CHEM100_11

Lecture 48. Electronic structure of atoms, Chapter 6.

Quiz#2 Feb. 16 (W)

Student's tutorial from 7-9pm Mondays and Tuesdays in NH246

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Quantized Energy and Photons

Three phenomena which caused development of quantum theory: black body radiation, photo-electronic effect, and emission spectra

Black-body radiation: read-hot objects are cooler than white-hot

- **Planck: energy can only be absorbed or released from atoms in certain amounts called quanta.**

The relationship between energy and frequency is

$$E = h\nu$$

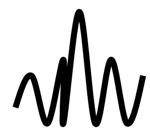
Matter can emit or absorb energy only in N×hν, where N is whole number

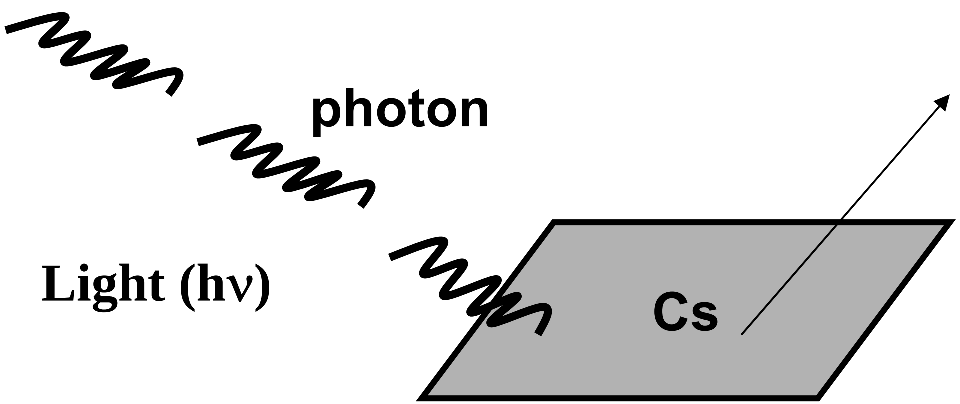
where h is **Planck's constant (6.626×10^{-34} Jxs).**

The Photoelectric Effect and Photons (Einstein's Noble prize)

- **light hits the surface of a light metal (Cs): electrons are ejected but only at certain frequencies.**

- **A photon transfers its energy to an electron. At sufficient amount of energy, an electron can escape the metal surface.**

