CHEM 205 section 03

LECTURE #18 Tues., March 11, 2008

LECTURE TOPICS:

TODAY'S CLASS: continue Ch.7

NEXT CLASS: **finish Ch.7, start Ch.8**

(1)

7.4 Wave properties of the electron

The Classical View:

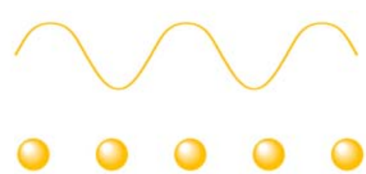
"PARTICLES" have mass, & position can be specified
"WAVES" are massless, & position cannot be specified

Problems recognized ~ 1900:

1.) In some ways, LIGHT acts like a stream of particles (Einstein's *photons*…).

Wave Properties:
diffraction

Particulate properties:
discrete bundles of E
= "photons"

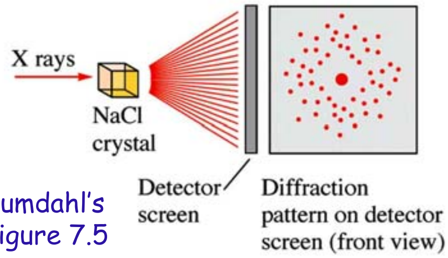


2.) As objects become smaller and smaller, their behaviour becomes less and less like particles…
…and more like waves!

(2)

So, what is an example of wave-like behaviour?

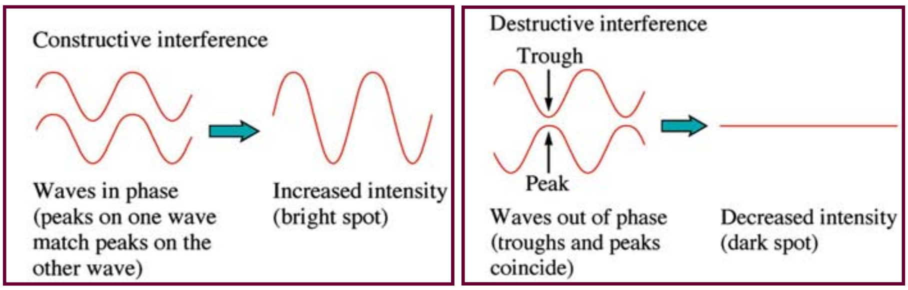
Diffraction = scattering of waves by regular array of objects



Zumdahl's Figure 7.5

Bright spots (red): due to constructive interference of waves

Dark areas (grey): due to destructive interference of waves



Surprising result: Beams of electrons can be diffracted!

Wave-Particle Duality

Matter exhibits properties of BOTH particles & waves !

Louis Victor de Broglie (1892-1987)

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

de Broglie's Equation

E = energy (in J)
definition: 1 J = 1 kg·m^2·s^{-2})

λ = wavelength, m

h = Planck's constant
6.626×10^{-34} J·s

m = mass, kg

v = velocity of object, m·s^{-1}

SMALL OBJECTS (PHOTONS)
$\lambda \gg$ object size
$\Rightarrow$ like WAVES

LARGE OBJECTS (BASEBALLS)
$\lambda \ll$ object size
$\Rightarrow$ like PARTICLES

INTERMEDIATE OBJECTS: (ELECTRONS)
$\lambda \approx$ object size $\Rightarrow$ behave as BOTH !!

Is the wave behaviour noticeable? How big is λ ?

1. If a ball with a mass of 0.450 kg is thrown at a speed of 102 km/h, what is its wavelength?

$\lambda = h/mv$

1 J = 1 N·m = 1 kg·m²·s⁻²

$= (6.626\times10^{-34}\ J\cdot s)/(0.450 kg)(\ \underline{28.3}\ m\cdot s^{-1})$

⇨ λ = **5.20×10^{-35} m**

$v = \frac{102\ km}{1\ h} \times \frac{1000\ m}{1\ km} \times \frac{1\ h}{3600\ s}$

$= 28.3\ m\cdot s^{-1}$

Wavelength « ball's size (d ≈ 0.1 m)

⇨ Wave properties NOT noticeable

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2. If an electron (mass 9.109×10^{-31} kg) is traveling at 40.0% the speed of light, what is its wavelength?

$\lambda = h/mv$

$= (6.626\times10^{-34}\ J\cdot s)/(9.109\times10^{-31} kg)(0.400 \times 2.998\times10^{8}\ m\cdot s^{-1})$

$= 6.06\times10^{-12}$ m

⇨ λ = **0.0606 Å**

↑ 1×10^{-10} m

Diameter of a H atom is ~ 0.7 Å

…wavelength of electron is almost 10% of this distance! VERY NOTICEABLE!

