Genel Kimya

Prensipler ve Modern Uygulamalar

Petrucci • Harwood • Herring

8. Baskı

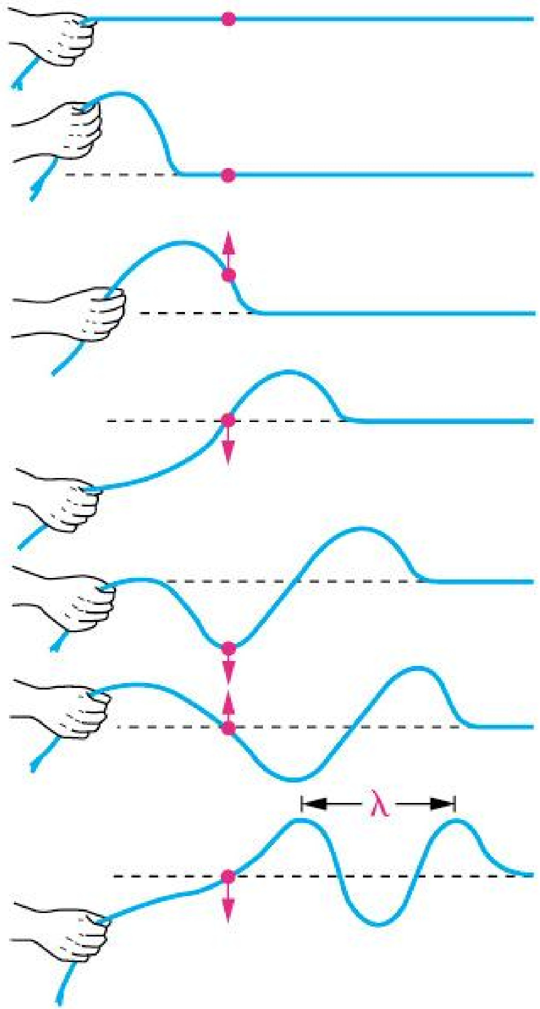
Bölüm 9: Atomun Elektron Yapısı

İçerik

İçerik

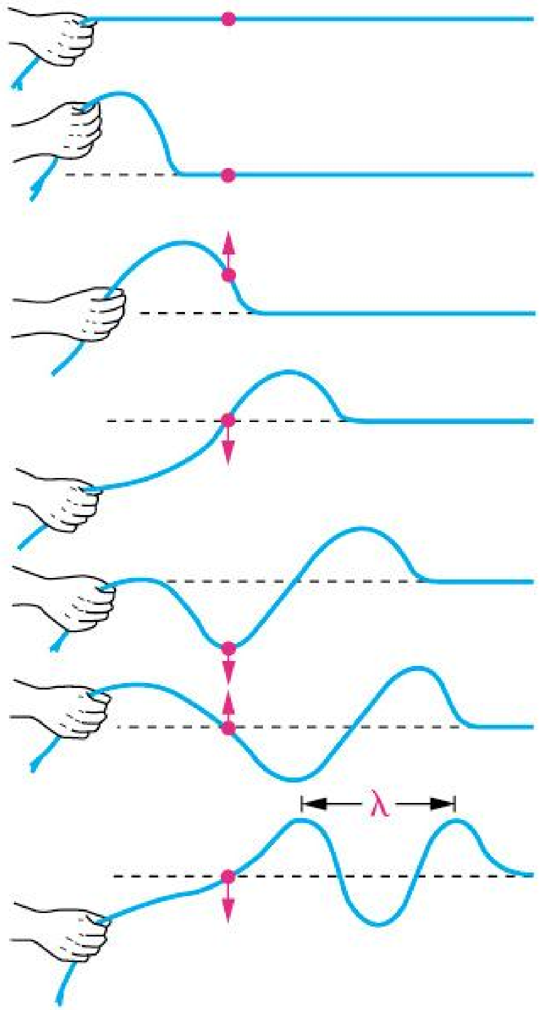
9-1 Elektromanyatik Işıma

- Elektromanyetik ışıma, elektrik ve manyetik alanın birbirine dik (boşlukta veya bir ortamda) dalgalar halinde yayılan enerji şeklidir.
- Dalga bir ortamda enerji taşıyan bir uyarıcıdır.
- Birbirini izleyen iki dalga tepesinin en üst noktaları arasındaki mesafeye **dalgaboyu** denir ve lamda (λ) ile gösterilir.

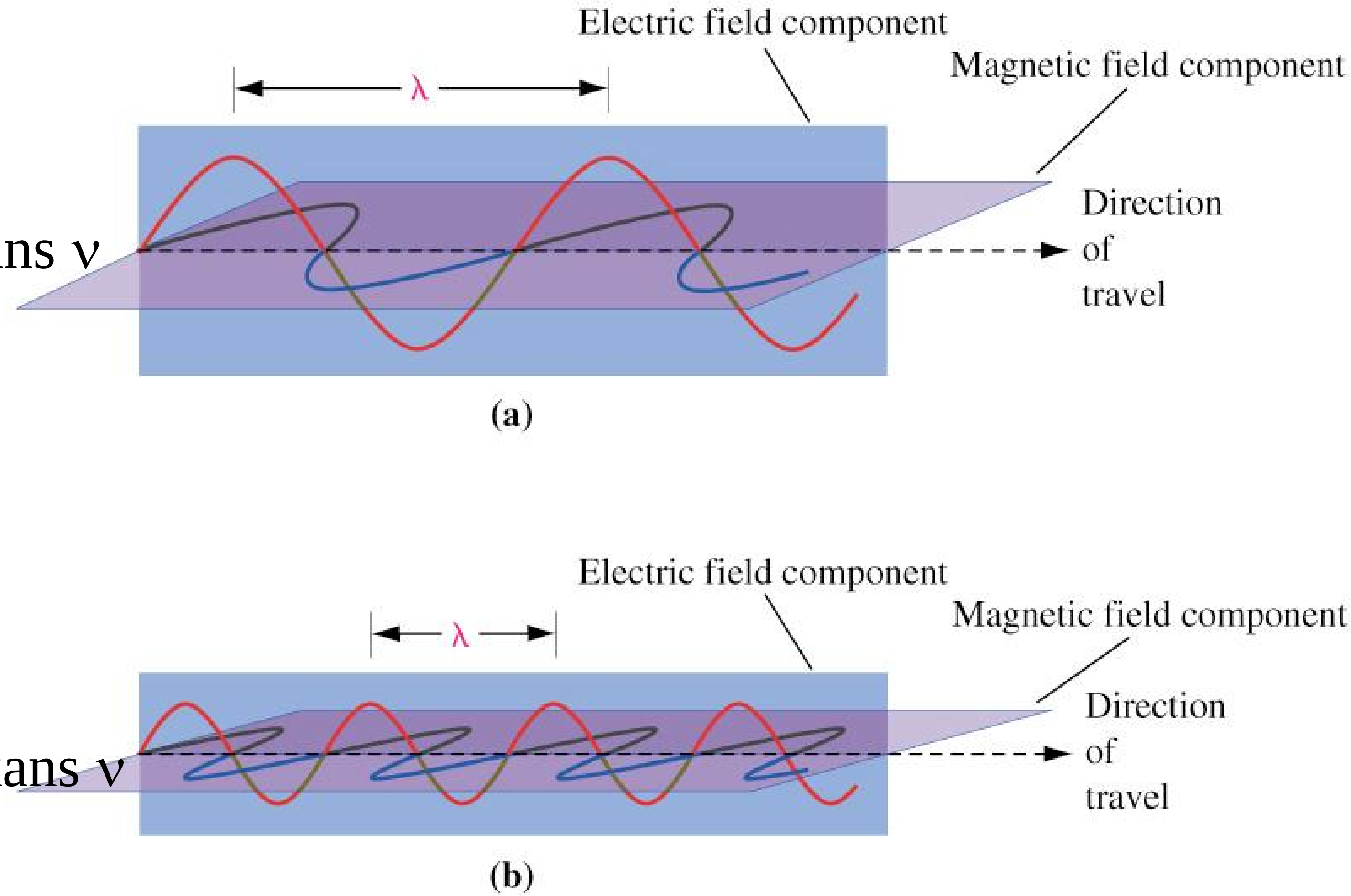


9-1 Elektromanyatik Işıma

- Dalgaboyu bir dalganın en önemli karakteristiğidir.
- Belirli bir noktadan birim zamanda geçen dalga sayısına **frekans** (υ), denir nü ile gösterilir.
- Frekansın birimi genelde 1/sn ve frekans ile dalga boyunun çarpımı dalganın birim zamanda aldığı yolu verir. Buna dalganın hızı denir.



Elektromanyetik Işıma



Düşük frekans ν

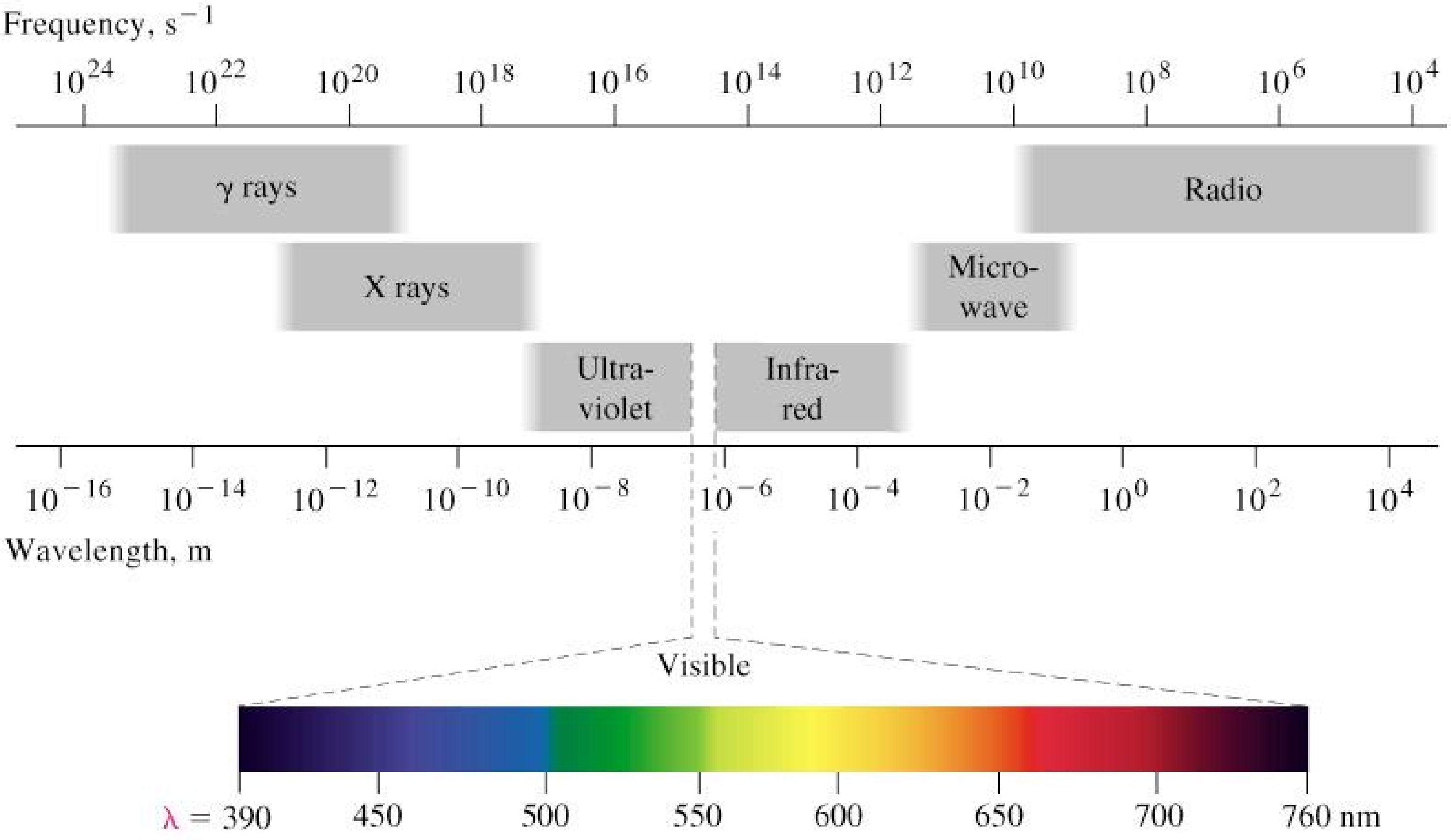
Yüksek frekans ν

Frekans, Dalgaboyu ve Hız

- Frekans (ν) Hertz—Hz veya s^{-1}.
- Dalgaboyu (λ)—m.
  - cm (10^{-2} m) μm (10^{-6} m) nm (10^{-9} m) A^o (10^{-10} m) pm (10^{-12} m)
- Hız (c)—2.997925×10^8 m s^{-1}.