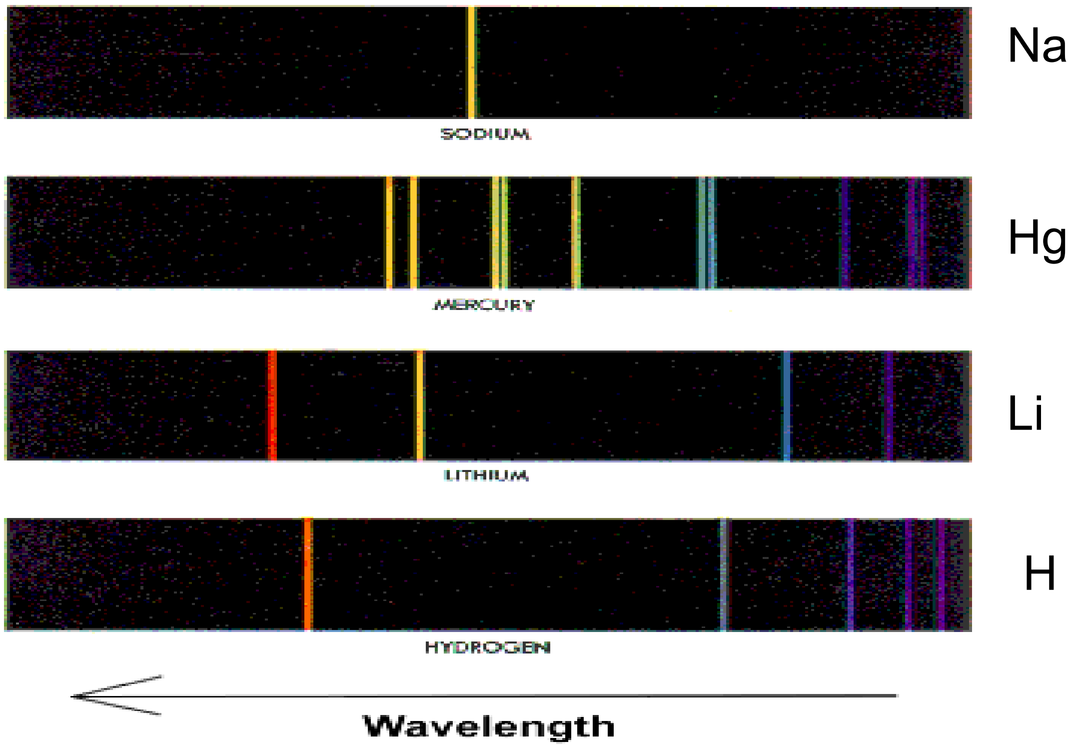
Light travels in packets: photons 

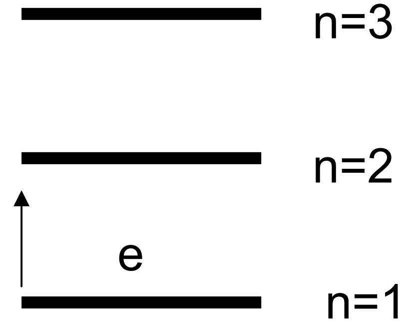


Emitted electron

Emission starts at $\nu \geq 4.6 \times 10^{14}\ s^{-1}$

Line Spectra of Atoms (radiation of only specific wavelengths)



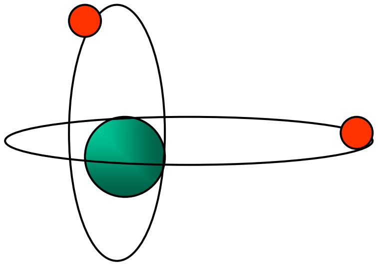


$E_2 – E_1 = hv$

Light hits an atom: atom absorbs certain frequencies (excited state)

atom in excited state emits light at certain frequencies

It is in contrast to continuous spectrum: rainbow



Bohr Model

- The first orbit in the Bohr model has *n* = 1, 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 (*hv*).
- The amount of energy absorbed or emitted on movement between states is given by

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

Duel nature of electron : wave + particle

Louis de Broglie (1924)

Small particles of matter exhibit wave-like properties

$$E = mc^2$$
$$E = h\nu$$

$$c = \nu\lambda$$

$$mc^2 = h\nu$$
$$\frac{h\nu}{c} = mc = p$$

$$\frac{h\nu}{\nu\lambda} = p$$
$$\frac{h}{\lambda} = p$$

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

De Broglie wave

What is the de Broglie wavelength (m) of a 60.0 kg athlete running at a speed of 10 m/s ?

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

h= 6.626×10^{-34} J s

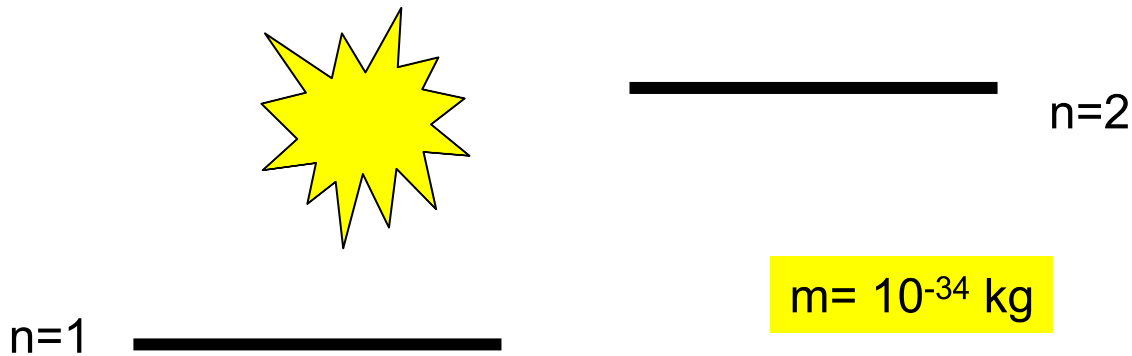
J = kg m^2 s^{-2}

$$\lambda = \frac{h}{mu} = \frac{6.626 \times 10^{-34} \frac{kg \times m^2}{s^2} \times s}{60kg \times 10 \frac{m}{s}} = 0.01104 \times 10^{-34} m$$

= 1.104×10^{-36}m

Gamma rays: 10^{-11}m

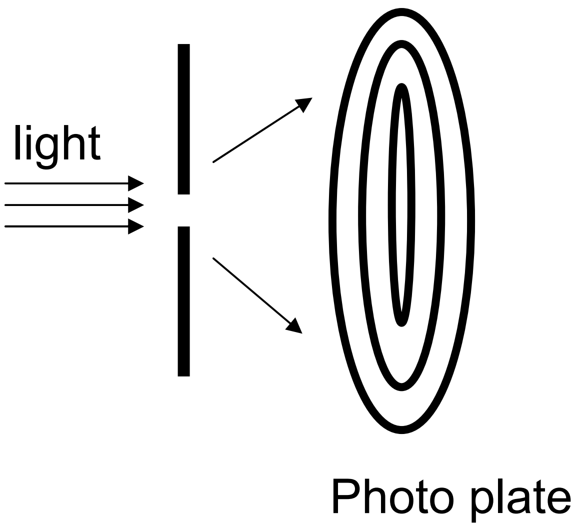
Electron acts as a particle:

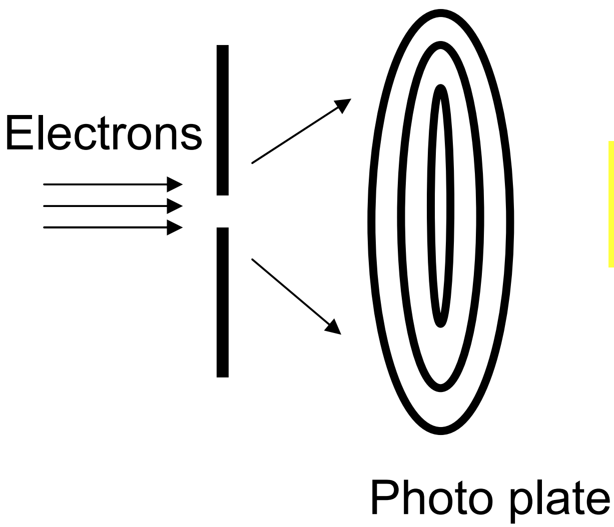


m= 10^{-34} kg

E=hν

Electron acts as a wave:

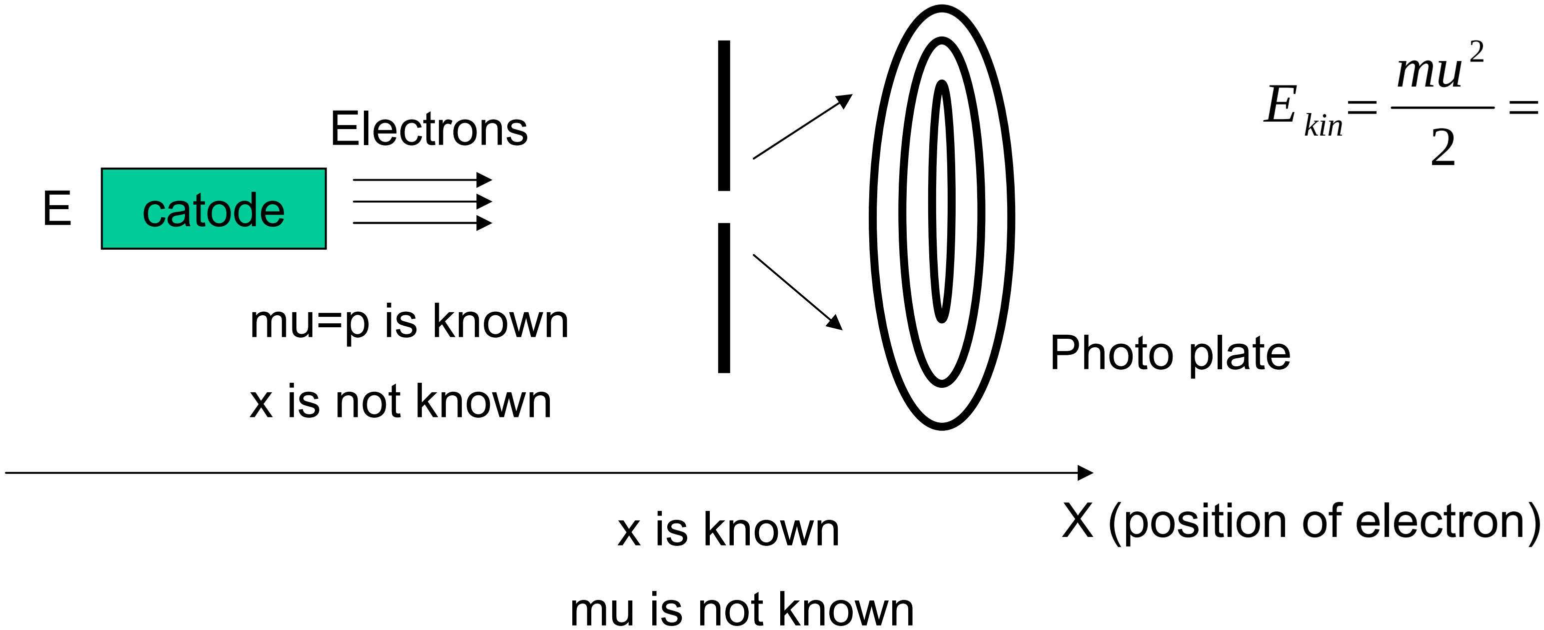


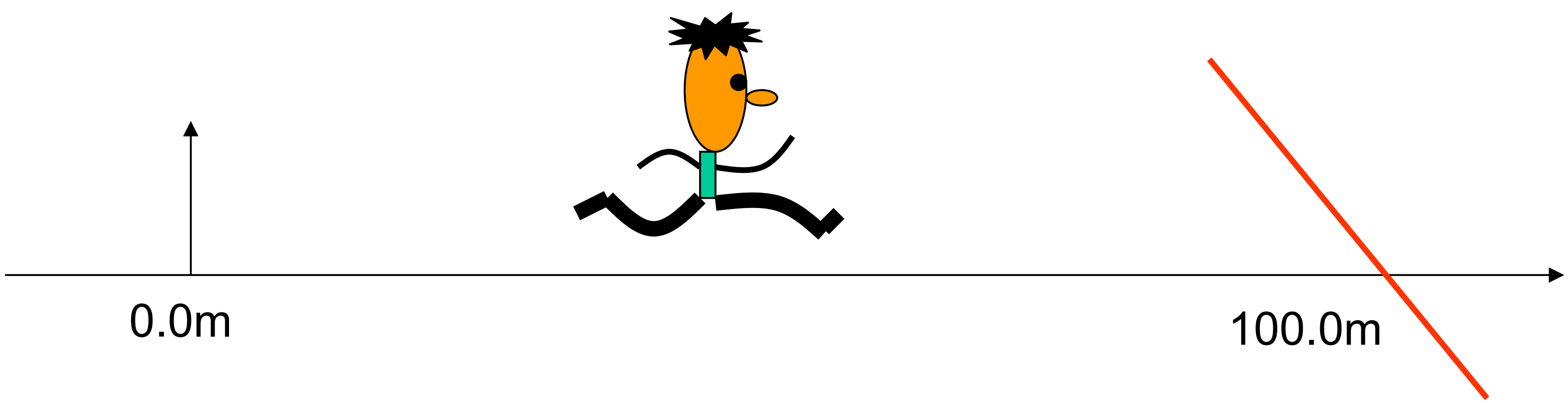


$$\lambda = \frac{h}{p} = \frac{h}{mu}$$

Heisenberg uncertainty principle

$$E_{kin} = \frac{mu^2}{2} = \frac{pu}{2}$$





The *process* of measurement of ē position changes the energy of the ē

We cannot know exact position and exact momentum of an electron at the same time

$$\Delta x \times \Delta p \approx h$$

