General Chemistry 1

Chem110

Section 1

Part 1: Understanding and describing an Atom – Introduction to Quantum Theory

Part 2: Understanding the properties of elements and their position in the periodic table

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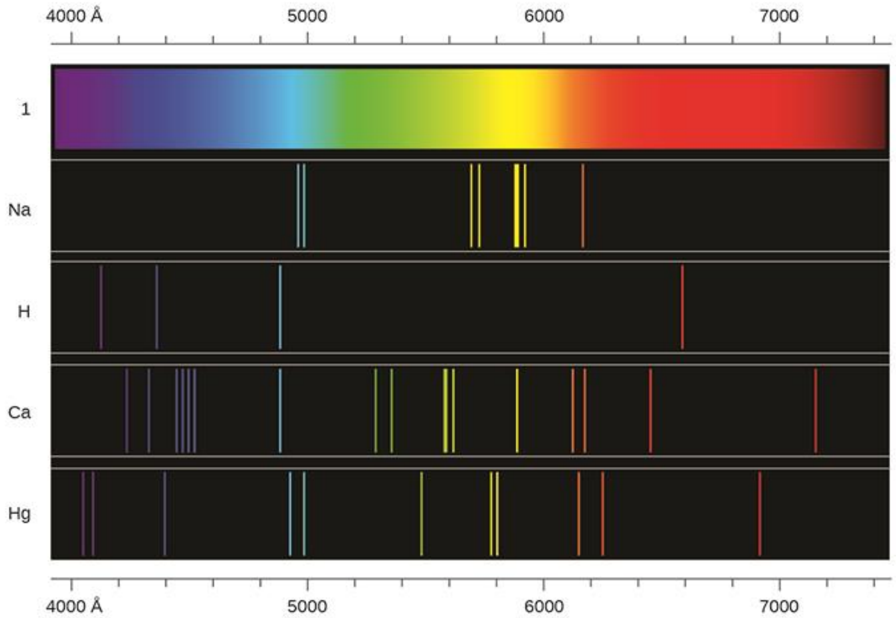
Atomic Spectra



Spectra is *unique to* and *characteristic of* each element

What does each spectral line represent?

What can you calculate from the spectral lines?

Section 1: Part 2 (Introduction to Quantum Theory)

- Concept Video 4
  - Bohr's Model – when it works and when it doesn't!
  - Wave and Particle nature of matter and light
  - Wavelength of matter and Uncertainty
- Concept Video 5
  - Schrodinger Equation
  - What is a wave function? What are orbitals?
- Concept Video 6
  - Why does Bohr's model work for H atom? H atom – A Special Case!

Bohr's Atomic Model

- Stationary States – H atom has only certain allowed energy levels where the electrons can reside. Higher the energy level – further from the nucleus the orbit is.
- Electron can move within the orbit without changing the atom's energy.
- The atom changes to another stationary state (the electron moves to another orbit) only by absorbing or emitting a photon.

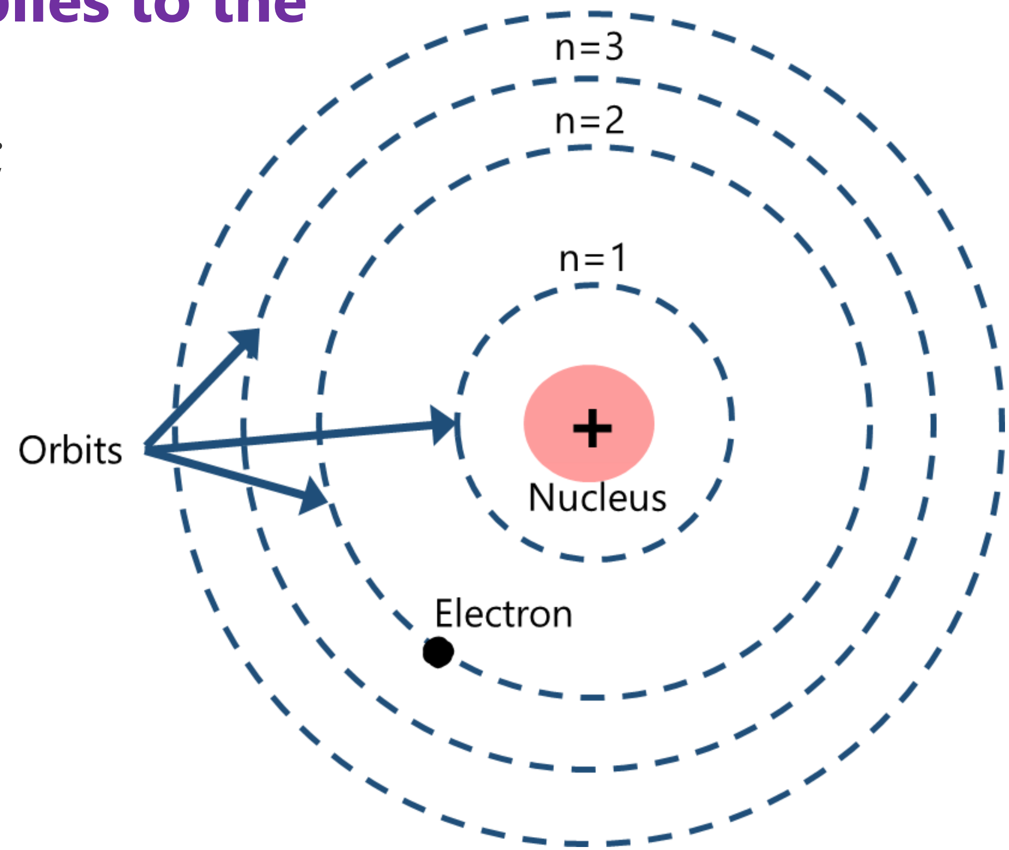
Energy (wavelength/frequency) of the photon (light) corresponds to the energy difference between the two stated.
So, in an electronic transition the electron can get excited to a higher energy state by absorbing the corresponding energy photon

