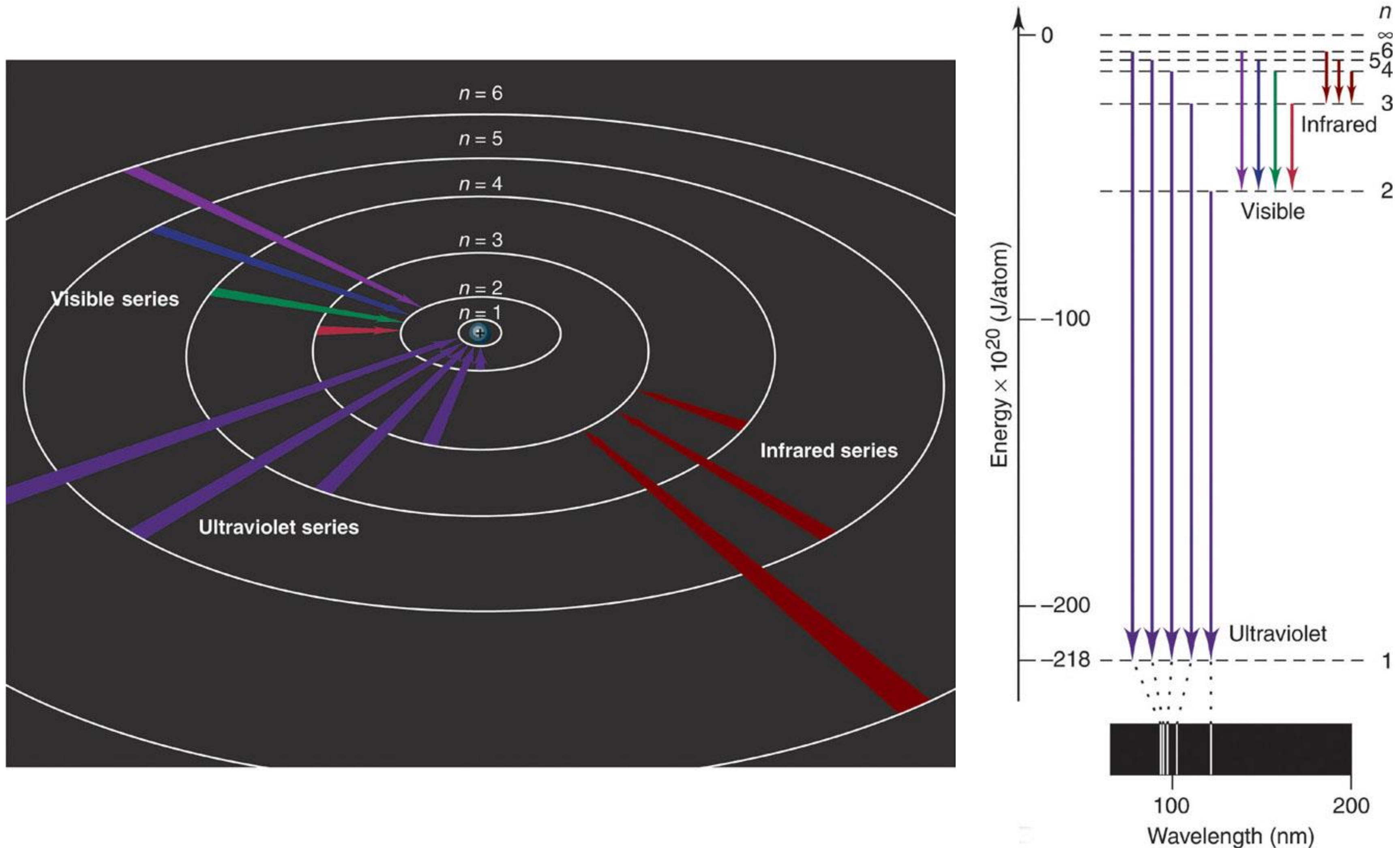
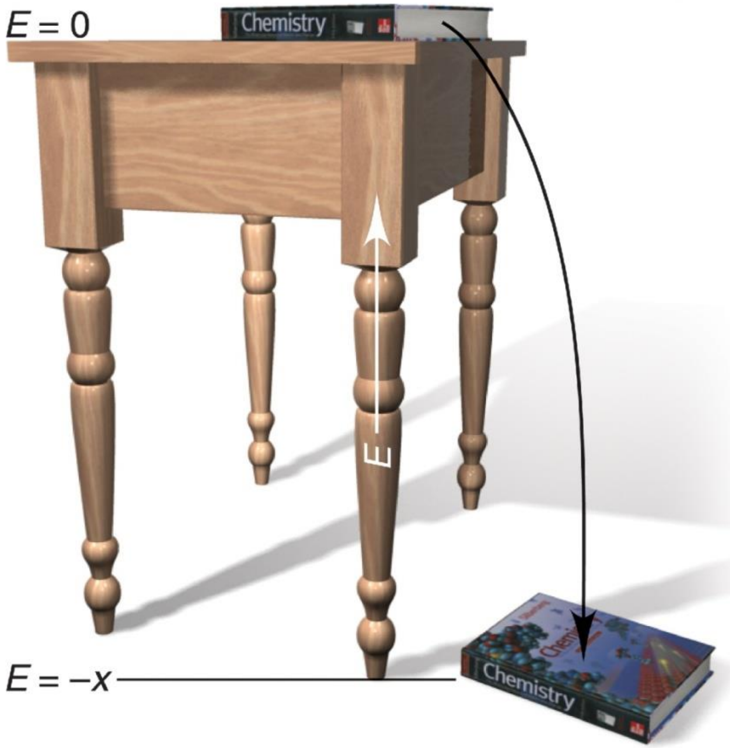