7.5 Quantum Mechanical View of the atom

ELECTRONS AS PARTICLES

- Niels Bohr & friends
- Predicted some properties of e⁻s…but failed for atoms with >1e⁻

<u>ELECTRONS AS WAVES</u>

- Building on deBroglie's ideas: Erwin Schrödinger & friends
- "wave mechanics" or "quantum mechanics"
- Treats electrons as "standing waves" surrounding nucleus

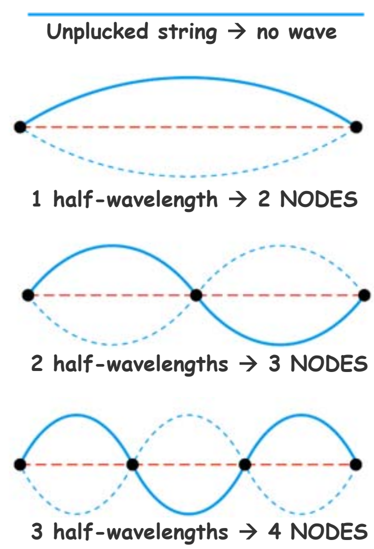
⇩

Correctly predicts some properties of electrons that Bohr's model can NOT

What are standing waves?

E.g., vibration of a guitar string fastened at both ends →

Z's Fig. 7.9; See Kotz Fig. 7.2 & Ex. 7.1



If standing wave's energy increases:

- Wave cannot propagate (trapped!)
- Maintains 1 node at each end
  - ⇨ Limited to integral # of half-wavelengths
- Number of nodes ↑ as E ↑

BY THEIR VERY NATURE, STANDING WAVES ARE QUANTIZED!

DESCRIBING ELECTRON WITH WAVE MECHANICS:
Electron is a standing wave centered on the nucleus
⇨ quantization is natural (in Bohr's model, it was imposed) !

Describing electrons as waves: Quantum Mechanics

$\hat{H}\psi = E\psi$ Schrödinger's equation

A special type of function that operates on the wavefunction… …it's NOT multiplication, but you don't need to understand it here.

Erwin Schrödinger (1887-1961) Nobel Prize 1933

ψ = a **wavefunction** = equation that describes the electron as a wave

$\hat{H}$ = mathematical operator
(very strange math involved-don't need to know)

E = total energy of the atom *(happens to = $-Rhc/n^2$, just like Bohr…)*

RESULT: Schrödinger's equation has many solutions (ψ)

- Each wavefunction (ψ) corresponds to a **standing wave** with a particular allowed energy

= *i.e.*, describes a way the electron can exist at that energy

Heisenberg's Uncertainty Principle

- If electron described as a wave:

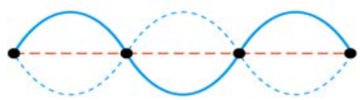
  cannot know BOTH position & energy with certainty at the same time

Werner Heisenberg (1901-1976)

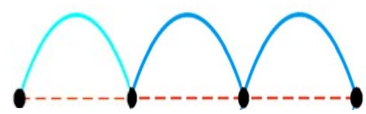
Nobel Prize 1932

THUS: can only find probability of finding e^- someplace

Simplified 1D wavefunction: ψ
- wave has + *vs.* - mathematical sign in different regions
- amplitude most important for now…

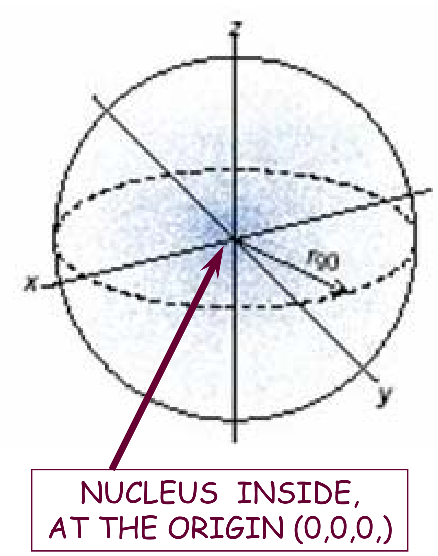


SQUARE of wavefunction: ψ^2
- removes sign
- represents probability



Where wavefunction has large value ⇨ e^- spends a lot of its time
⇨ high *ELECTRON DENSITY*
In 3D ⇨ describes e^-'s *ORBITAL*

THE GROUND STATE for HYDROGEN: e^- in "1s" orbital

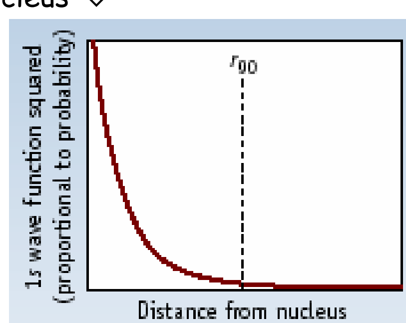


Kotz Fig. 7.14a,b

the 1s orbital

SPHERICAL REGION OF SPACE SURROUNDING NUCLEUS in which have 90% chance of finding the electron

…highest probability is very close to the nucleus ⇩



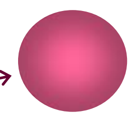
So, what is an "orbital" ?

