ECE 340: Semiconductor Electronics

Chapter 2: Atoms and Electrons

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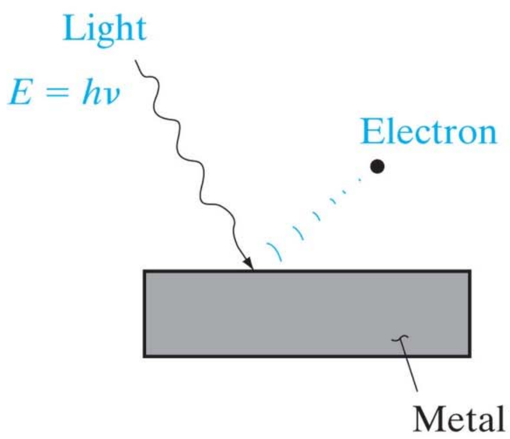
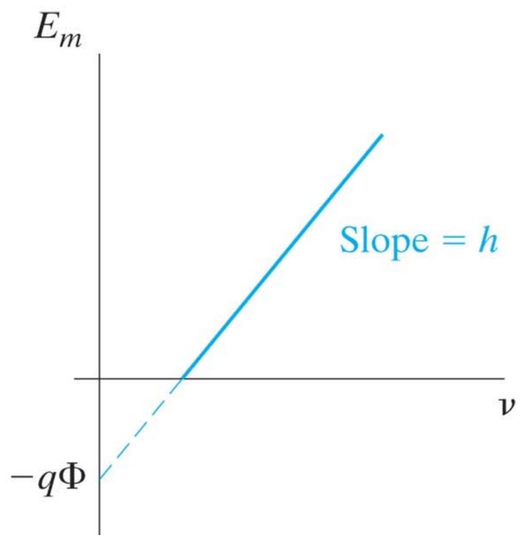
Outline

- Experimental observation of quantization
    - Photoelectric effect
    - De Broglie relationship
    - Atomic spectra
- Quantum mechanics
- Atomic structure and periodic table

Photoelectric effect





Maximum energy of ejected electrons: $\boldsymbol{E_m = h\nu - q\varphi}$

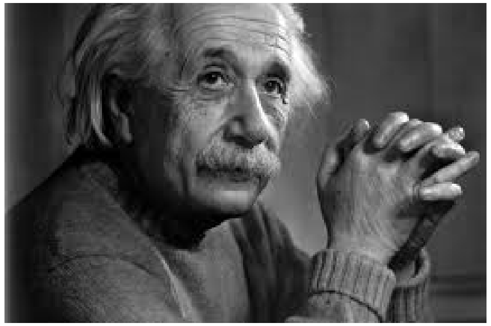
h: plank constant ν: light frequency $q\varphi$: work function

Light has both wave and particle nature. Light energy is quantized (called photon):