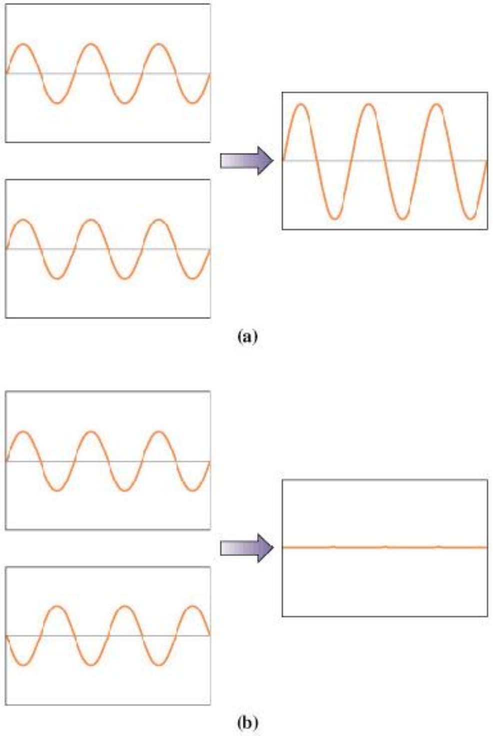
$$c = \lambda\nu \qquad \lambda = c/\nu \qquad \nu = c/\lambda$$

Elektromanyetik Spektrum



Elektromanyetik dalgaların özelliği

Elektromanyetik dalgaların en önemli iki özelliği girişim ve kırınımdır.

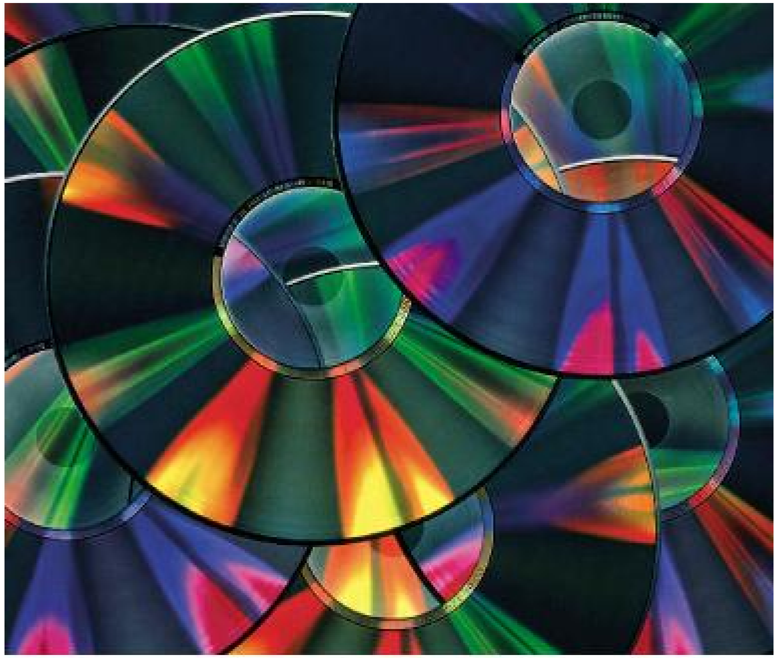


Şiddetlendirici

Yokedici

Dalgaların Girişimi

(a)



(b)

Işığın Kırılımı ve Kırınımı

Bir ışın demetinin yivli bir yüzeyden yansımasıyla oluşan girişimden kaynaklanan farklı dalgaboyundaki bileşenlşerinin saçılımına kırınım(difraksiyon) denir.

(a)

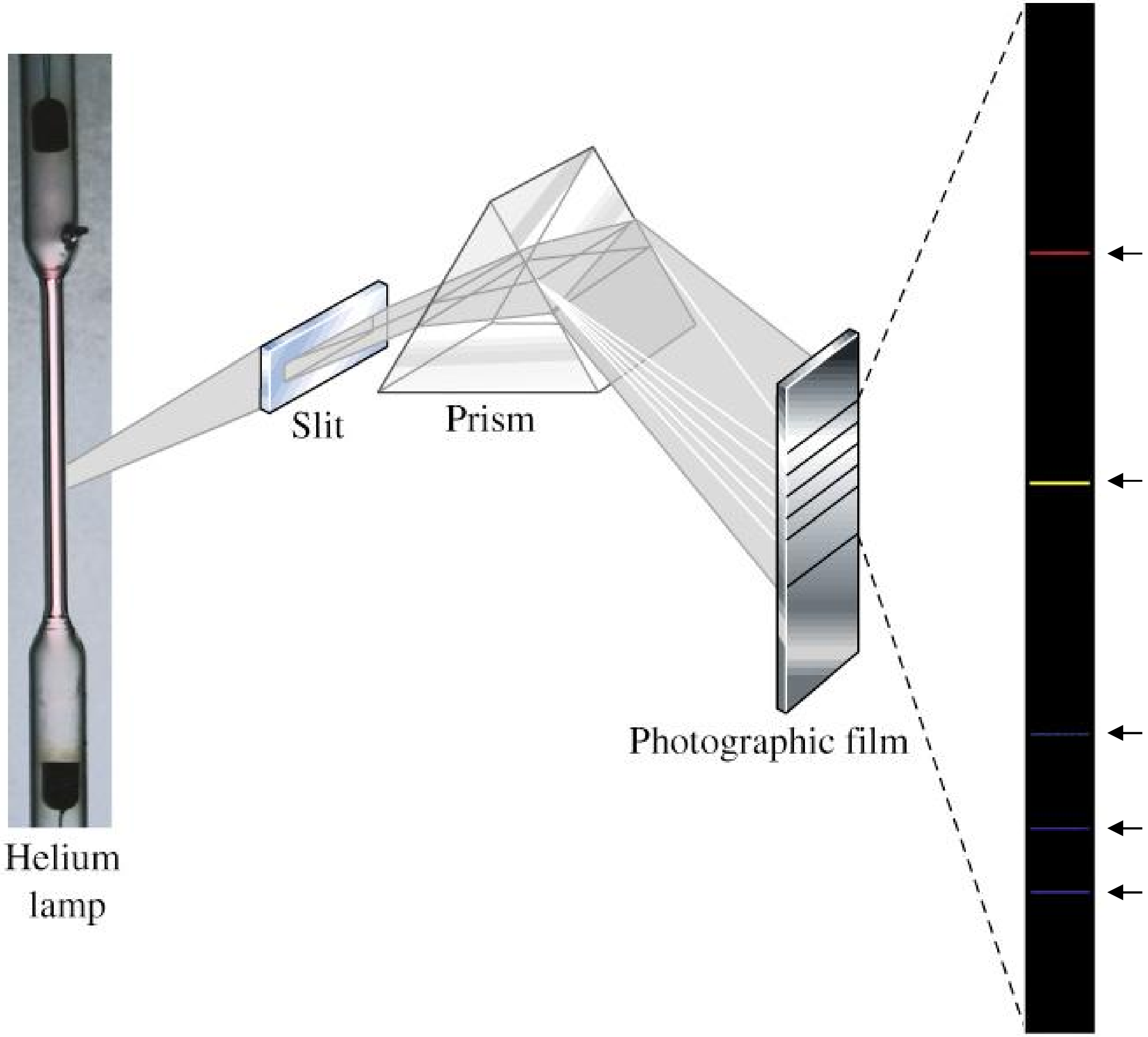
(b)

Işık bir ortamdan farklı bir ortama geçerken kırılır(bükülür). Beyaz bir ışık prizmadan geçirildiğinde kırmızı ışık en az mor ışık en çok kırılır.

Atom Spektrumları

(a) Hidrojen, (b) Helyum, (c) Lityum, (d) Sodyum, (e) Potasyum

Atom Spektrumu

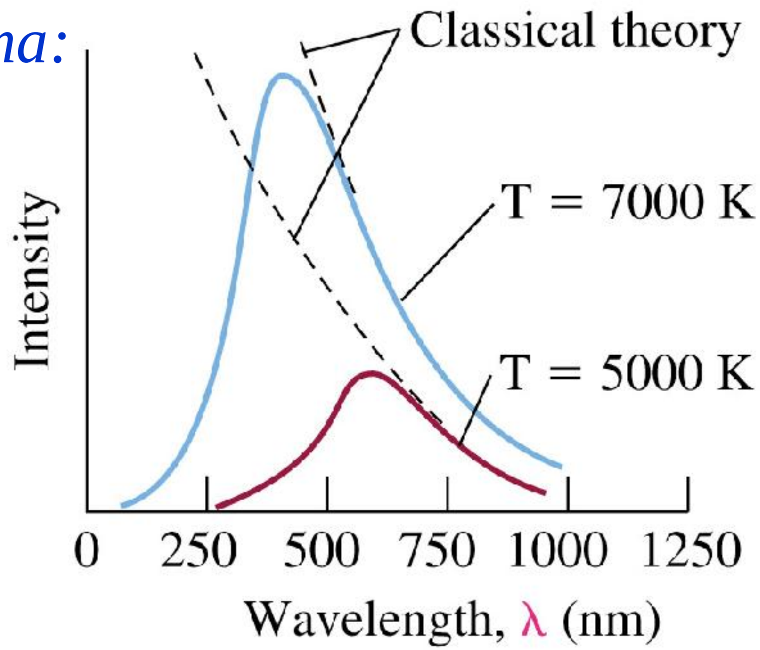


Kuantum Teorisi

Isıtılmış bir cisimden yayılan ışıma:

Siyah cisim ışıması

$$\epsilon = h\nu$$



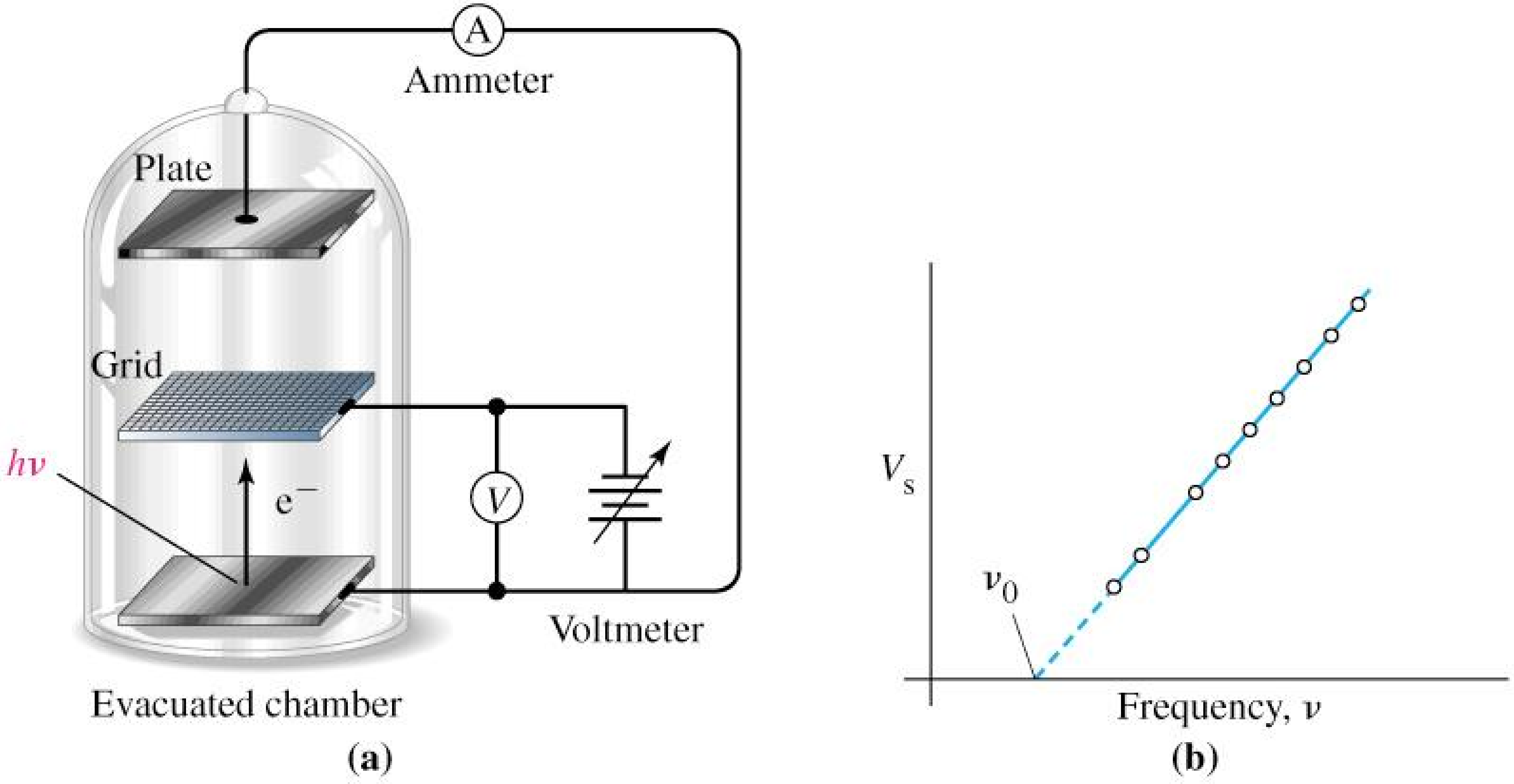
Max Planck, 1900:

Enerji de madde gibi sürekli değildir. Klasik fizik bir sistemin sahip olduğu enerji için sınırlandırma getirmezken Planck kunatum teorisine göre sistem belirli paketler halindeki enerjilere sahiptir. Herbir enerji paketine enerji kuantumu denir.

Fotoelektrik Olayı

- 1888 de Heinrich Hertz, belirli metallerin yüzeyine ışık çarptığında metalden elektron boşaldığını bulmuştır.
- Elektron yayılımı yalnızca gelen ışığın frekansının eşik değerinin üzerine çıkınca olur.
- Bu koşul sağlandığında yayılan elektron sayısı gelen ışığın şiddetine bağlıdır.
- Yayılan elektronların kinetik enerjisi ışığın frekansına bağlıdır.
- $\nu > \nu_o$ eşik frekansı
- Elektromanyetik ışımanın taneciklerine foton denir.

Fotoelektrik Olayı



Fotoelektrik Olayı

- Durdurma potansiyelindeki yayılan elektronun kinetik enerjisi potansiyel enerji olarak ifade edilebilir.(Vs: durdurma potansiyeli)

$$\frac{1}{2} mu^2 = eV_s$$

- Eşik frekansı ν_o ve gelen ışığın frekansı ν :

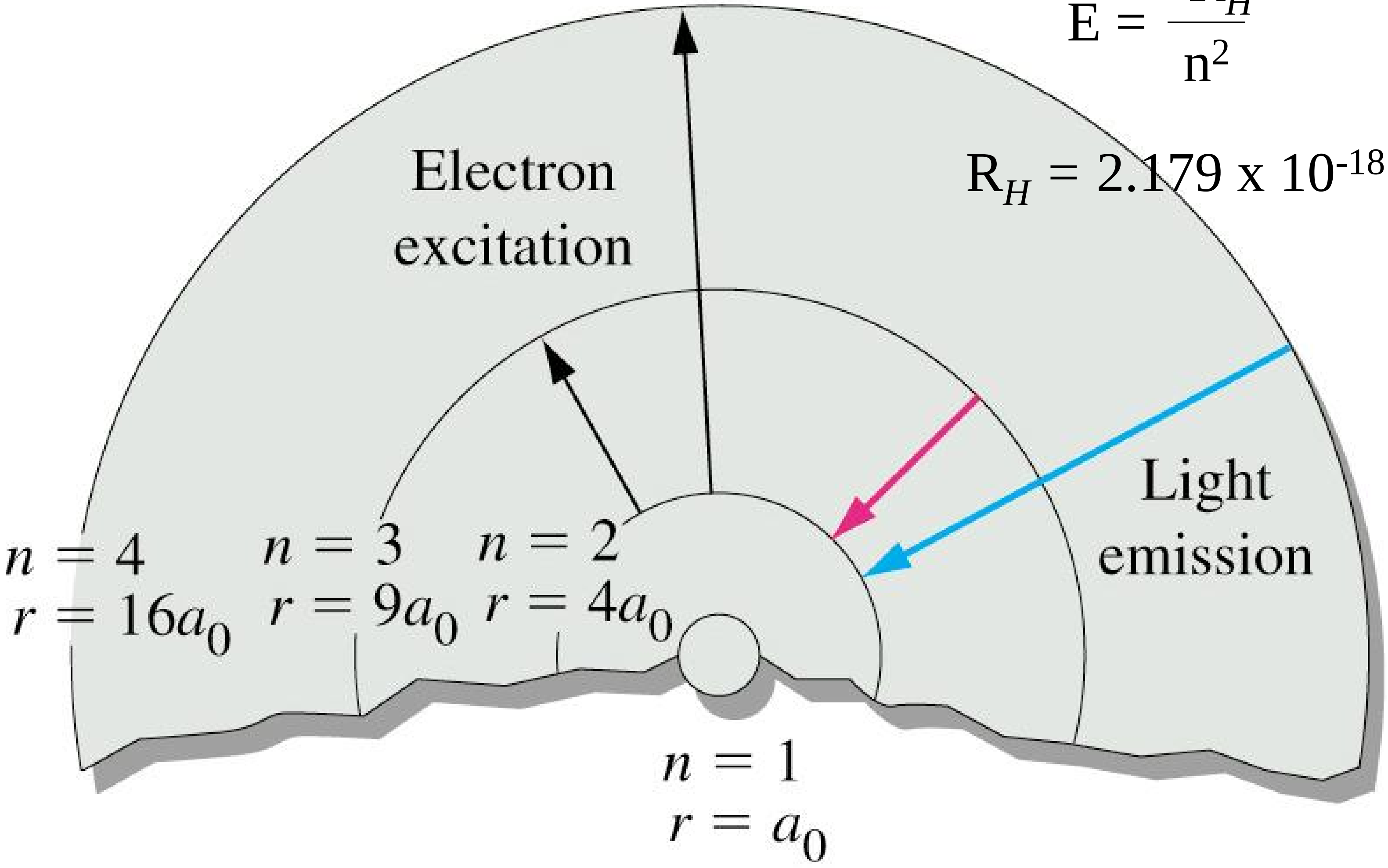
ν_o her metal için farklıdır. Eğer frekans eşik frekansının altındaysa fotoelektrik oluşmaz. Vs ışığın şiddetine değil frekansına bağlıdır.