Figure 7.10 **The Bohr explanation of three series of spectral lines emitted by the H atom.**



A tabletop analogy for the H atom's energy.



$$\Delta E = E_{final} - E_{initial} = -2.18\text{x}10^{-18}\ \text{J} \left(\frac{1}{n^2_{final}} - \frac{1}{n^2_{initial}} \right)$$

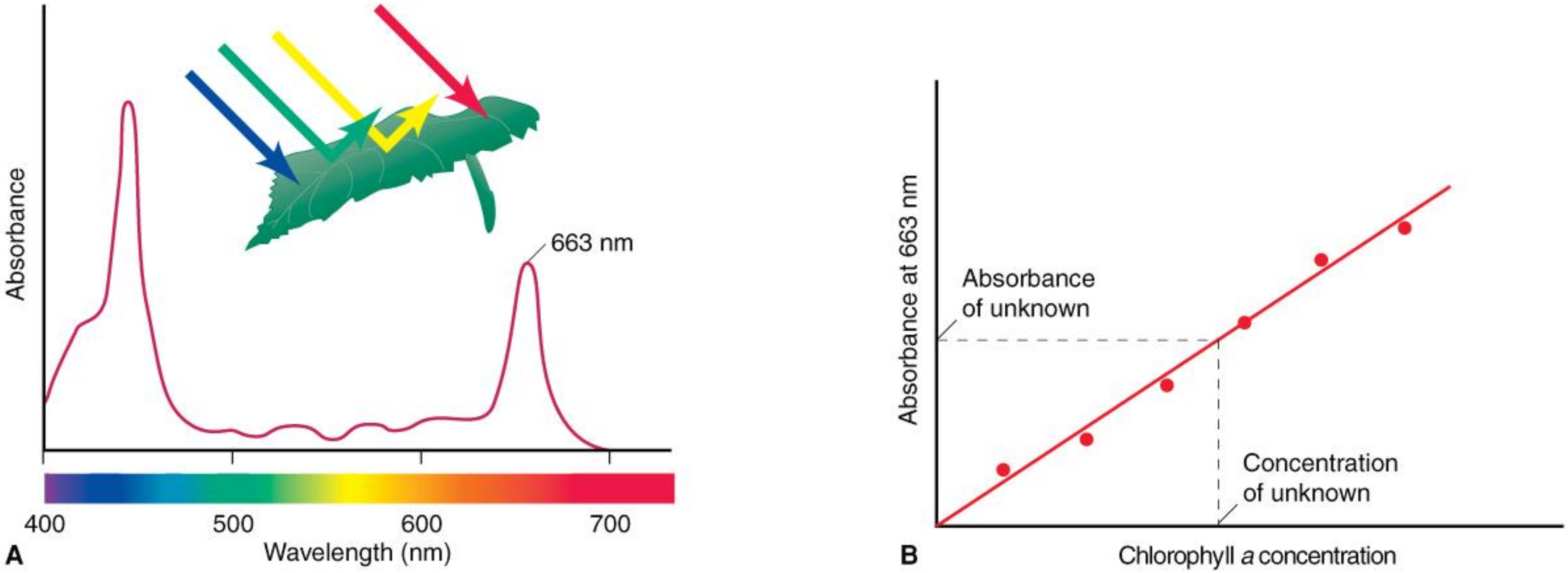
Sample Problem 7.3

Determining ΔE and λ of an Electron Transition

PROBLEM: A hydrogen atom absorbs a photon of UV light (see Figure 7.10) 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.

Sample Problem 7.3

Figure 7.11 Measuring chlorophyll *a* concentration in leaf extract.



The Wave-Particle Duality of Matter and Energy

Matter and Energy are alternate forms of the same entity.

$$\boxed{E = mc^2}$$

All matter exhibits properties of ***both particles and waves***. Electrons have wave-like motion and therefore have only certain allowable frequencies and energies.

Matter behaves as though it moves in a wave, and the ***de Broglie wavelength*** for any particle is given by:

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

m = mass

u = speed in m/s

Figure 7.12 Wave motion in restricted systems.