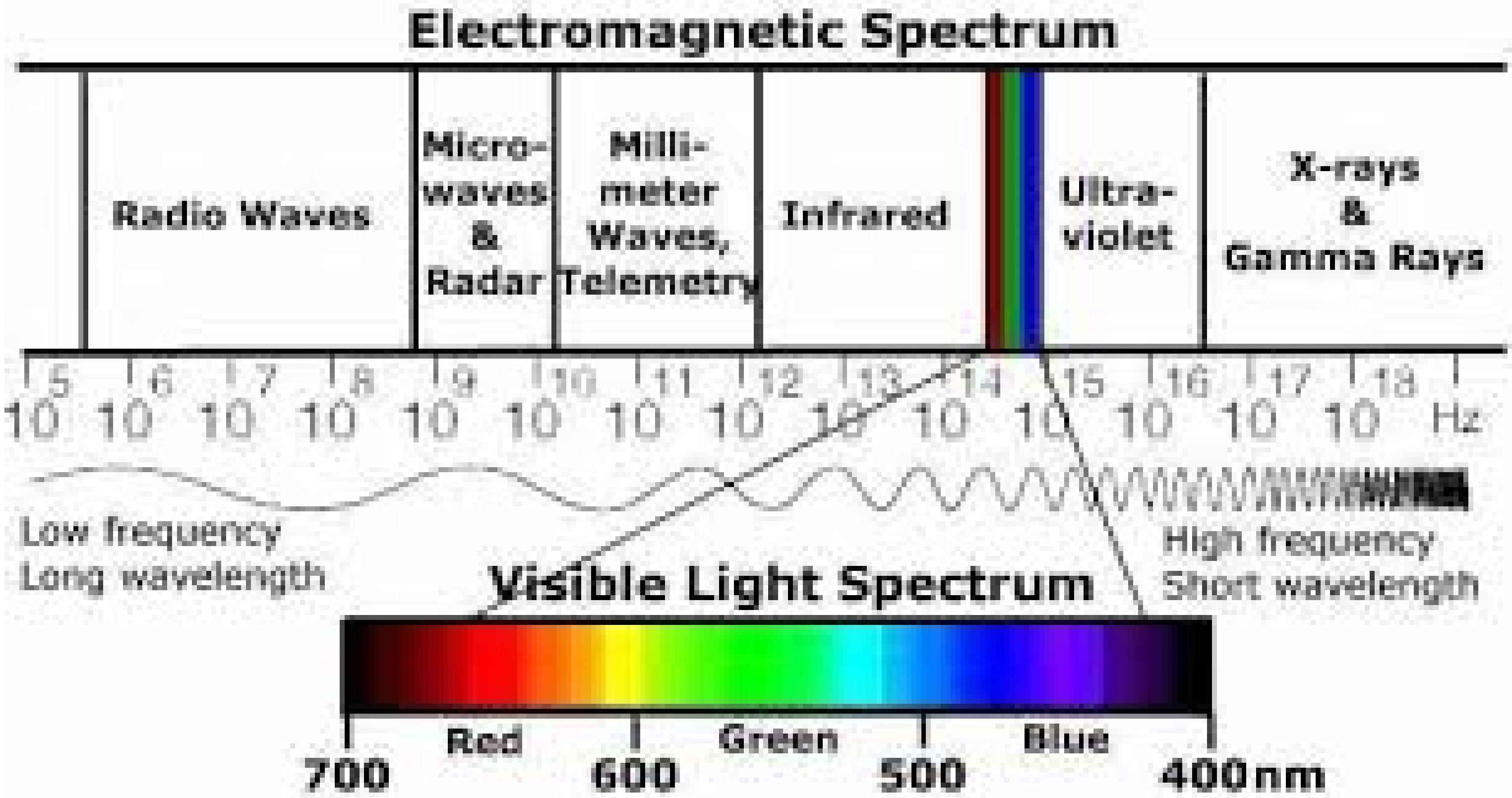
$$\boldsymbol{E = h\nu = \frac{h}{2\pi}2\pi\nu = \hbar\omega}$$

$\hbar$ is reduced plank constant, ω is angular frequency

Albert Einstein



Electromagnetic spectrum



De Broglie relationship and dispersion relationship

- Particles of matter (such as electrons) could manifest wave character.
- A particle of momentum p=mv has a wavelength given by:

$$\lambda = h/p$$ **De Broglie relationship**

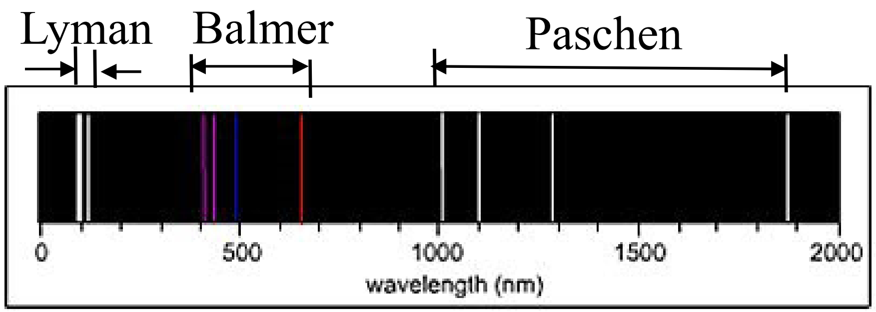
$$\Longrightarrow p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k$$ (k is angular wavenumber $k = \frac{2\pi}{\lambda}$)