$$V_s = k (\nu - \nu_o)$$

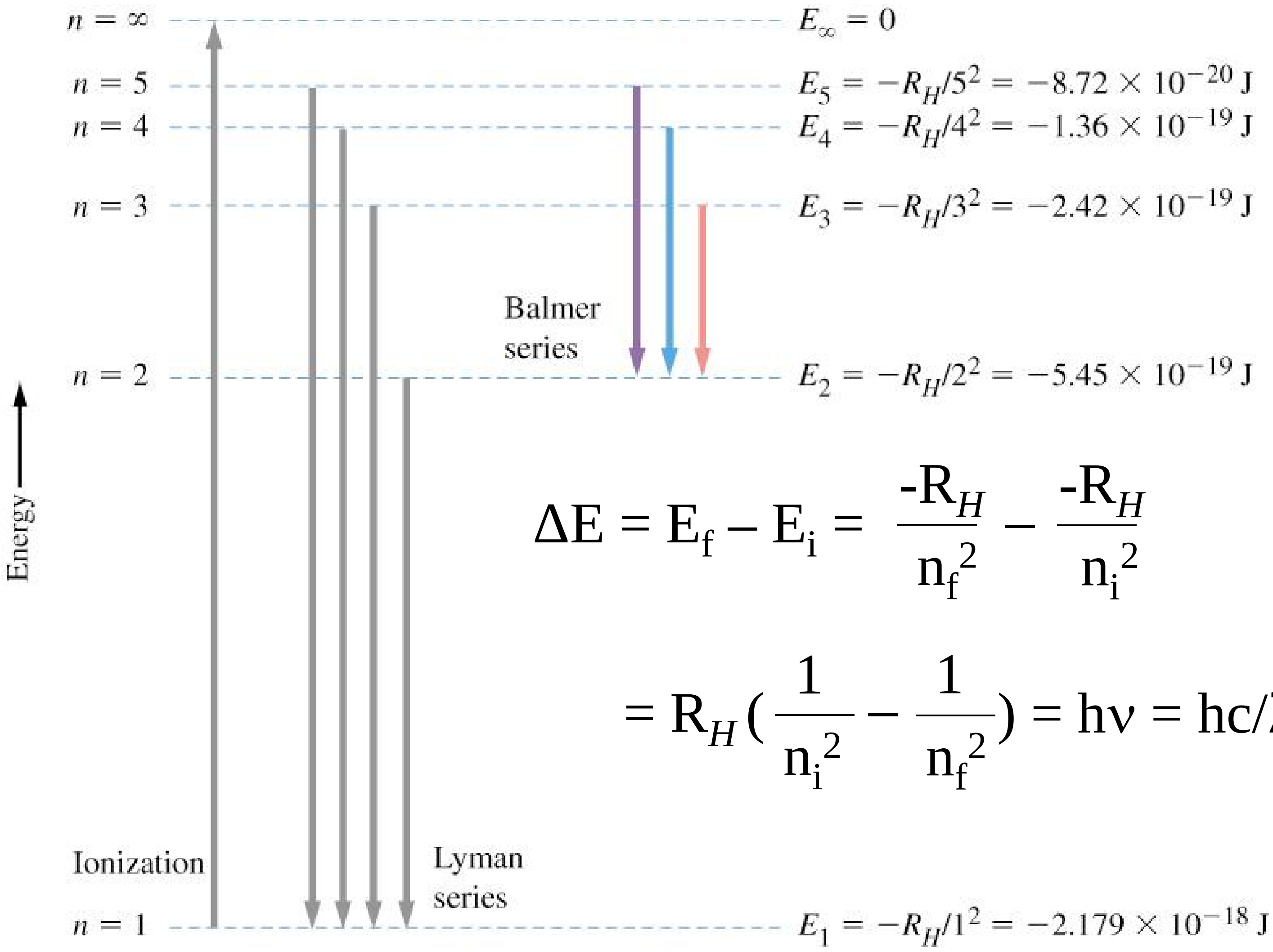
Bohr Atom Modeli

$$E = \frac{-R_H}{n^2}$$

$R_H = 2.179 \times 10^{-18}$ J



Enerji-Düzeyi Diyagramı



$$\Delta E = E_f - E_i = \frac{-R_H}{n_f^2} - \frac{-R_H}{n_i^2}$$

$$= R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = h\nu = hc/\lambda$$

Ionization Energy of Hydrogen

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

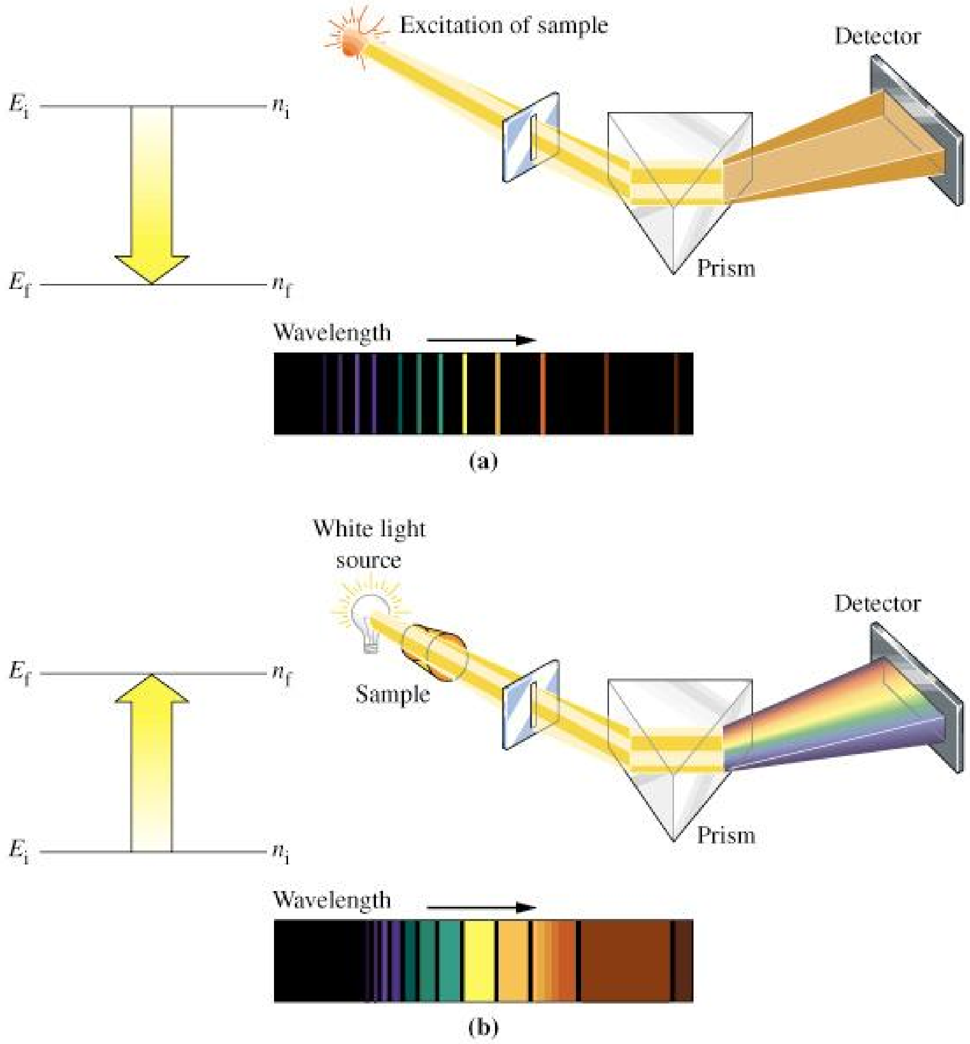
As n_f goes to infinity for hydrogen starting in the ground state:

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

This also works for hydrogen-like species such as He^+ and Li^{2+}.

$$h\nu = -Z^2 R_H$$

Emission and Absorption Spectroscopy



9-5 Two Ideas Leading to a New Quantum Mechanics

- Wave-Particle Duality.
  - Einstein suggested particle-like properties of light could explain the photoelectric effect.
  - But diffraction patterns suggest photons are wave-like.
- deBroglie, 1924
  - Small particles of matter may at times display wavelike properties.

deBroglie and Matter Waves

$$E = mc^2$$

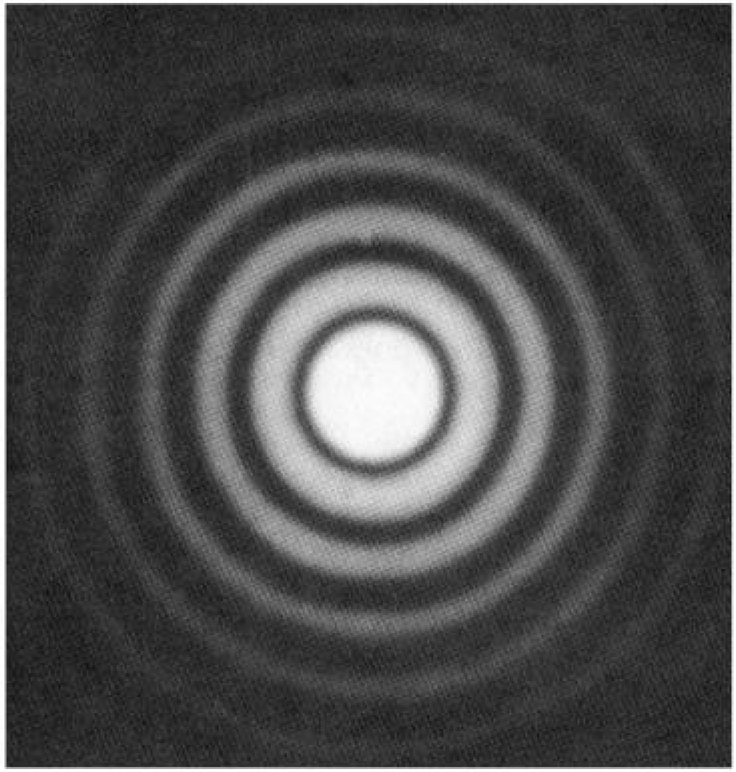
$$h\nu = mc^2$$

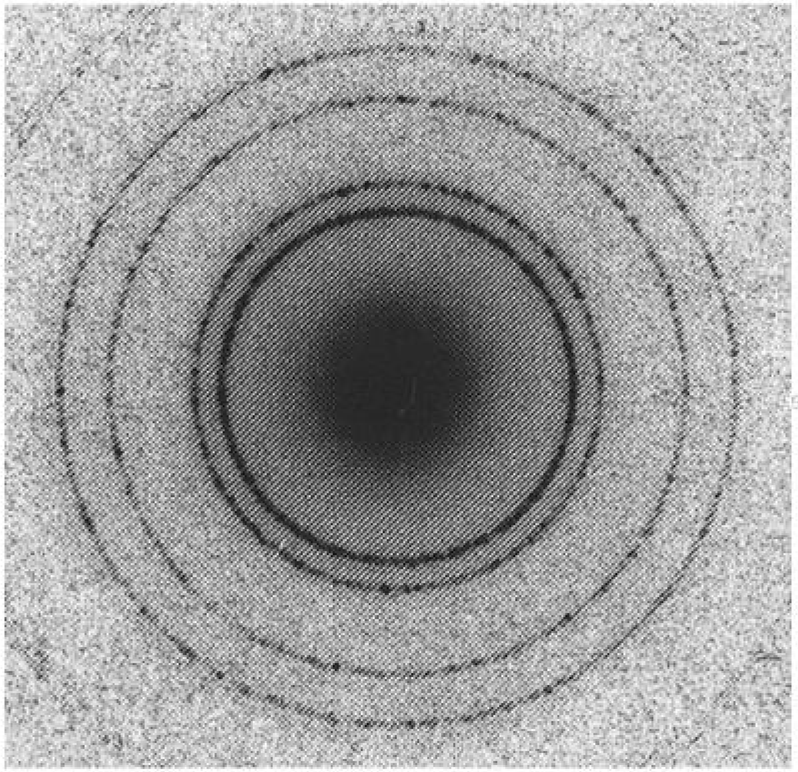
$$h\nu/c = mc = p$$

$$p = h/\lambda$$

$$\lambda = h/p = h/mu$$

X-Ray Diffraction

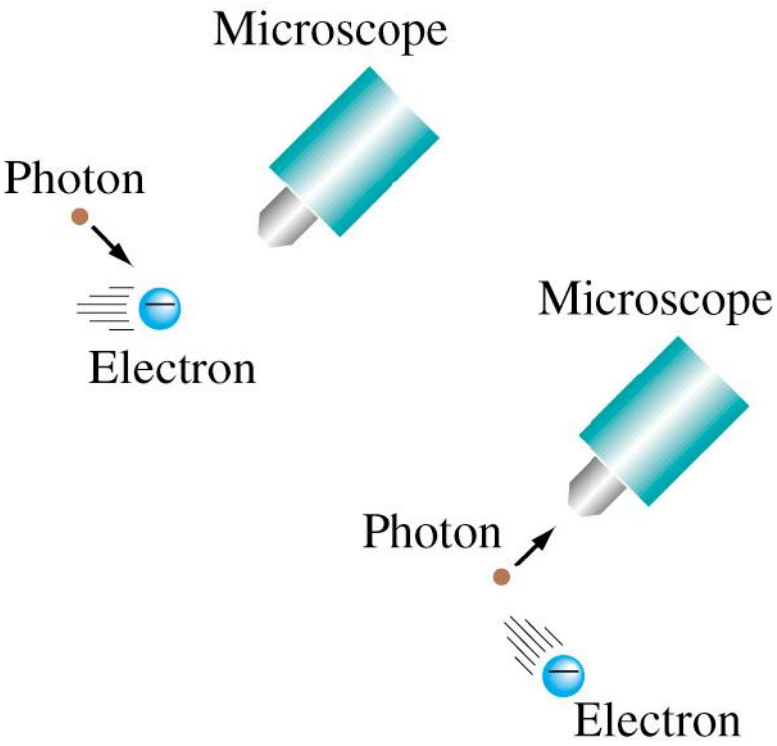




The Uncertainty Principle

- Werner Heisenberg

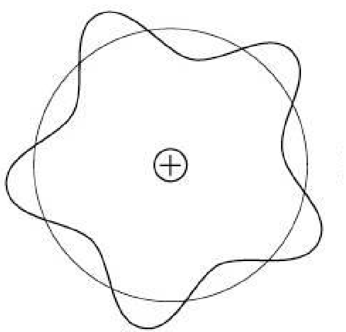
$$\Delta x \, \Delta p \geq \frac{h}{4\pi}$$

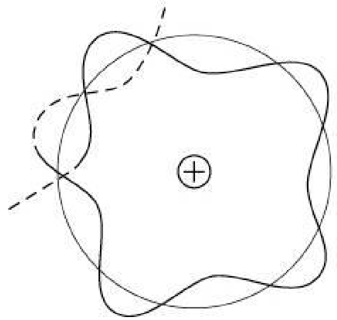


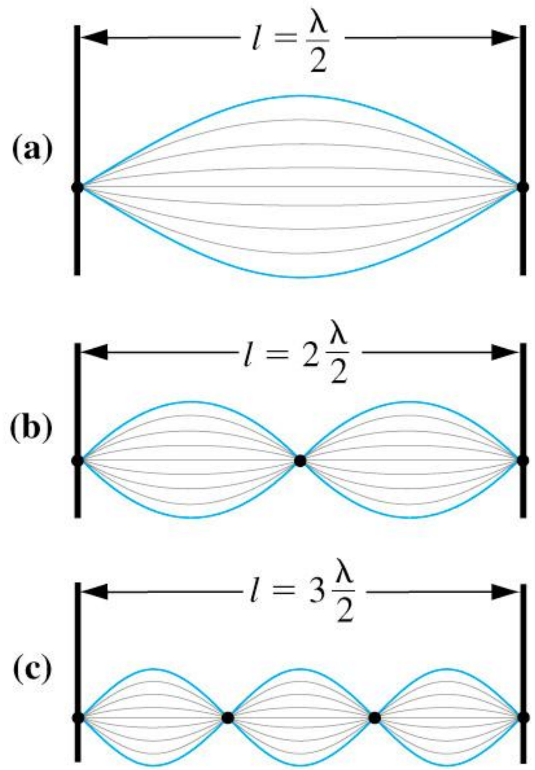
9-6 Wave Mechanics

- Standing waves.
  - Nodes do not undergo displacement.