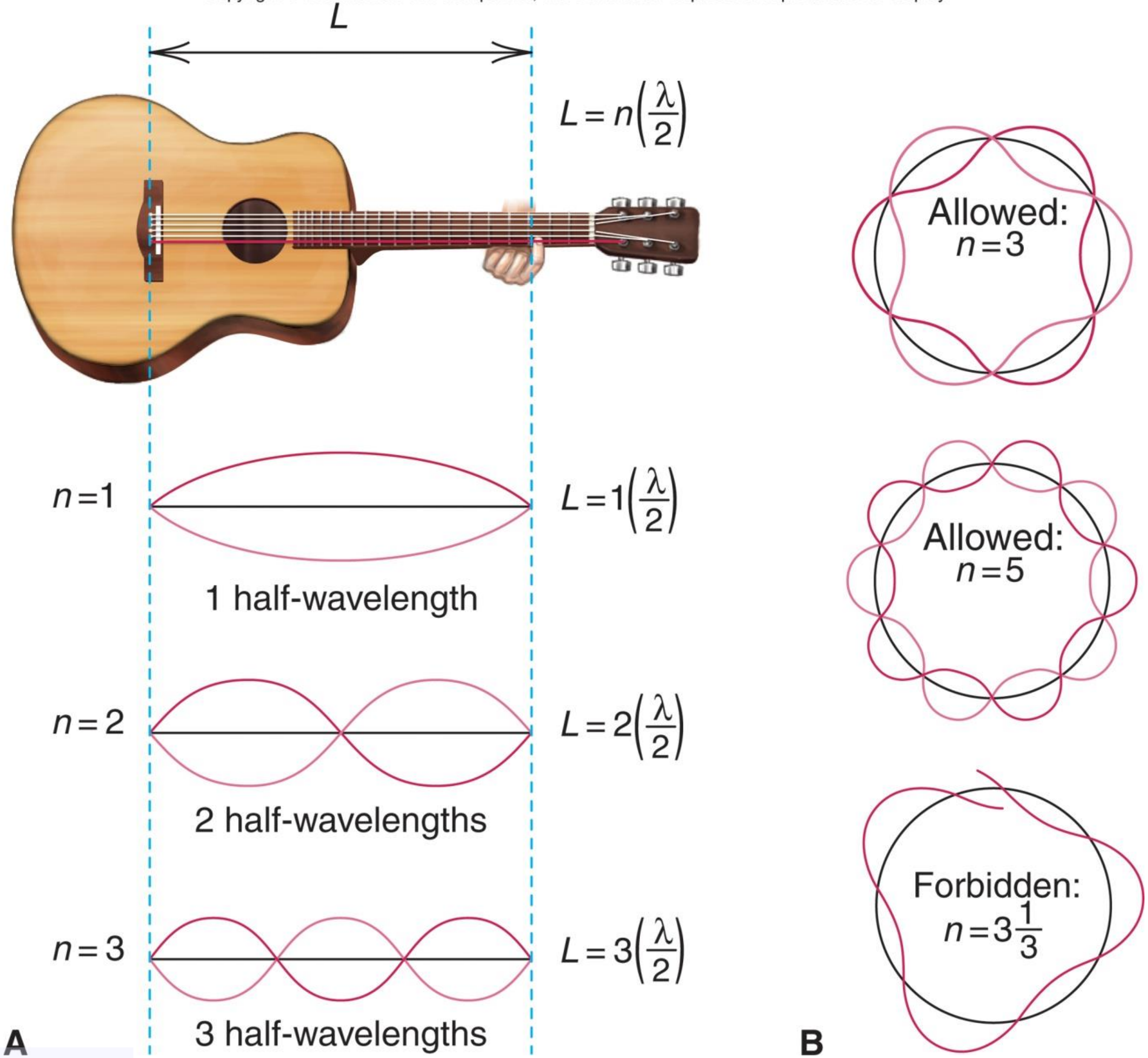


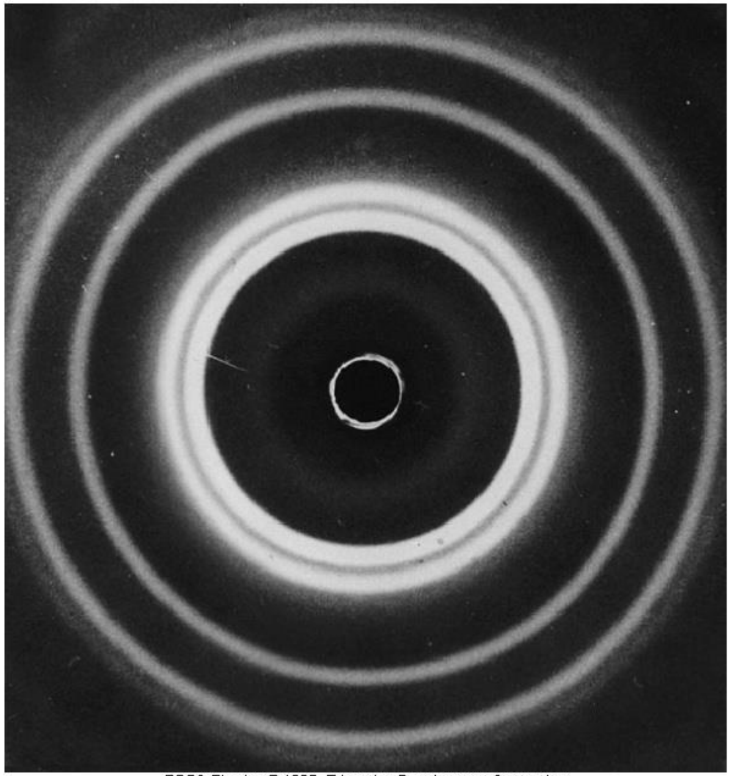
Table 7.1 The de Broglie Wavelengths of Several Objects

Substance	Mass (g)	Speed (m/s)	λ (m)
slow electron	9×10^{-28}	1.0	7×10^{-4}
fast electron	9×10^{-28}	5.9×10^{6}	1×10^{-10}
alpha particle	6.6×10^{-24}	1.5×10^{7}	7×10^{-15}
one-gram mass	1.0	0.01	7×10^{-29}
baseball	142	25.0	2×10^{-34}
Earth	6.0×10^{27}	3.0×10^{4}	4×10^{-63}

Sample Problem 7.4 **Calculating the de Broglie Wavelength of an Electron**

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

Figure 7.13 Diffraction patterns of aluminum with x-rays and electrons.