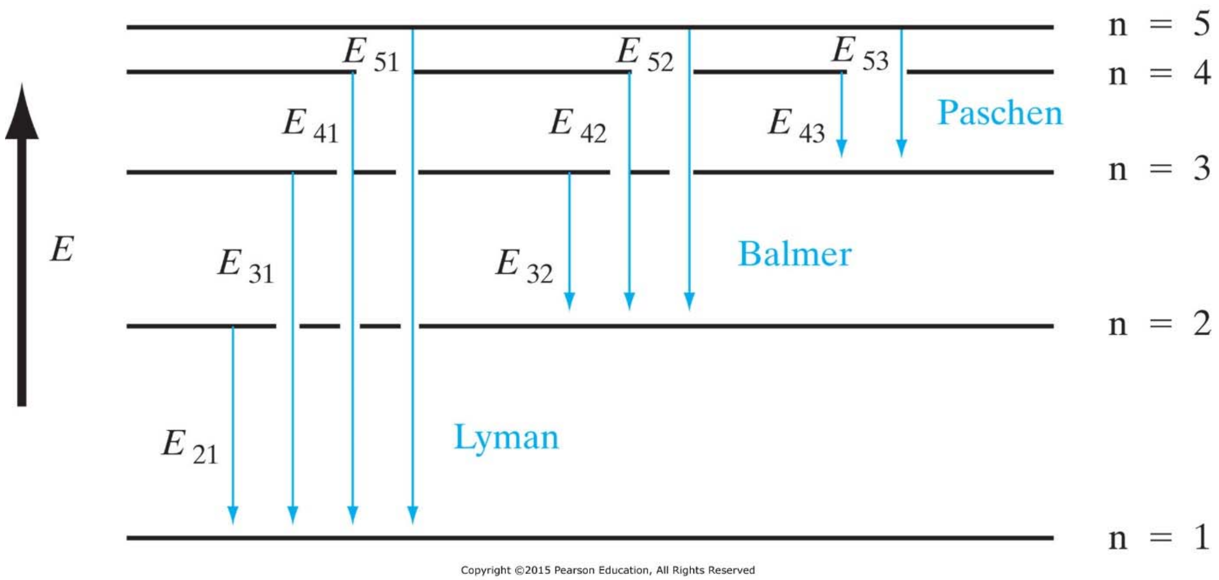
- Wave-particle duality are valid for situation and objects.
- Dispersion relationship: relation between frequency and wavelength (or energy and momentum)

For photons:

$$\upsilon = \frac{c}{\lambda} \quad \Rightarrow \quad E = h\nu = h\frac{c}{\lambda} = cp$$

Hydrogen atom emission spectrum





Lyman: $v = CR\left(\frac{1}{1^2} - \frac{1}{n^2}\right)$

Balmer: $v = CR\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$

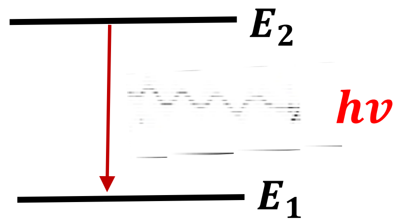
Balmer: $v = CR\left(\frac{1}{3^2} - \frac{1}{n^2}\right)$

- Light emission spectrum of hydrogen contains a series of discrete lines instead of a continuous distribution.

Bohr's Model

Postulate:

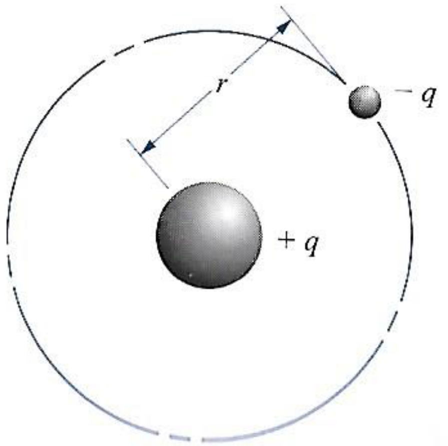
1. Electron moves in circular orbits where it does not radiate (stationary state)
2. Radiation emitted in transition between stationary states