- TECHNICALLY: orbital = wavefunction, ψ
- EVERYDAY USE: orbital refers to ψ^2
  = probability of finding an electron at a given position

ψ^2 **represents the PHYSICAL MEANING of "ORBITAL"**

<u>**Probability distributions**</u> = visual representations of orbitals
Most common: **"boundary surface"** showing 3D space inside which can "find" electron 90% of the time

e.g., 1s orbital



***Alternatively:* can look INSIDE the space to get an accurate view…**

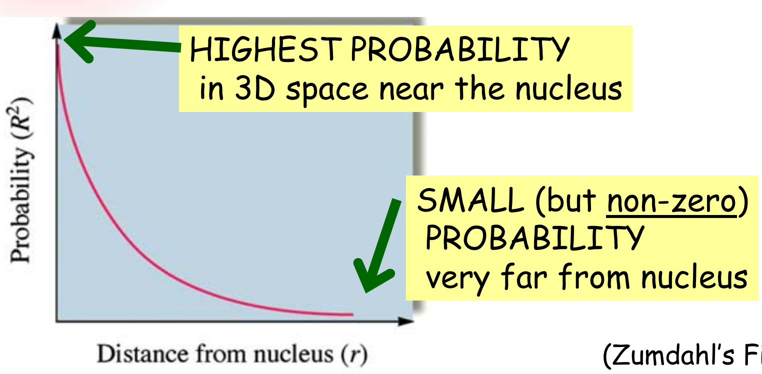
VIEW #1.) At any given point: probability *vs.* distance from nucleus
e.g., Figure 7.14b

VIEW #2.) Radial probability distribution: for spherical shells surrounding nucleus (like LAYERS OF AN ONION)

VIEW #1: PROBABILITY *vs* DISTANCE FROM NUCLEUS

THE GROUND STATE for HYDROGEN: e^- in "1s" orbital

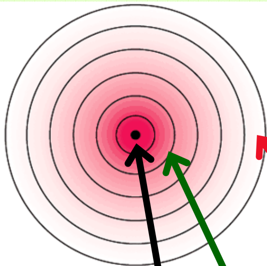
A slice through the 1s orbital (SPHERICAL region surrounding nucleus), crossing through the nucleus…
NOTE: node EXACTLY AT nucleus…



(Zumdahl's Fig. 7.11)

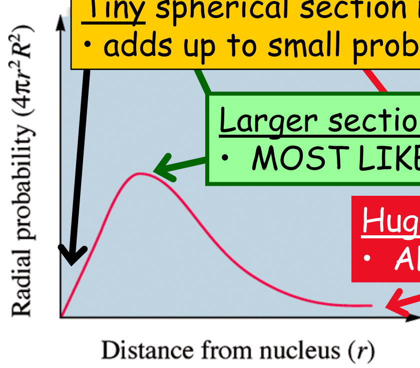
VIEW #2: RADIAL PROBABILITY DISTRIBUTION

Zumdahl's Fig. 7.12: like K&T's "A Closer Look"



Hydrogen's *1s* orbital divided into successive thin spherical layers.

like LAYERS OF AN ONION considered one at a time



Tiny spherical section nearest nucleus
- adds up to small probability

Larger section a bit farther away
- MOST LIKELY to find e^- there…

Huge section very far away
- ALMOST ZERO probability

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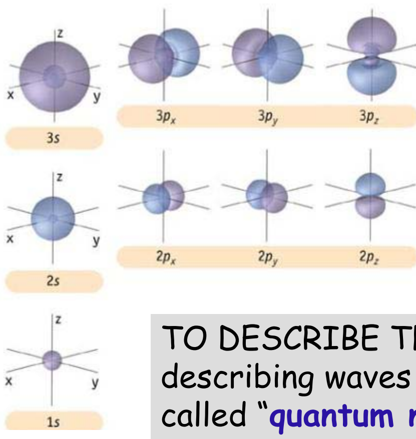
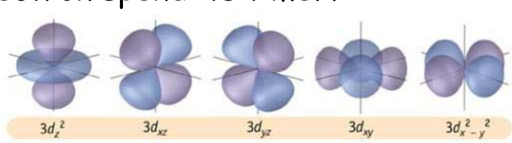
Views of orbitals for electron in an H atom… in ground state and in higher E states

Kotz Fig. 7.15

What do other (higher energy) atomic orbitals "look like"?
Where else can the H's electron spend its time??





⇨ these shapes represent ψ^2 's
for ground state & higher E's
for the hydrogen atom
i.e., probability maps of solutions to Schrodinger's equation…

TO DESCRIBE THEM: mathematical functions describing waves are defined by many variables… called "**quantum numbers**"

→ 3 important ones: n, ℓ, m_ℓ (ℓ = a hand-written small L)

→ have certain allowed integer values

ASSIGNED READINGS

- **BEFORE NEXT CLASS:**

read up to & including Ch.8.2

master orbital names, shapes & energies,
assigning/using quantum numbers

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