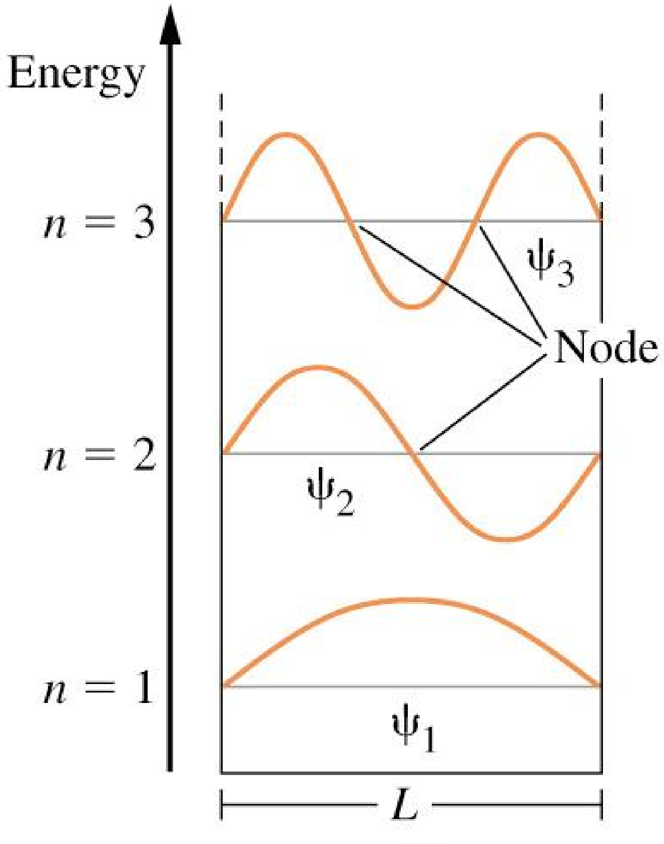
$$\lambda = \frac{2L}{n},\ n = 1, 2, 3\ldots$$







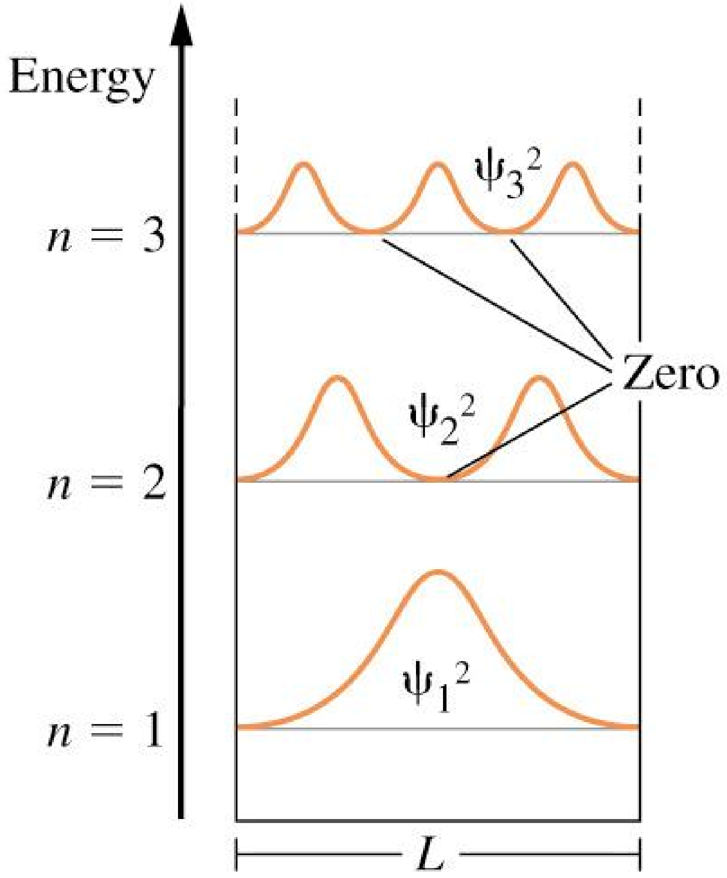
Wave Functions



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

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

Probability of Finding an Electron



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

The probabilities

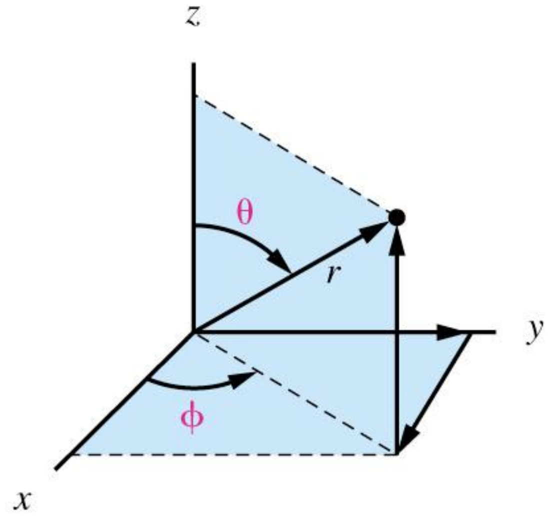
Wave Functions for Hydrogen

- Schrödinger, 1927 $E\psi = \mathcal{H}\psi$
  - $\mathcal{H}(x,y,z)$ or $\mathcal{H}(r,\theta,\varphi)$

$$\psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$$

R(r) is the radial wave function.

Y(θ,φ) is the angular wave function.



Spherical polar coordinates

$x^2 + y^2 + z^2 = r^2$

$x = r \sin\theta \cos\phi$

$y = r \sin\theta \sin\phi$

$z = r \cos\theta$

Principle Shells and Subshells

- Principle electronic shell, n = 1, 2, 3…
- Angular momentum quantum number, ℓ= 0, 1, 2…(n-1)

ℓ= 0, s

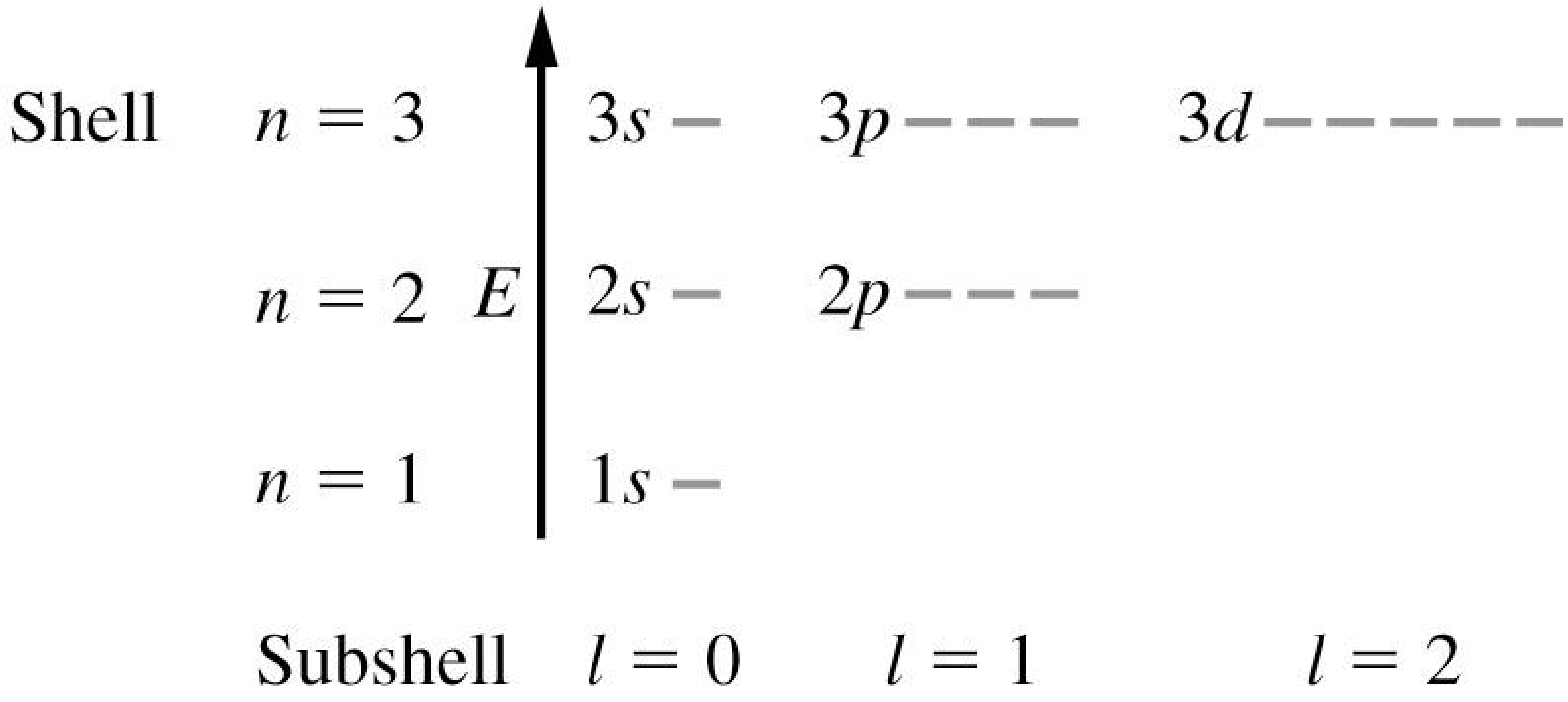
ℓ= 1, p

ℓ= 2, d

ℓ= 3, f

- Magnetic quantum number, m_l= - ℓ…-2, -1, 0, 1, 2…+ℓ

Orbital Energies

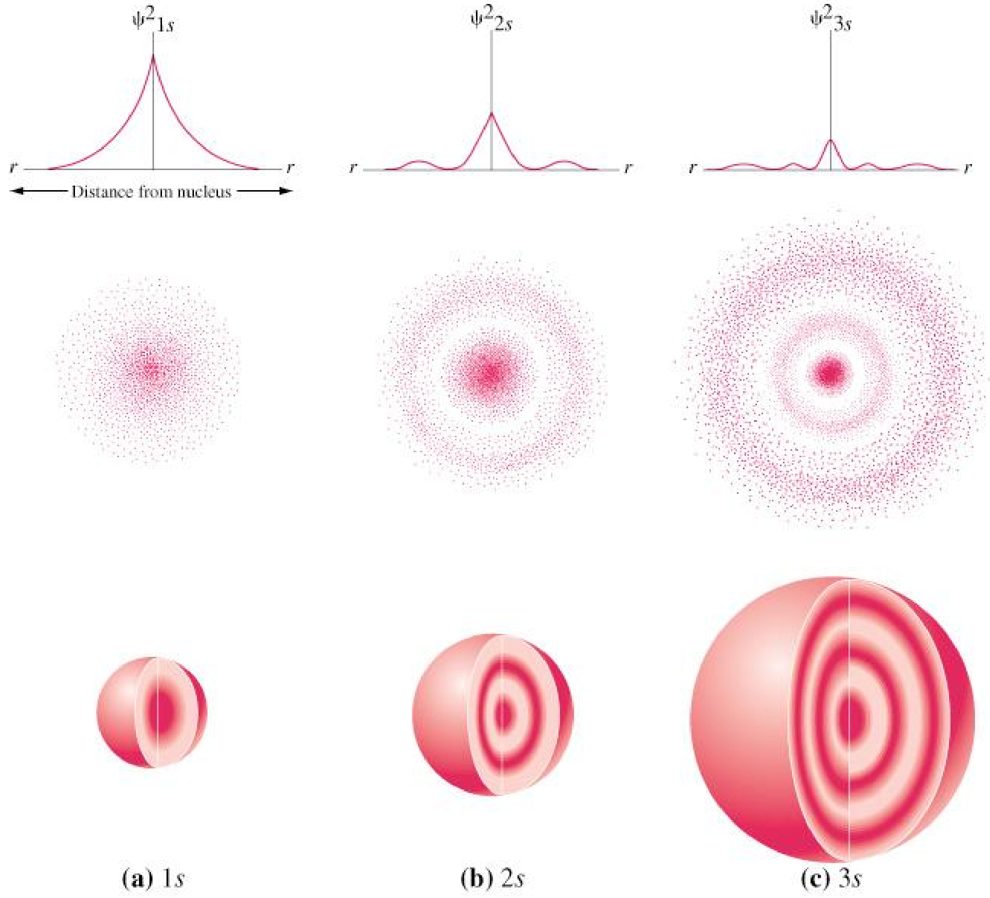


Each subshell is made up of $(2l + 1)$ orbitals.