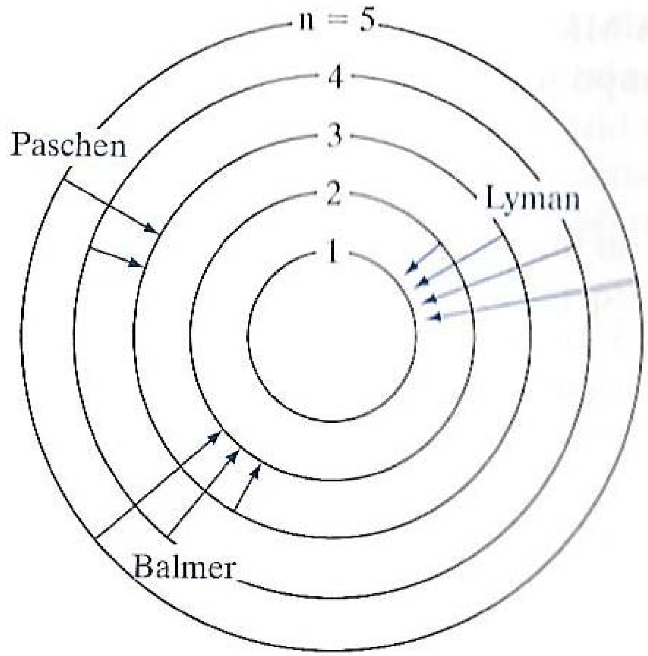


$$hv = E_2 - E_1$$

3. Orbital angular momentum quantized

$$P_\theta = n\hbar, \qquad n = 1,2,3,\ldots$$





Bohr model: $E_H = -\dfrac{mq^4}{2(4\pi\varepsilon\hbar \mathbf{n})^2} = -\dfrac{13.6}{\mathbf{n}^2}\,\text{eV}$

Main Ideas of Quantum mechanics

- Use wave mechanics – Schrödinger equation
- Based on three essential postulates:
  - Each particle in the system is defined by a wavefunction. The wavefunction and its space derivative are continuous, finite and single valued.
  - We must express the normal classical quantities with the new quantum mechanical operators.

Classical variable	Quantum operator
x	x
$f(x)$	$f(x)$
$p(x)$	$\frac{\hbar}{j}\frac{\partial}{\partial x}$
E	$-\frac{\hbar}{j}\frac{\partial}{\partial t}$

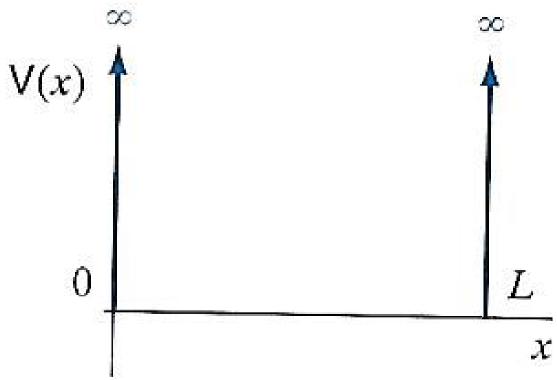
Schrödinger equation

Classical equation for the energy of a particle:

$$\frac{P^2}{2m}+\mathrm{V}=\mathrm{E}$$

In quantum mechanics, it is describes by Schrödinger equatic

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi$$

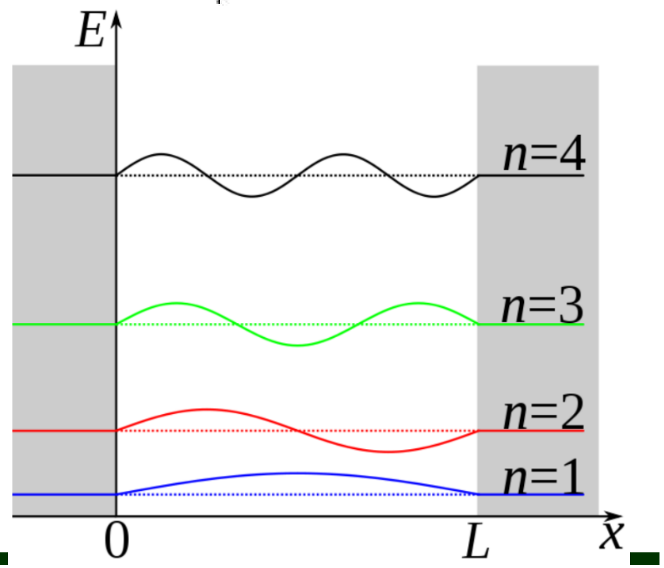


Particle in a box (potential well)