In quantum mechanics, a particle does not have well-defined position and velocity

Heisenberg uncertainty principle

A particle (electron) CAN BE represent by WAVE FUNCTION (Ψ)

Ψ is a number at each point of space that will give the probability of finding the particle at this position.

Schrődinger equation: gives a rate at which Ψ is changing with time

$$ih\frac{\partial}{\partial t}\Psi(\vec{x},t) = \widehat{H}\Psi(\vec{x},t)$$

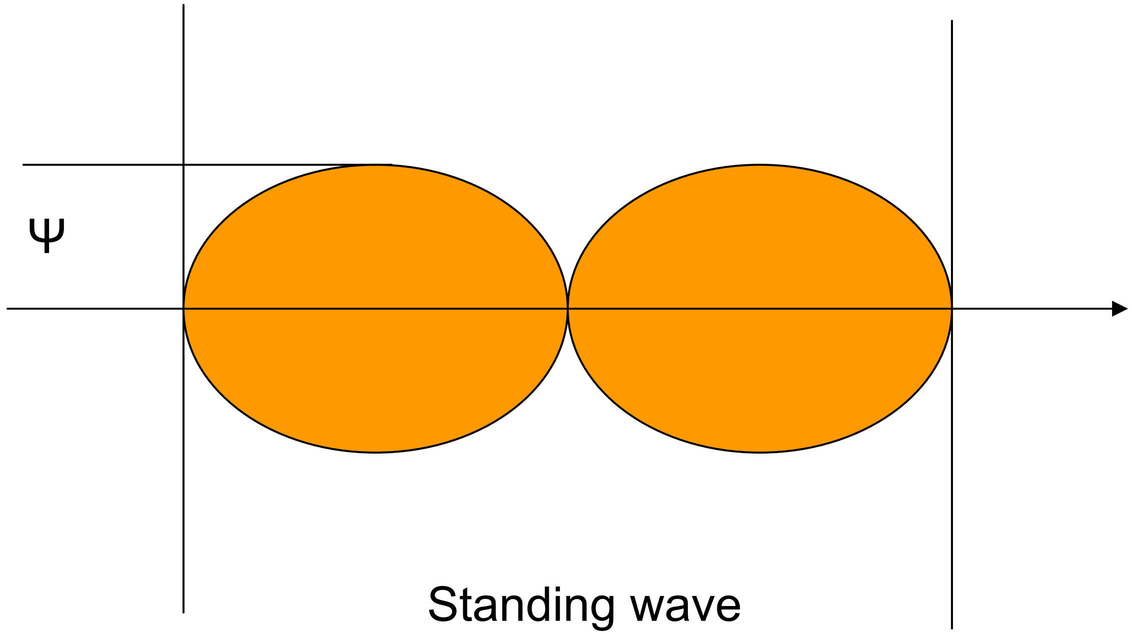
H is energy operator, x is space coordinate, t is time