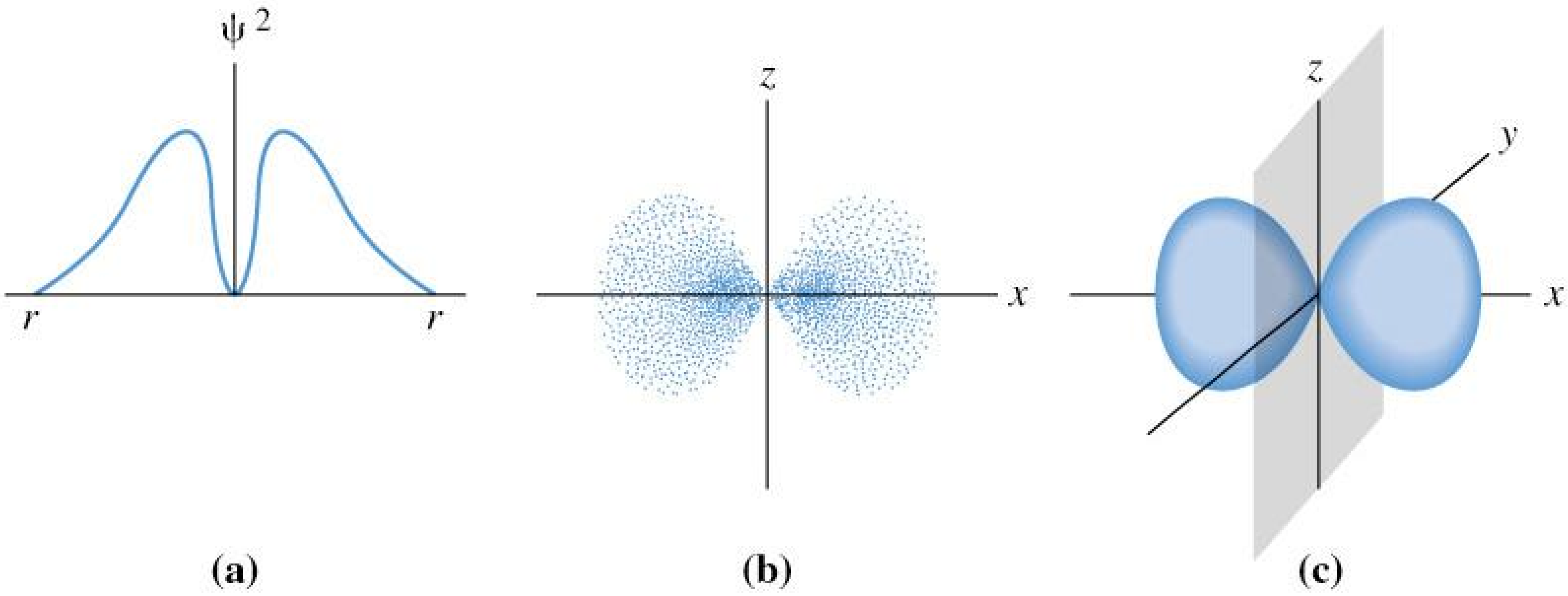
TABLE 9.1 The Angular and Radial Wave Functions of a Hydrogen-like Atom