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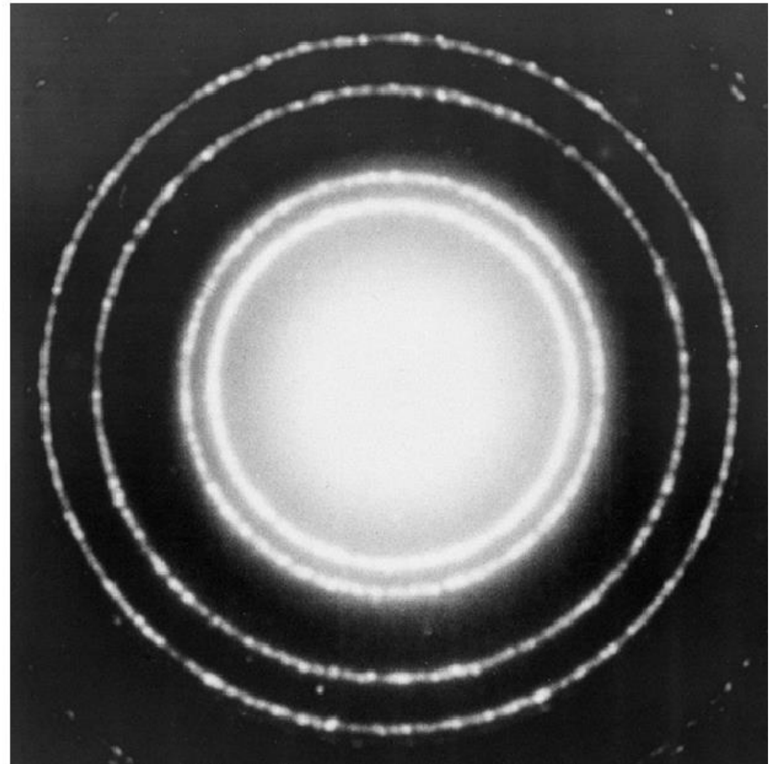
x-ray diffraction of aluminum foil



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electron diffraction of aluminum foil

Figure 7.14

Major observations and theories leading from classical theory to quantum theory

CLASSICAL THEORY

Matter	**Energy**
particulate, massive	**continuous, wavelike**

Since *matter* is discontinuous and particulate, perhaps *energy* is discontinuous and particulate.

Observation		***Theory***	
Blackbody radiation	→	Planck:	Energy is quantized; only certain values allowed
Photoelectric effect	→	Einstein:	Light has particulate behavior (photons)
Atomic line spectra	→	Bohr:	Energy of atoms is quantized; photon emitted when electron changes orbit.

Figure 7.14 continued

Since *energy* is wavelike, perhaps *matter* is wavelike.	
Observation	***Theory***
Davisson/Germer: Electron beam is diffracted by metal crystal ←	deBroglie: All matter travels in waves; energy of atom is quantized due to wave motion of electrons
Since *matter* has mass, perhaps *energy* has mass	
Observation	***Theory***
Compton: Photon’s wavelength increases (momentum decreases) after colliding with electron ←	Einstein/deBroglie: Mass and energy are equivalent; particles have wavelength and photons have momentum.

QUANTUM THEORY

Energy *and* Matter
particulate, massive, wavelike

Heisenberg's Uncertainty Principle

Heisenberg's Uncertainty Principle states that it is not possible to know both the position *and* momentum of a moving particle at the same time.

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

x = position

u = speed

The more accurately we know the speed, the less accurately we know the position, and vice versa.

The Quantum-Mechanical Model of the Atom

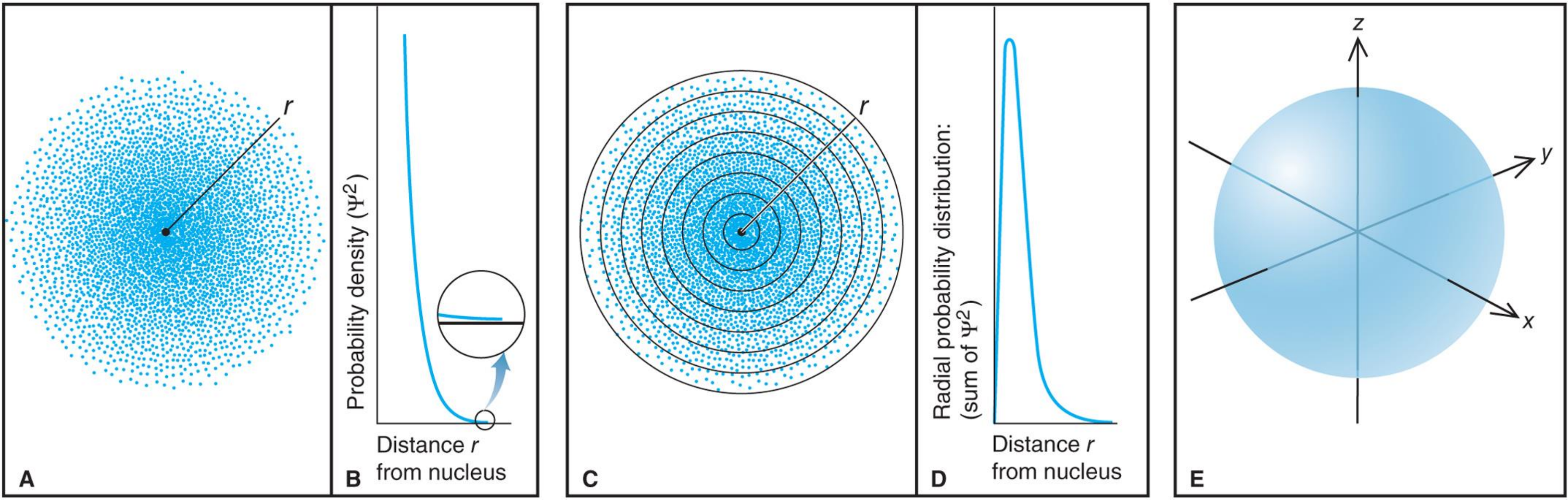
The matter-wave of the electron occupies the space near the nucleus and is continuously influenced by it.