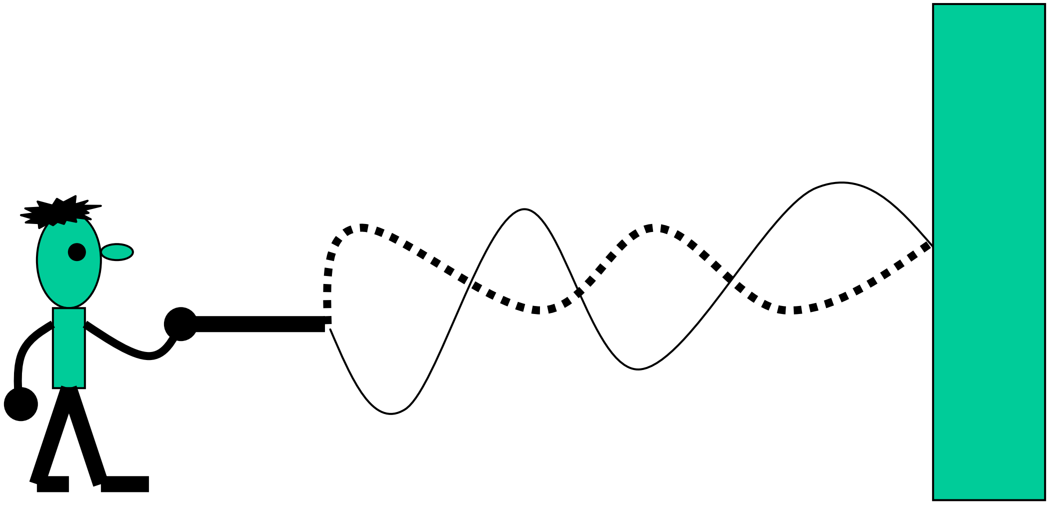
If time is constant

$$\widehat{H}\Psi(\vec{x}) = E\Psi(\vec{x})$$

$$\widehat{H} = \widehat{T} + \widehat{V}$$

T is kinetic energy, V is potential energy


Ψ
Standing wave



Solution of Sch. Eq. gives the energy of the system and Ψ

Physical meaning of Ψ, postulated by **Born**

Ψ^2 gives a probability of finding electron in elementary volume of space

Quantum mechanics is a theory of probabilities, the values, predicted with Q.M. are average values

Solving Schr. Eq:

Solution gives Ψ for each electron in atom which we called orbitals

Each orbital has energy

Each orbital has properties described by quantum numbers

Ψ and Ψ^2 have approximately the same shape- shape of an orbital

Quantum numbers

Principle q. n. $n = 1, 2, 3, \ldots\ldots$

Orbital angular momentum $\ell = 0, 1, 2, 3, \quad (n-1)$

Magnetic quantum number $m_l = -\ell, \quad -\ell+1, \quad \ldots.0 \ldots.. \quad +\ell$