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

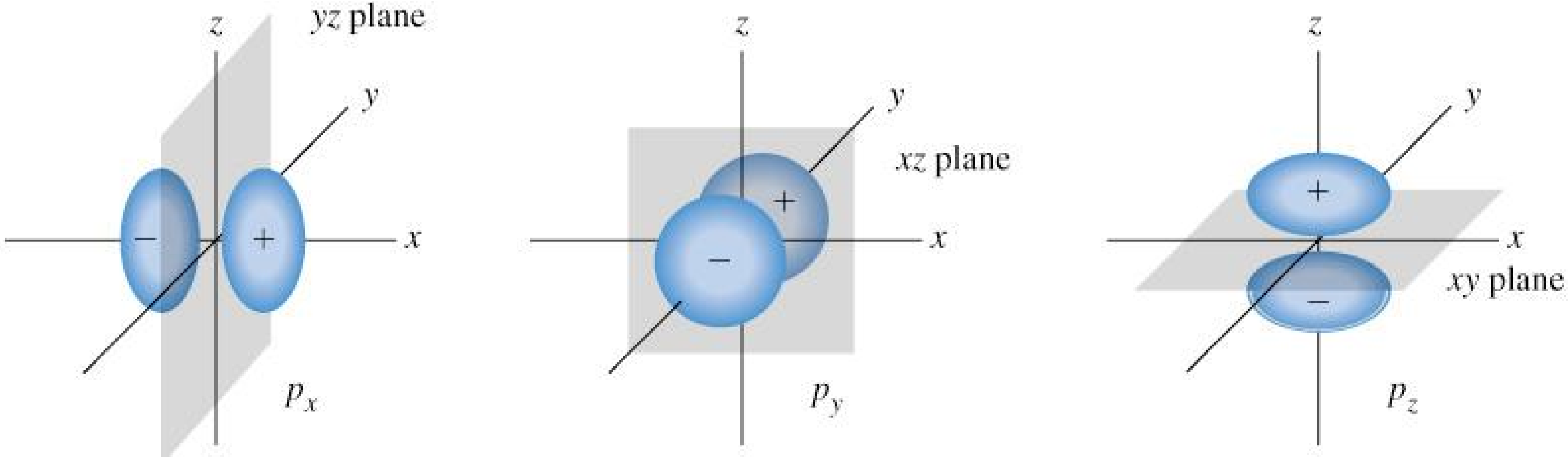
s orbitals



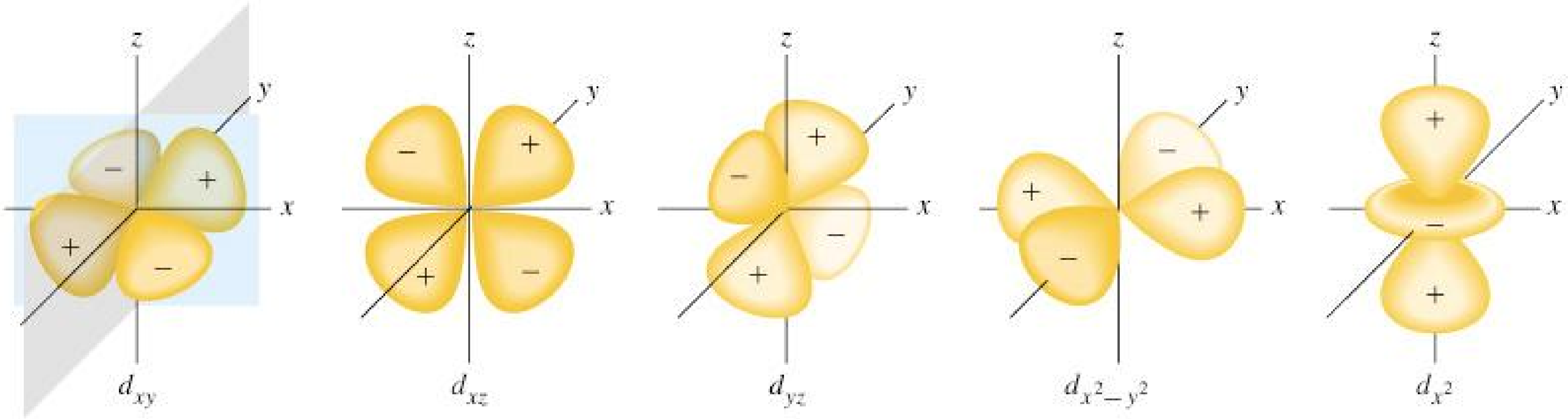
p Orbitals



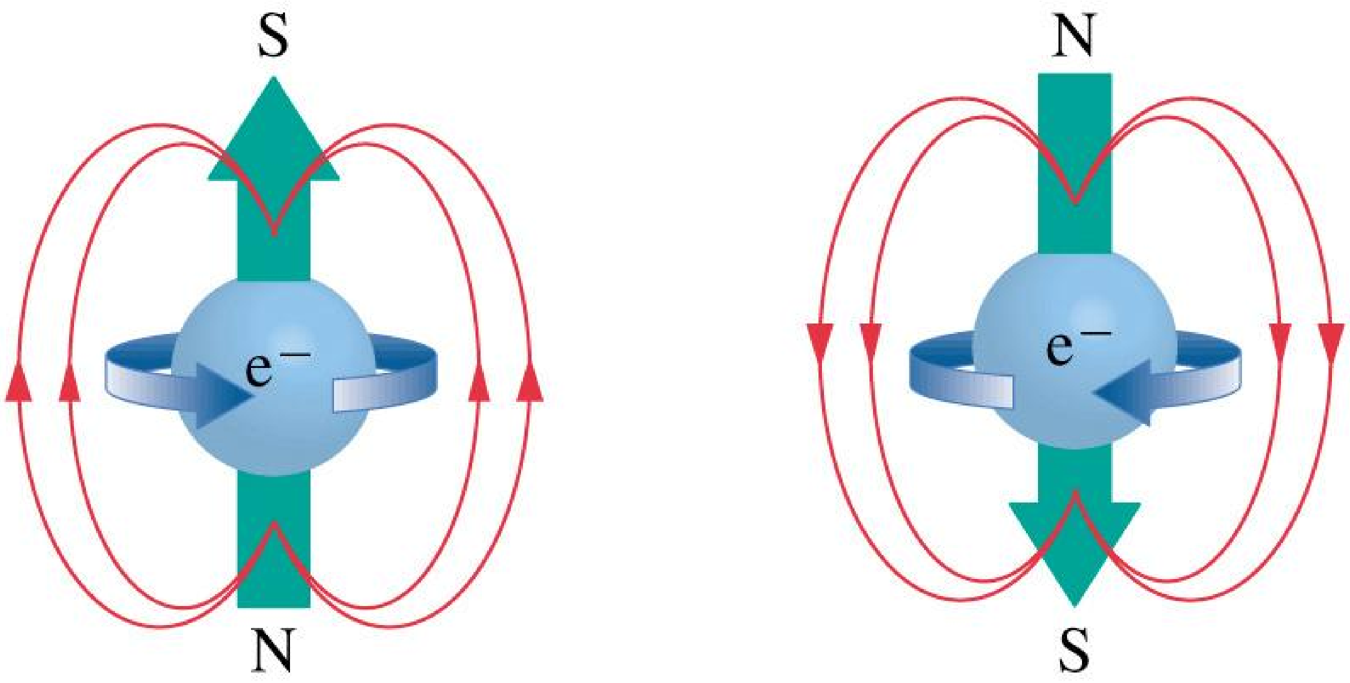
p Orbitals



d Orbitals



9-9 Electron Spin: A Fourth Quantum Number

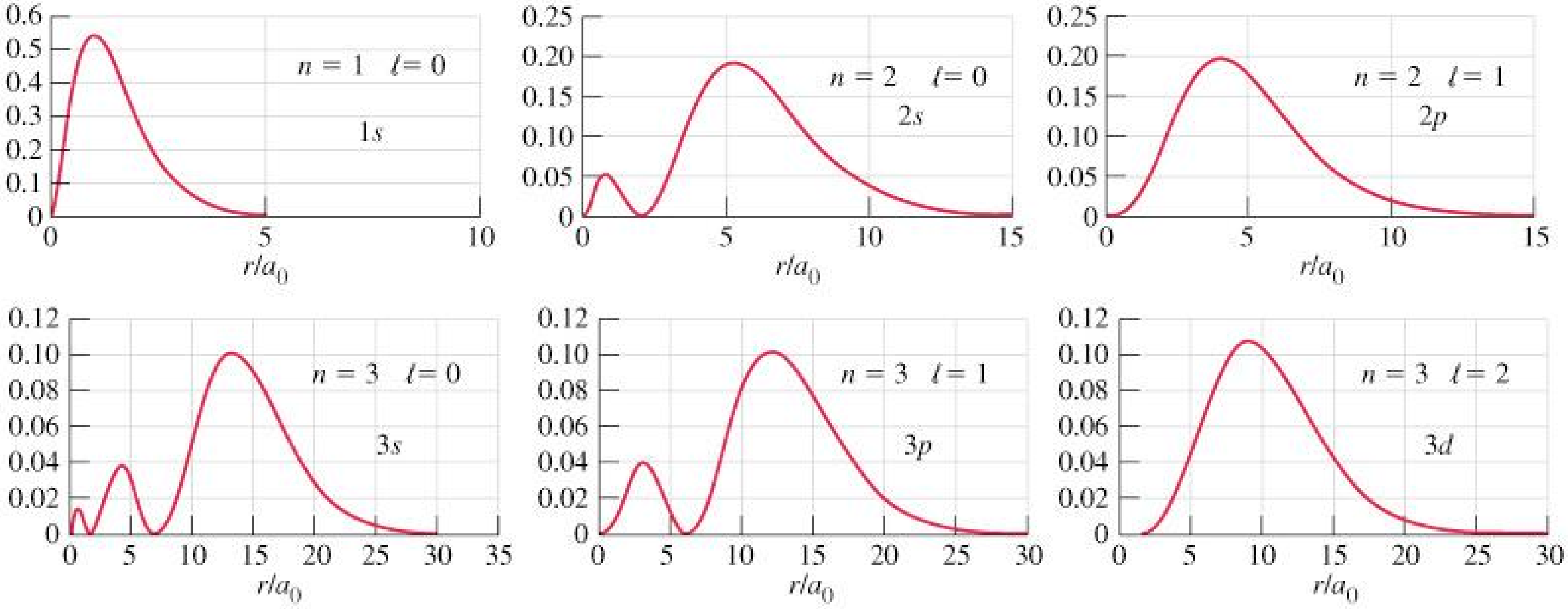


$m_s = +\frac{1}{2}$ $\qquad$ $m_s = -\frac{1}{2}$

9-10 Multi-electron Atoms

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

Penetration and Shielding

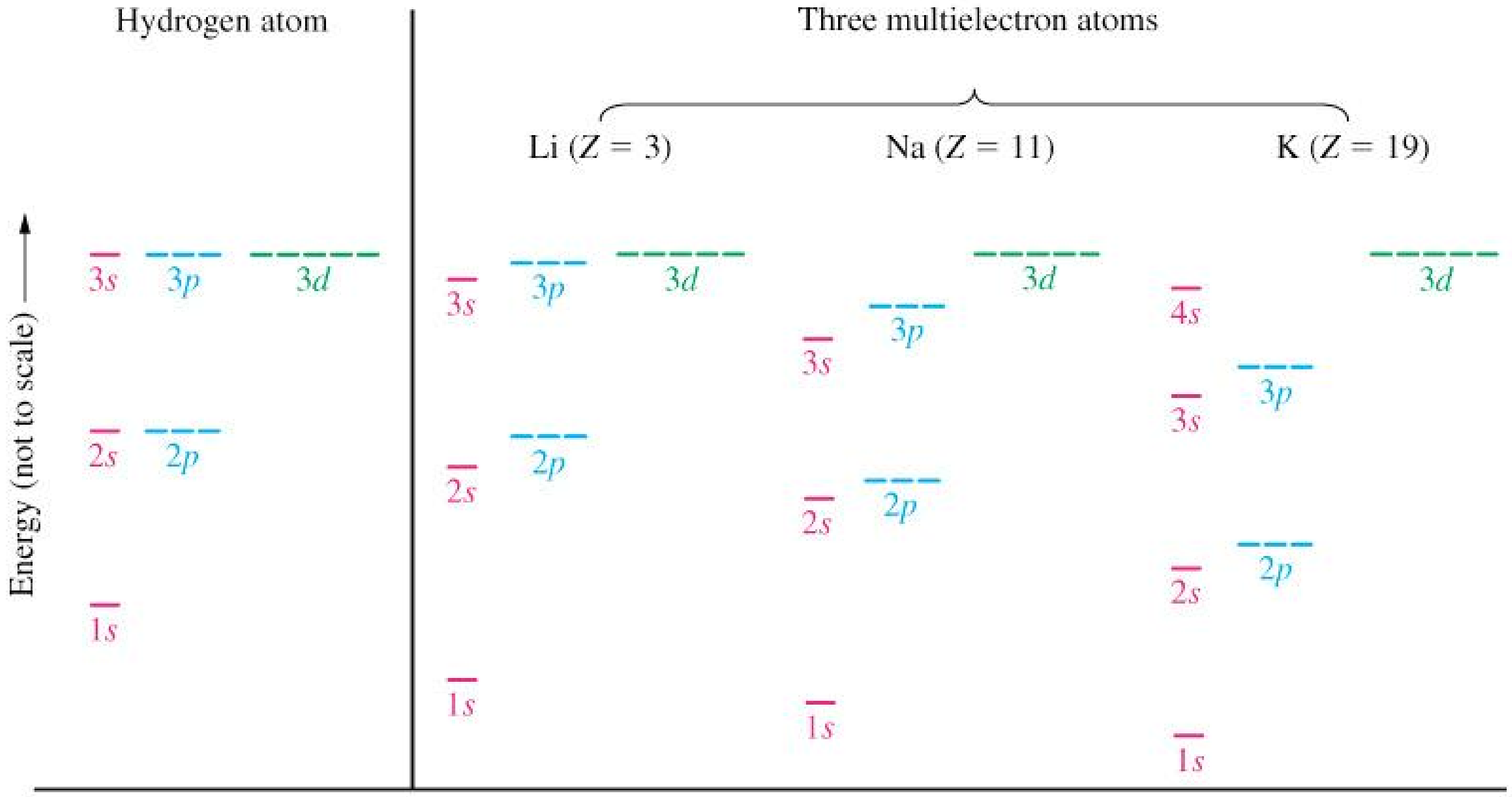


Z_{eff} is the effective nuclear charge.

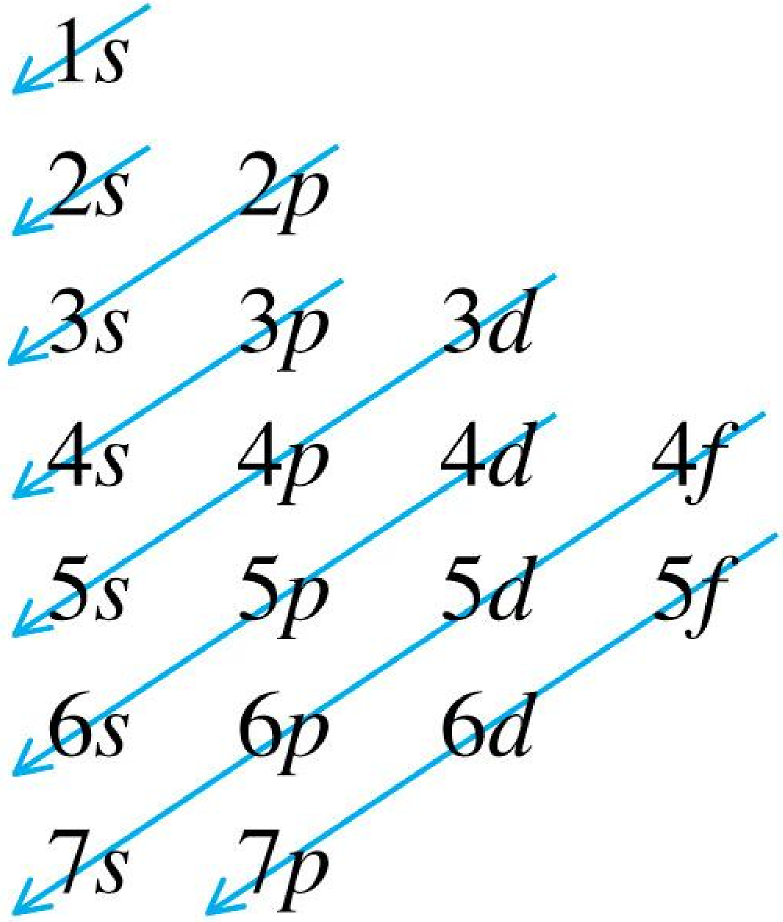
9-11 Electron Configurations

- 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.