Potential well: V (x)=0, 0<x<L
V(x)=∞, x≤0 or ≥L

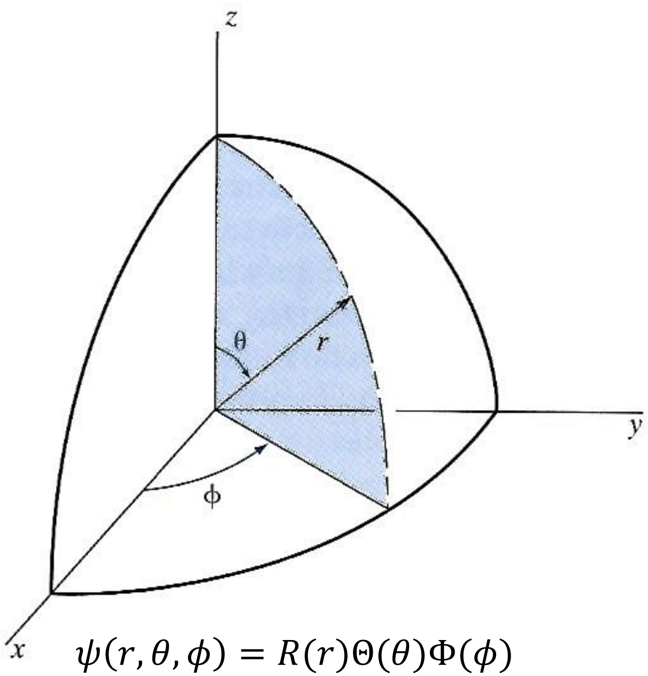
Particle will have discrete, separated energy levels:

$$E_n=\frac{n^2\hbar^2\pi^2}{2ma^2}\qquad n=1,2,3,...$$



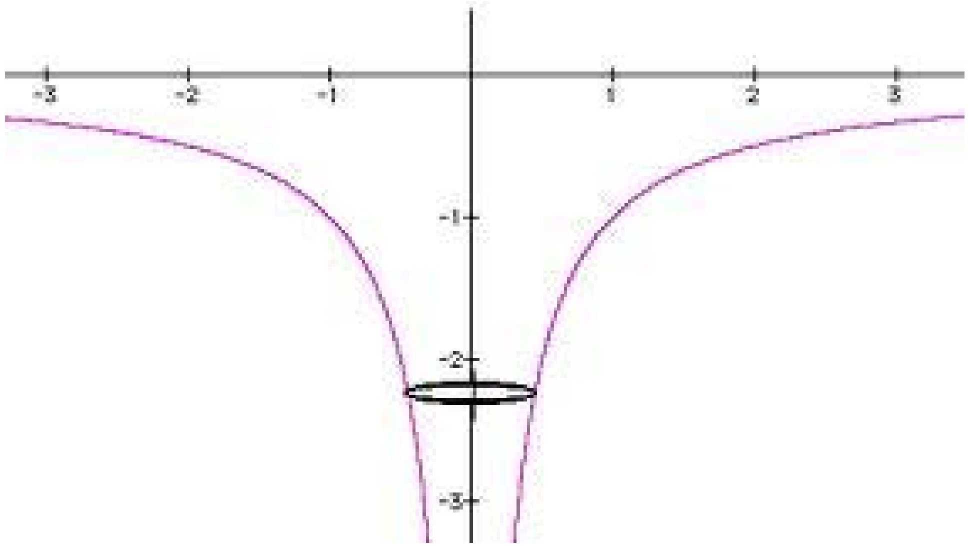
Hydrogen Atom

Spherical coordinate system



$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$

Columbic potential



$$V(r,\theta,\phi) = V(r) = -(4\pi\epsilon_0)^{-1}\frac{q^2}{r}$$

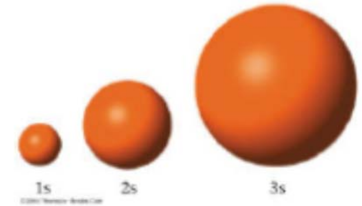
The wavefunction for the hydrogen atom is a solution of the Schrodinger equation in three dimensions for a Columbic potential field.