The ***Schrödinger wave equation*** allows us to solve for the energy states associated with a particular atomic orbital.

The square of the wave function gives the ***probability density***, a measure of the ***probability*** of finding an electron of a particular energy in a particular region of the atom.

Figure 7.15

Electron probability density in the ground-state H atom.



Quantum Numbers and Atomic Orbitals

An atomic orbital is specified by three quantum numbers.

The ***principal*** quantum number (***n***) is a positive integer.

The value of *n* indicates the relative ***size*** of the orbital and therefore its relative ***distance*** from the nucleus.

The ***angular momentum*** quantum number ***(l)*** is an integer from 0 to (*n* -1).

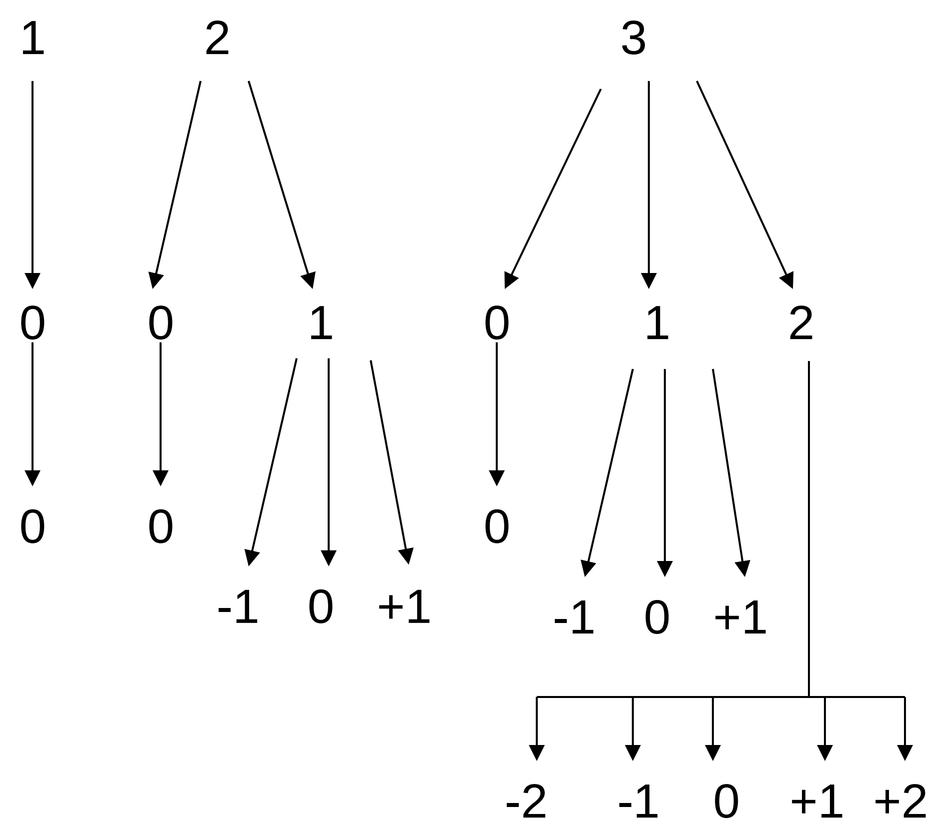
The value of *l* indicates the ***shape*** of the orbital.

The ***magnetic*** quantum number **(m_l)** is an integer with values from $-l$ to $+l$

The value of m_l indicates the spatial ***orientation*** of the orbital.

Table 7.2 The Hierarchy of Quantum Numbers for Atomic Orbitals

Name, Symbol (Property)	Allowed Values	Quantum Numbers
Principal, n (size, energy)	Positive integer (1, 2, 3, ...)	1 2 3
Angular momentum, l (shape)	0 to n – 1	0 0 1 0 1 2
Magnetic, m_l (orientation)	$-l,\ldots,0,\ldots,+l$	0 0 -1 0 +1 0 -1 0 +1 -2 -1 0 +1 +2



Sample Problem 7.5 **Determining Quantum Numbers for an Energy Level**

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

Sample Problem 7.6 **Determining Sublevel Names and Orbital 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)** $n = 4$, $l = 3$

Sample Problem 7.7 — Identifying Incorrect 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	1*p*
(b)	4	3	+1	4*d*
(c)	3	1	-2	3*p*

Figure 7.16 The 1*s*, 2*s*, and 3*s* orbitals.