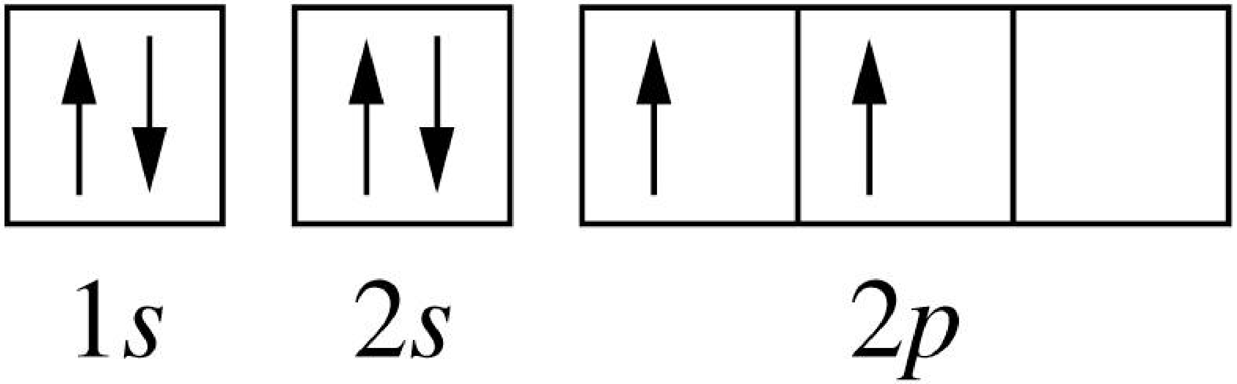
Orbital Energies



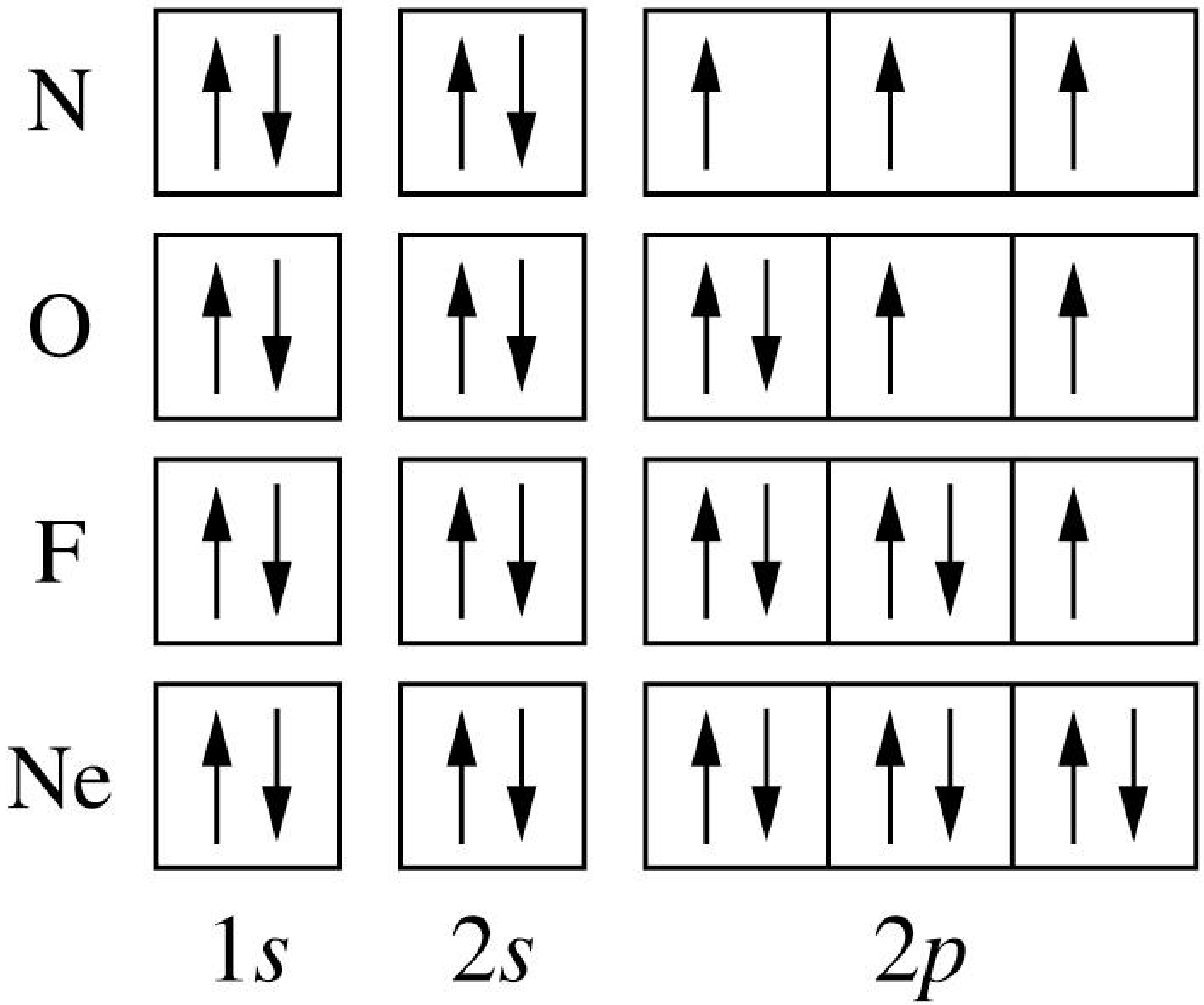
Orbital Filling



Aufbau Process and Hunds Rule



Filling p Orbitals

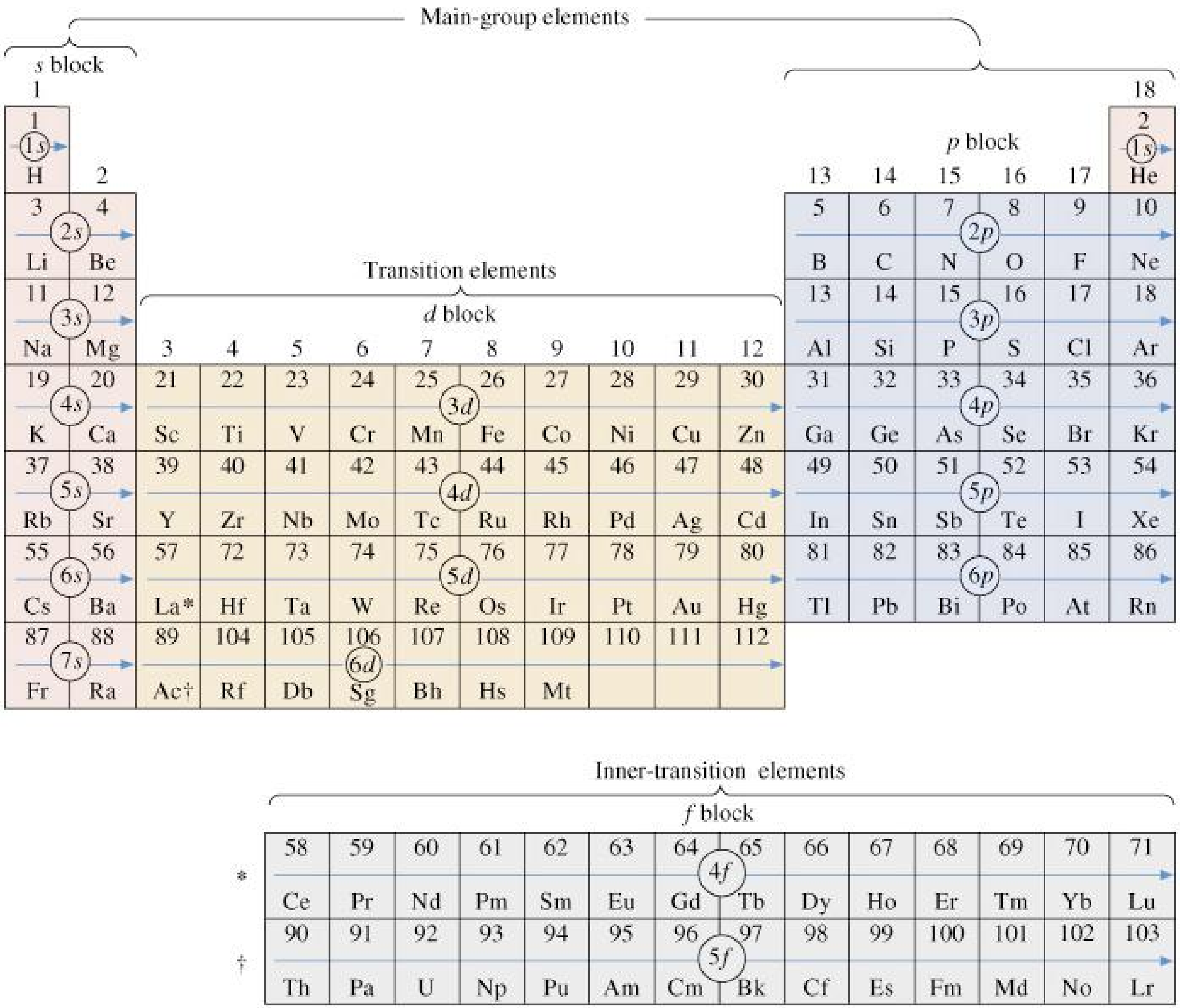


Filling the d Orbitals

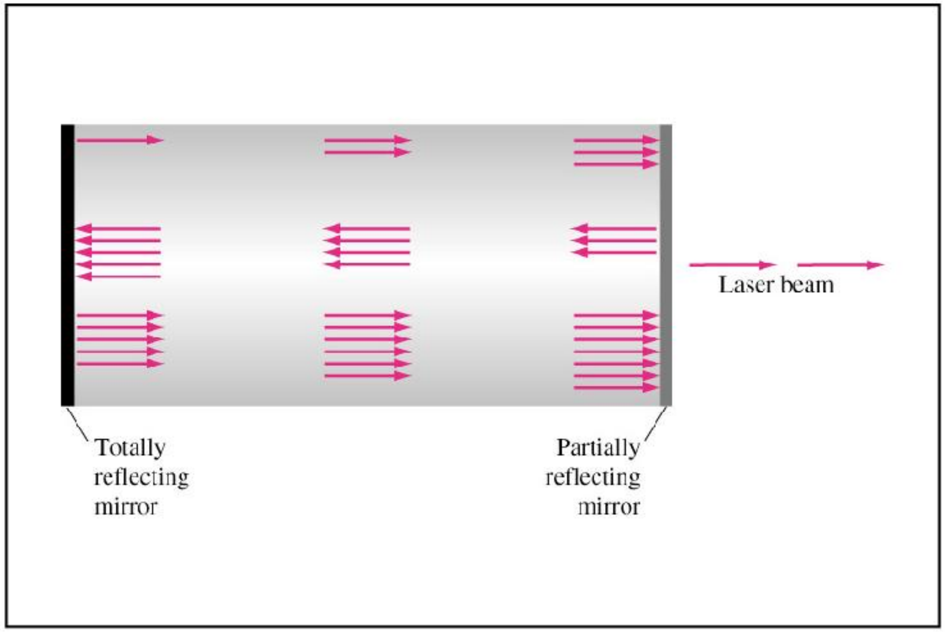
		3d					4s	
Sc:	[Ar]	↑					↑↓	$[Ar]3d^{1}4s^{2}$
Ti:	[Ar]	↑	↑				↑↓	$[Ar]3d^{2}4s^{2}$
V:	[Ar]	↑	↑	↑			↑↓	$[Ar]3d^{3}4s^{2}$
Cr:	[Ar]	↑	↑	↑	↑	↑	↑	$[Ar]3d^{5}4s^{1}$
Mn:	[Ar]	↑	↑	↑	↑	↑	↑↓	$[Ar]3d^{5}4s^{2}$
Fe:	[Ar]	↑↓	↑	↑	↑	↑	↑↓	$[Ar]3d^{6}4s^{2}$
Co:	[Ar]	↑↓	↑↓	↑	↑	↑	↑↓	$[Ar]3d^{7}4s^{2}$
Ni:	[Ar]	↑↓	↑↓	↑↓	↑	↑	↑↓	$[Ar]3d^{8}4s^{2}$
Cu:	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$[Ar]3d^{10}4s^{1}$
Zn:	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	$[Ar]3d^{10}4s^{2}$

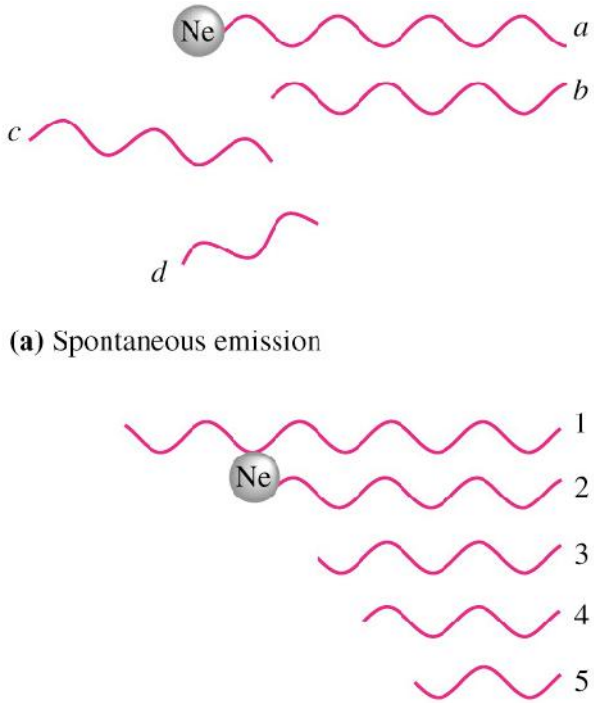
TABLE 9.2	Electron Configurations of Some Groups of Elements	
Group	**Element**	**Configuration**
1	H	$1s^1$
	Li	$[He]2s^1$
	Na	$[Ne]3s^1$
	K	$[Ar]4s^1$
	Rb	$[Kr]5s^1$
	Cs	$[Xe]6s^1$
	Fr	$[Rn]7s^1$
17	F	$[He]2s^2 2p^5$
	Cl	$[Ne]3s^2 3p^5$
	Br	$[Ar]3d^{10} 4s^2 4p^5$
	I	$[Kr]4d^{10} 5s^2 5p^5$
	At	$[Xe]4f^{14} 5d^{10} 6s^2 6p^5$
18	He	$1s^2$
	Ne	$[He]2s^2 2p^6$
	Ar	$[Ne]3s^2 3p^6$
	Kr	$[Ar]3d^{10} 4s^2 4p^6$
	Xe	$[Kr]4d^{10} 5s^2 5p^6$
	Rn	$[Xe]4f^{14} 5d^{10} 6s^2 6p^6$

9-12 Electron Configurations and the Periodic Table



Focus on He-Ne Lasers





(a) Spontaneous emission

(b) Stimulated emission

Chapter 9 Questions

1, 2, 3, 4, 12, 15,
17, 19, 22, 25, 34,
35, 41, 67, 69, 71,
83, 85, 93, 98