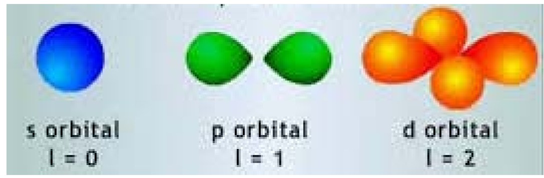
$$E_H = -\frac{mq^4}{2(4\pi\varepsilon\hbar\mathbf{n})^2} = -\frac{13.6}{\mathbf{n}^2}\,\text{eV} \qquad \text{n=1, 2, 3…}$$

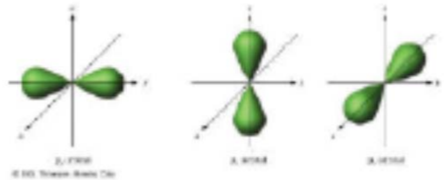
Quantum number selection rule

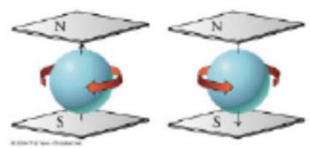
- Quantum number: the sets of numerical values which give acceptable solutions to the Schrödinger wave equation for the Hydrogen atom

Name	Symbol	Orbital meaning	Values
principal quantum number	n	energy shell	$n = 1, 2, 3, \ldots$
azimuthal quantum number (angular momentum)	ℓ	subshell (shape of the sublevel orbital)	$\ell = 0, 1, 2 \ldots, (n-1)$
magnetic quantum number, (projection of angular momentum)	m	spacial orientation of the sublevel orbital	$m = -\ell, \ldots -1, 0, 1, \ldots \ell$
spin projection quantum number	s	spin of the electron	$s = -\frac{1}{2}, \frac{1}{2}$









Pauli exclusion principle and allowed states

- Pauli exclusion principle: no two electrons in an interacting system can have the same set of quantum number n, l, m, and s.
- Quantum numbers and allowed states:

n	l	m	$s/\hbar$	Allowable states in subshell	Allowable states in complete shell
1	0	0	$\pm\frac{1}{2}$	2	2
2	0	0	$\pm\frac{1}{2}$	2	8
	1	-1	$\pm\frac{1}{2}$	6	
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
3	0	0	$\pm\frac{1}{2}$	2	18
	1	-1	$\pm\frac{1}{2}$	6	
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
	2	-2	$\pm\frac{1}{2}$	10	
		-1	$\pm\frac{1}{2}$		
		0	$\pm\frac{1}{2}$		
		1	$\pm\frac{1}{2}$		
		2	$\pm\frac{1}{2}$		