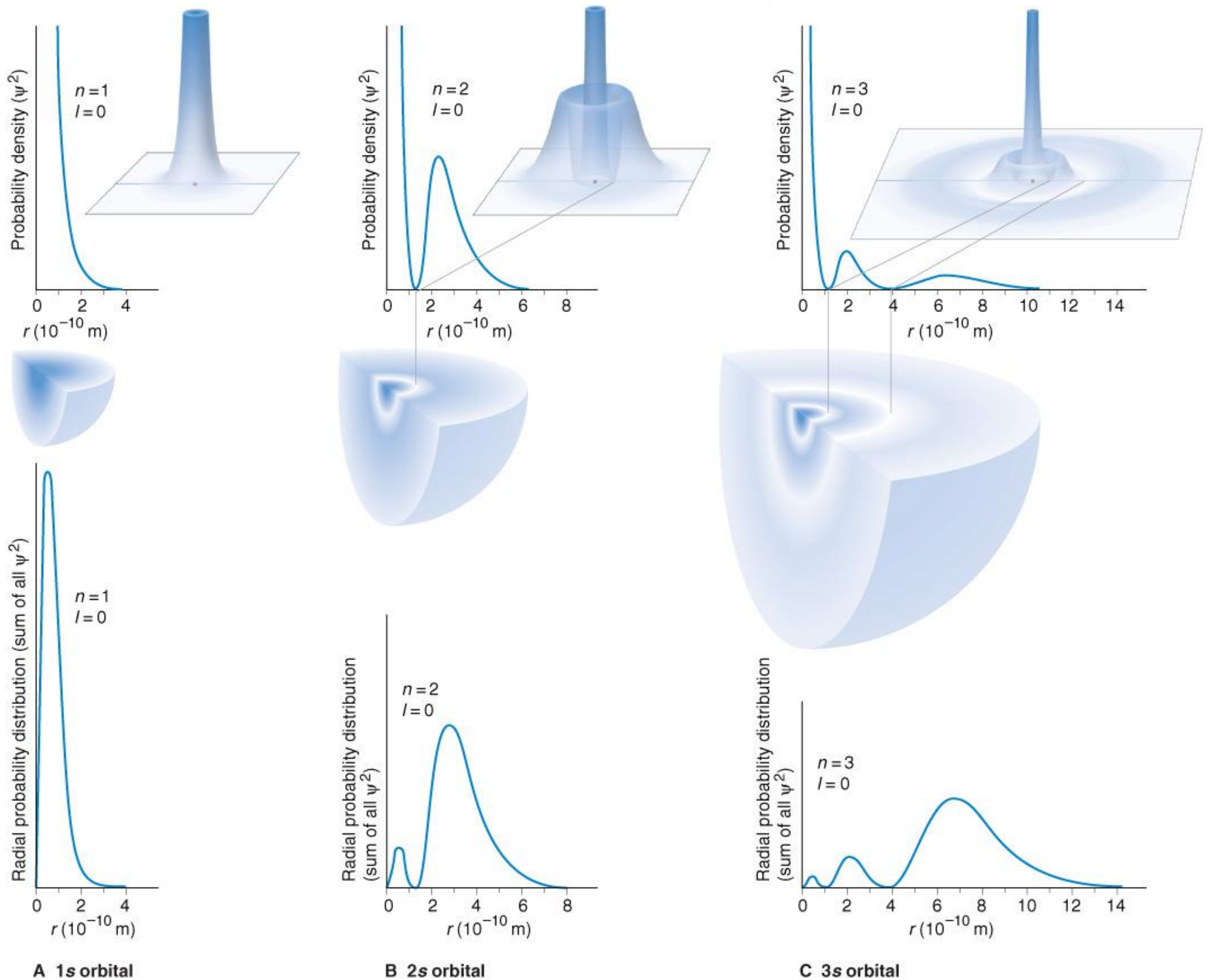
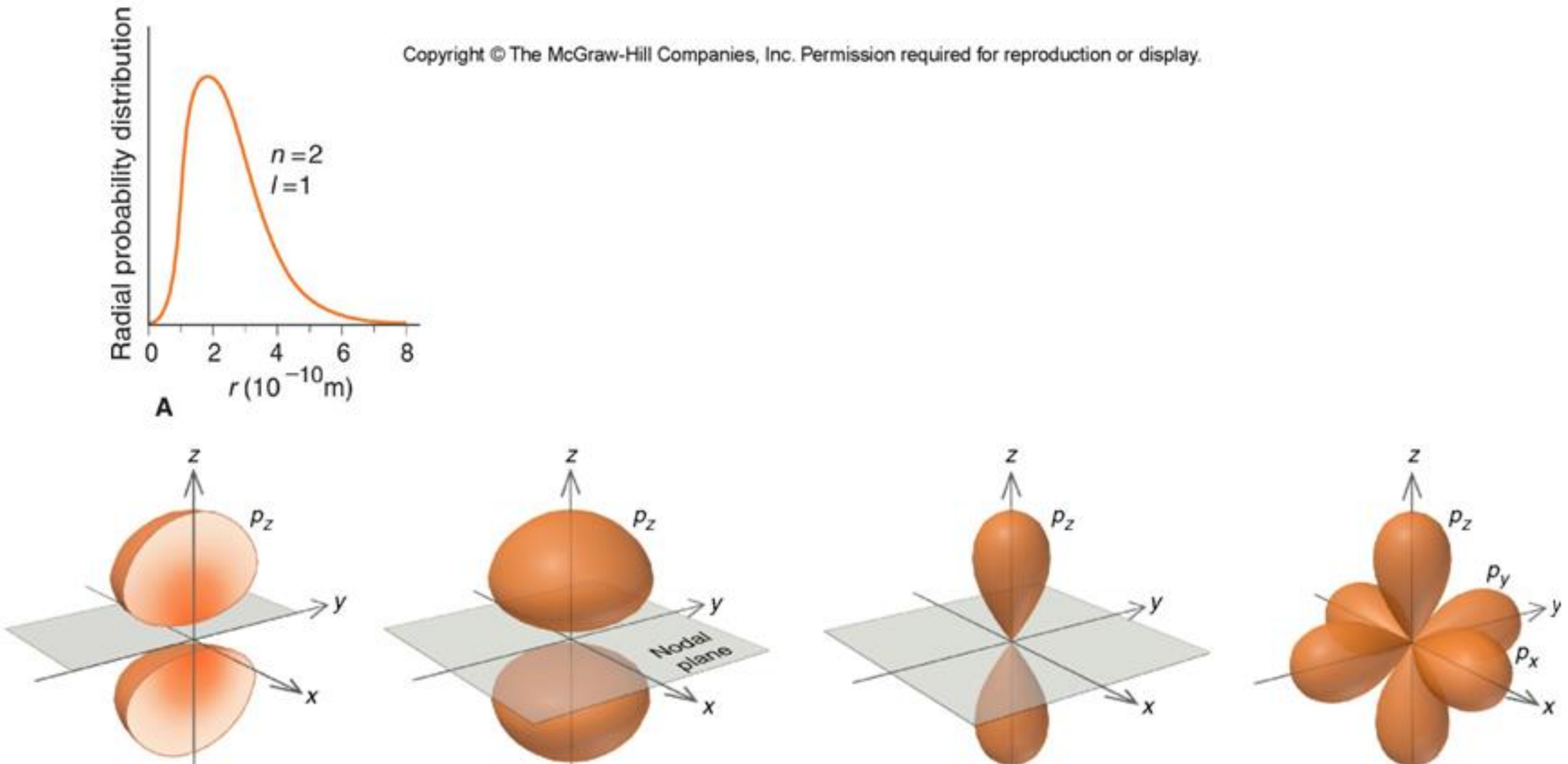