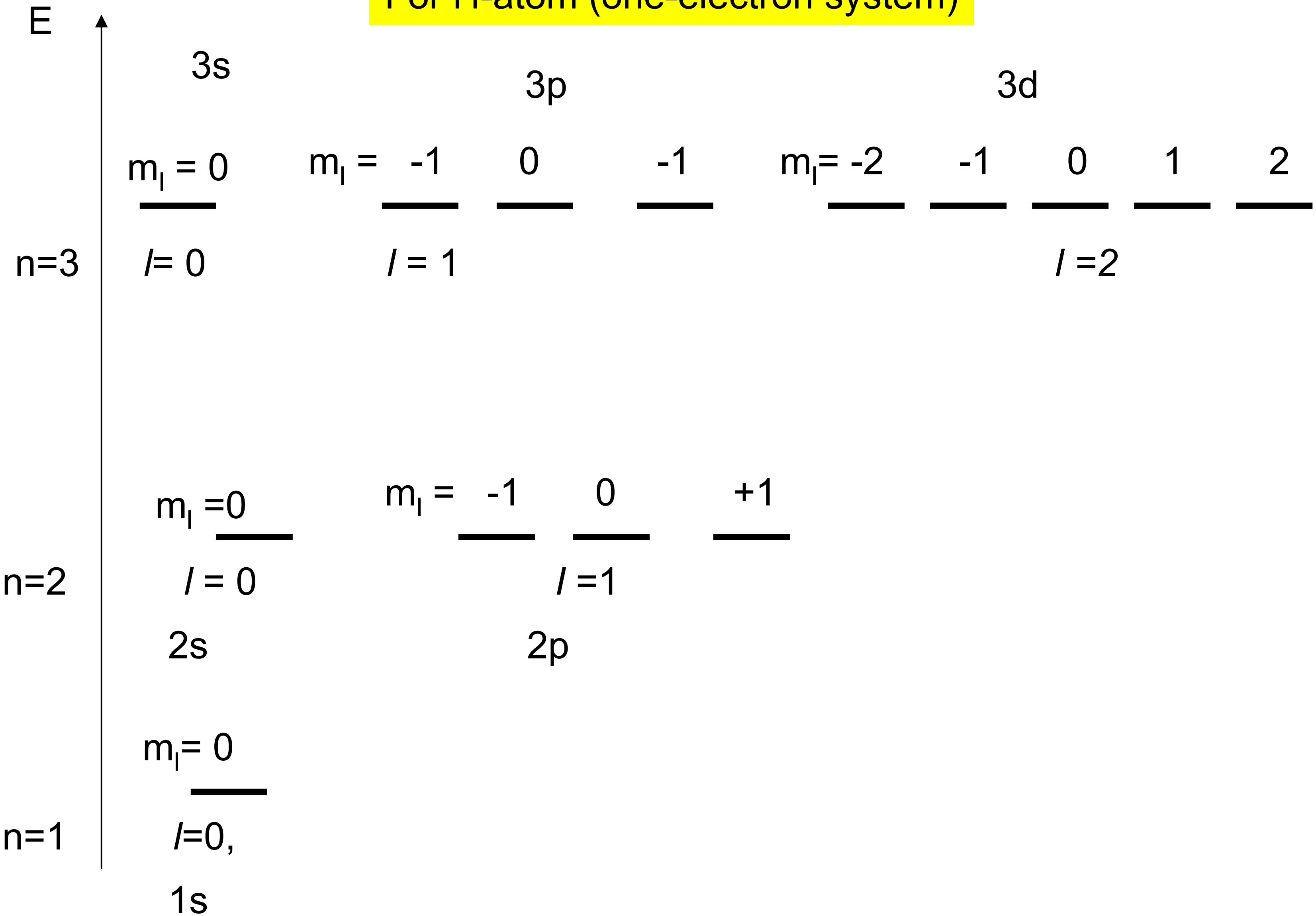
Electronic shells

All orbitals with the same n - principle electronic shell

All orbitals with the same n and ℓ - subshell

$\ell =$ 0	1	2	3	4	5
s-subsh	p-subsh	d-subsh	f-subsh	g-subsh	h-subsh

For H-atom (one-electron system)

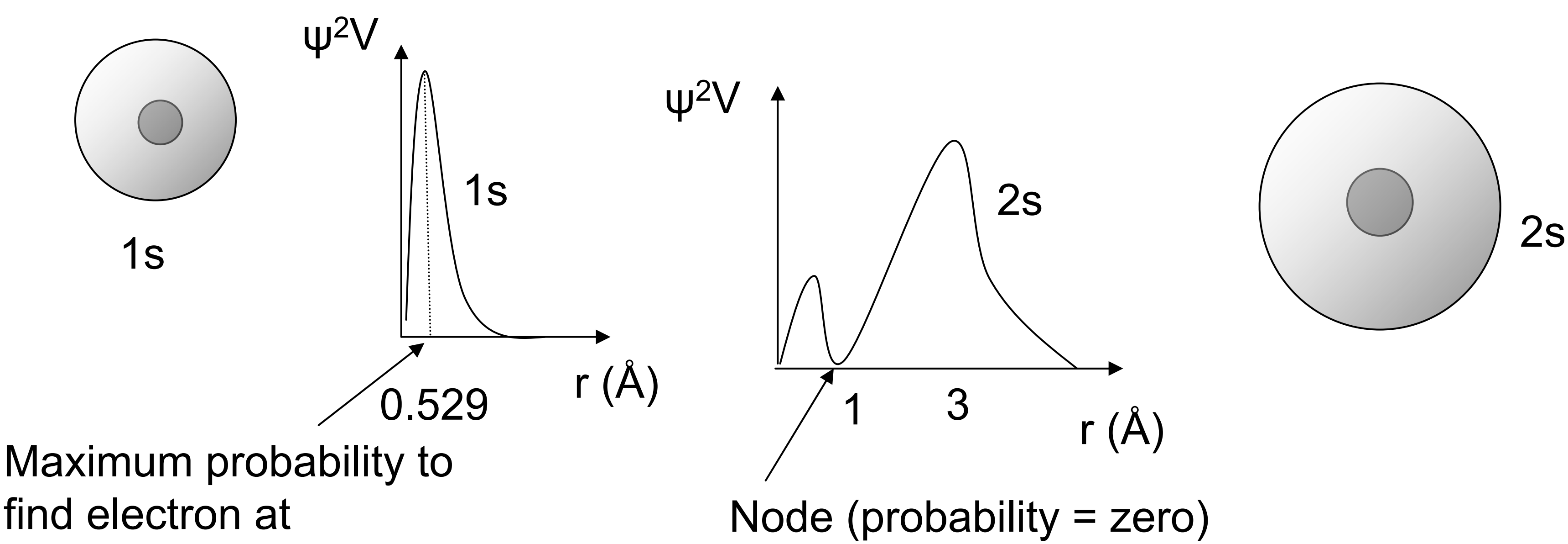


Ψ^2 – gives the probability of finding electron at the certain point in space, i.e.