Electronic Configuration of Elements

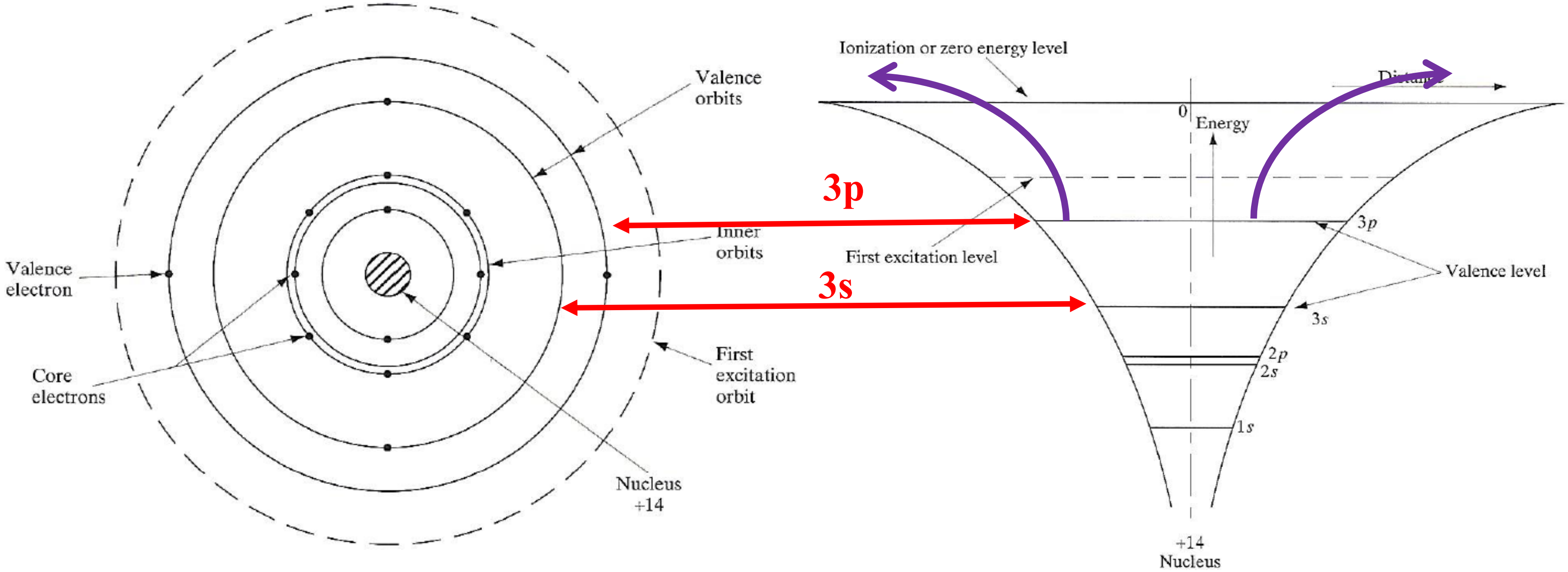
ℓ=0, 1, 2, 3, 4 …
s, p, d, f, g …

		Number of electrons								
		n = 1	2		3			4		
		l = 0	0	1	0	1	2	0	1	
Atomic number (Z)	**Ele-ment**	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	**Shorthand notation**
1	H	1								$1s^1$
2	He	2								$1s^2$
3	Li	helium core, 2 electrons	1							$1s^2\ 2s^1$
4	Be		2							$1s^2\ 2s^2$
5	B		2	1						$1s^2\ 2s^2\ 2p^1$
6	C		2	2						$1s^2\ 2s^2\ 2p^2$
7	N		2	3						$1s^2\ 2s^2\ 2p^3$
8	O		2	4						$1s^2\ 2s^2\ 2p^4$
9	F		2	5						$1s^2\ 2s^2\ 2p^5$
10	Ne		2	6						$1s^2\ 2s^2\ 2p^6$
11	Na	neon core, 10 electrons			1					[Ne] $3s^1$
12	Mg				2					$3s^2$
13	Al				2	1				$3s^2\ 3p^1$
14	Si				2	2				$3s^2\ 3p^2$
15	P				2	3				$3s^2\ 3p^3$
16	S				2	4				$3s^2\ 3p^4$
17	Cl				2	5				$3s^2\ 3p^5$
18	Ar				2	6				$3s^2\ 3p^6$

Electronic structure and energy levels in a silicon atom

Orbital model of a Si atom

Energy levels in the Coulomb potential



Si: $1s^2 2s^2 2p^6 3s^2 3p^2$

- There are 4 valence electrons of Si (two in 3s states and two in 3p states).
- A Coulomb potential varies as 1/r as a function of distance from the nucleus. Similar to "particle in a box", the energy level is discrete.

Summary

- Wave-particle duality:
  - Light with frequency $\boldsymbol{v}$ has photon energy $\boldsymbol{E = hv}$
  - Particles with momentum p has a wavelength $\lambda = h/p$
- The energy level in atom is discrete. The states of the electron can be identified using four quantum numbers.
- Quantum number selection rule:
  - n=1, 2…; ℓ =0, ..n-1; m=-ℓ , …0, …ℓ ; s=$\pm\frac{1}{2}$
- Pauli exclusion principle: no two electrons can have the same set of quantum number
- Silicon has 4 valence electrons.