Figure 7.17 The 2*p* orbitals.



B Cross section of electron cloud depiction

C Accurate probability contour

D Stylized probability contour

E The three *p* orbitals

Figure 7.18 The 3*d* orbitals.

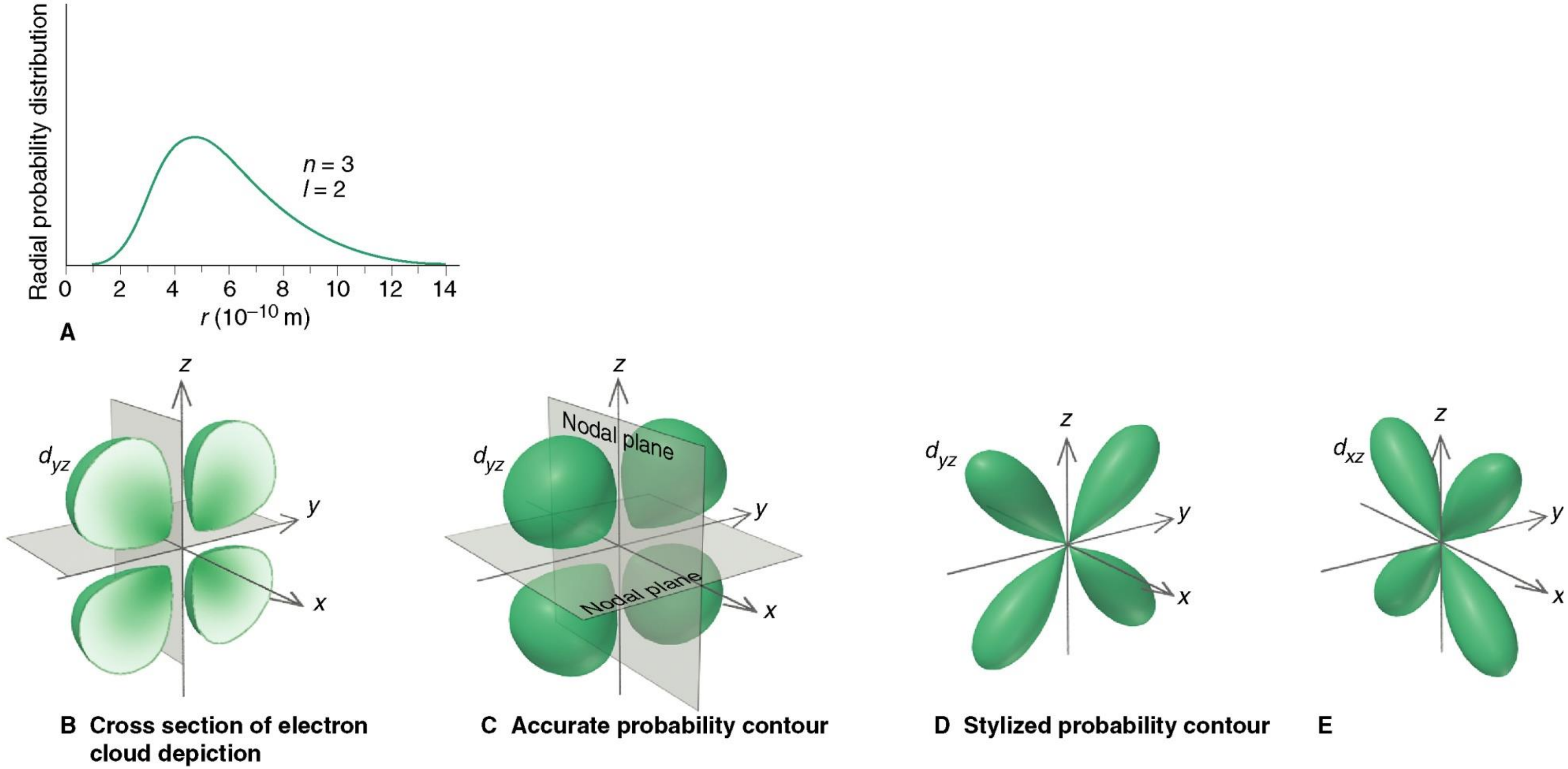