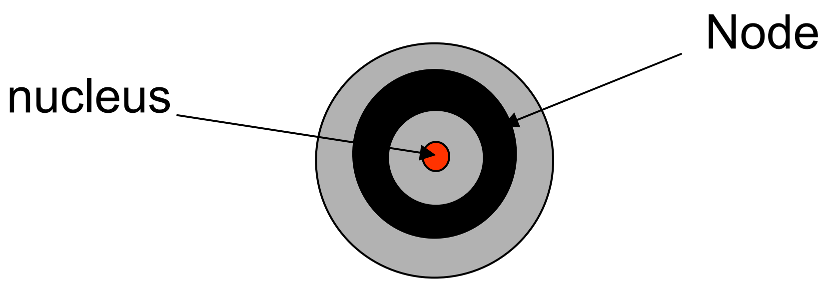
the <u>probability density</u>

Ψ^2 x Volume = probability of finding electron in that volume – all the space around atom

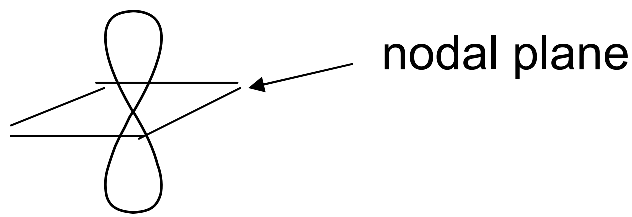
Orbital (solution of Schr. Eq.) – is the probability of finding electron in the space around the nucleus



Section of 2s:

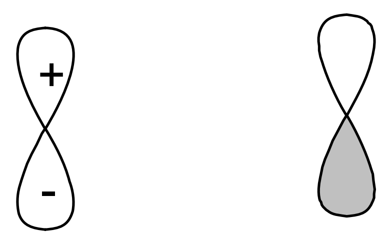


For l =1



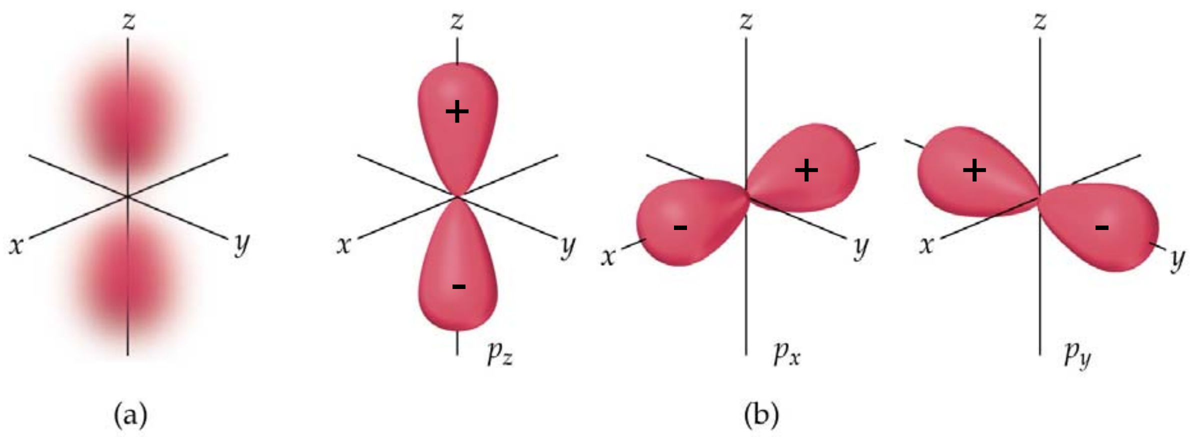
2p

Ψ has the same shape as Ψ^2 but it has a sign (opposite phase)