Figure 7.18

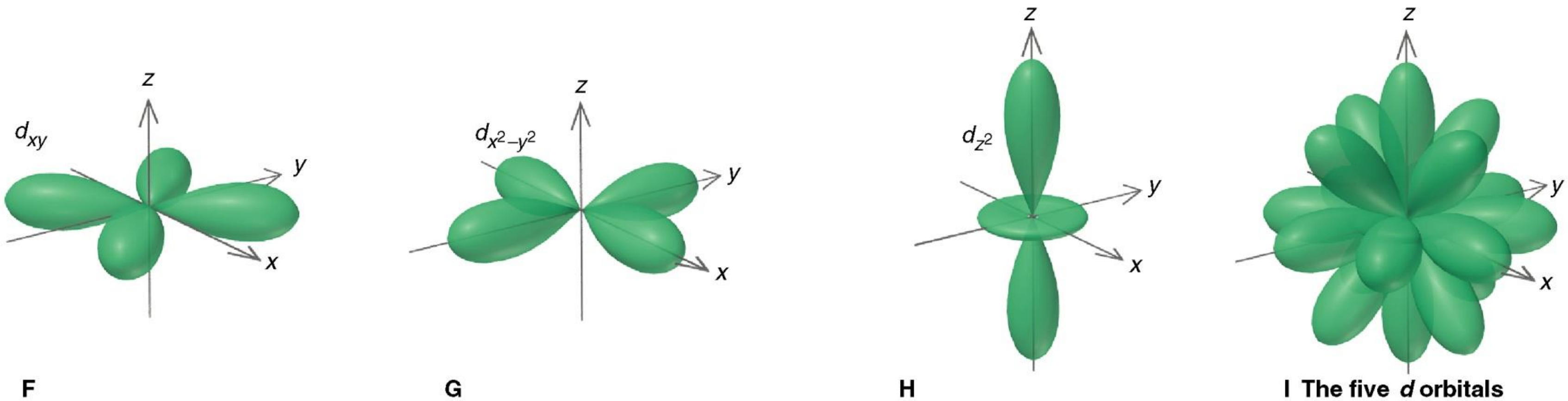


Figure 7.19 **The $4f_{xyz}$ orbital, one of the seven $4f$ orbitals.**

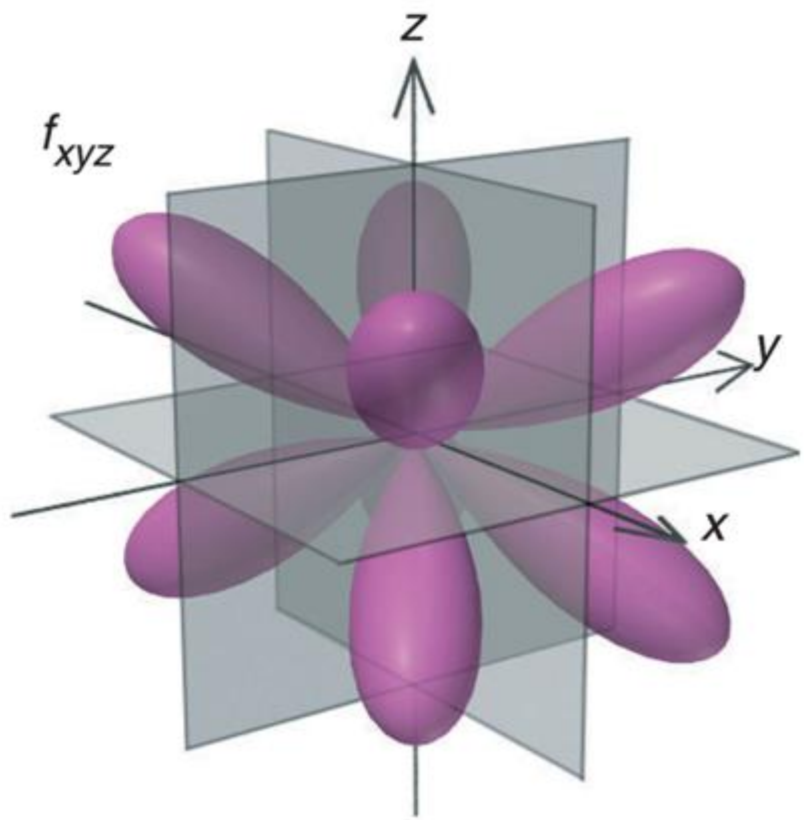


Figure 7.20 **Energy levels of the H atom.**