ℓ gives shapes of orbitals

m_l = gives the orientation of atomic orbitals in Cartesian coordinates



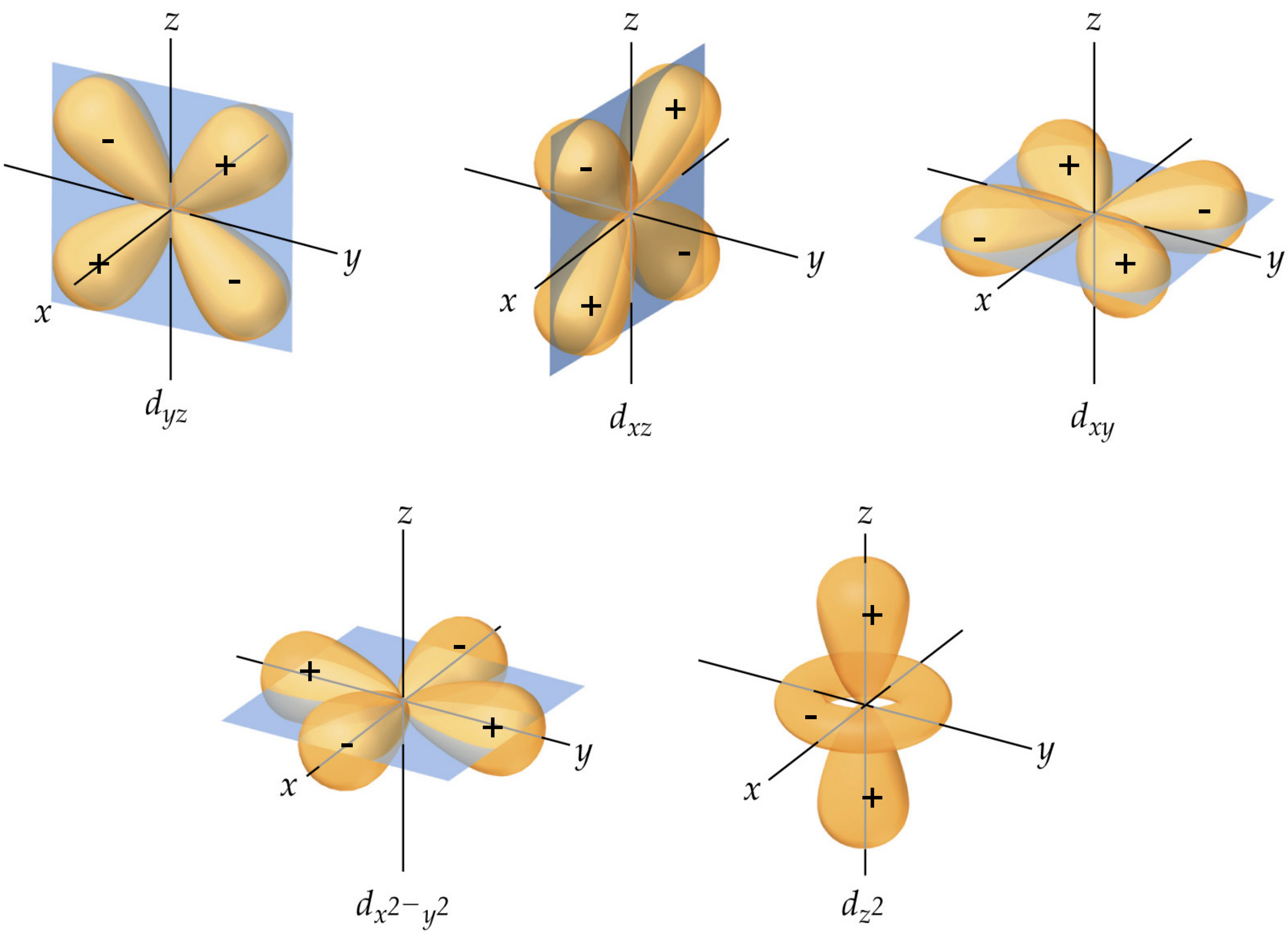
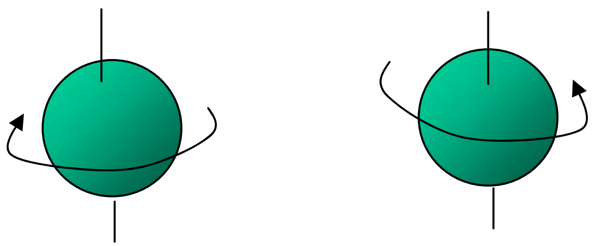


Figure 6.24 in the text

Magnetic spin number: m_s

$m_s = +1/2;\ -1/2$

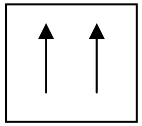
Spin UP and spin DOWN



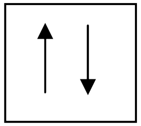
Building the electronic configurations for atoms

Pauli Exclusion Principle:

Two electrons in an atom cannot have the same set of quantum numbers (n, l, m_l, and m_s). Two electrons on the same orbital (n,l,m are the same) must have opposite spins.



$n=1,\ l=0,\ m_l=0,\ m_s=1/2$



$n=1,\ l=0,\ m_l=0,\ m_s = 1/2$

$n=1,\ l=0,\ m_l=0,\ m_s = -1/2$