$$E_{\text{photon}} = h\nu = hc/\lambda = \Delta E = E_f - E_i$$

h is Planck's constant
E_i and E_f are the initial and final orbit energies, respectively.

Bohr's Atomic Model

n is a **quantum number – applies to the electron**
It can only have integer values;
$n \geq 1$.



What does the value *n* tell us about the electron in an atom?

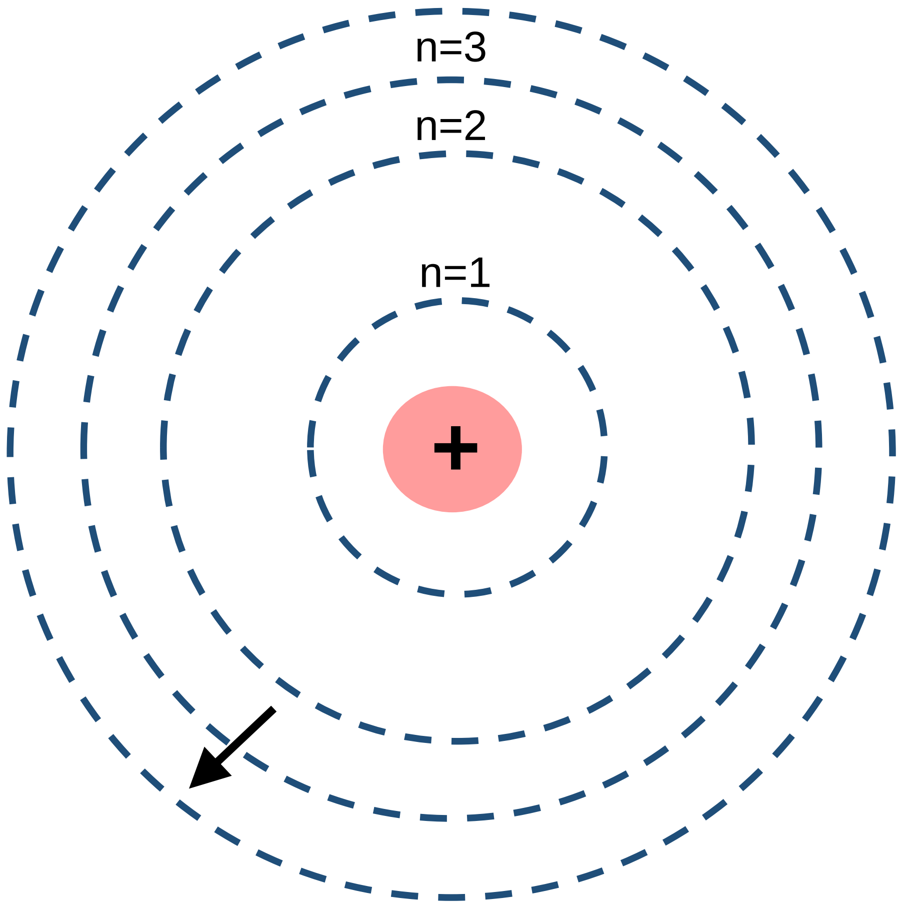
Distance from the nucleus
Energy

When the electron is in the first orbit ($n = 1$) closest to the nucleus, and the H atom is in its lowest (first) energy level, called the **ground state.**
If the electron is in any other orbit – **excited state**

Bohr’s Model of Hydrogen atom (or any 1-electron species)

Absorption: If an electron *absorbs* a photon whose energy equals the *difference* between lower and higher energy levels, the electron moves to the outer (higher energy) level.

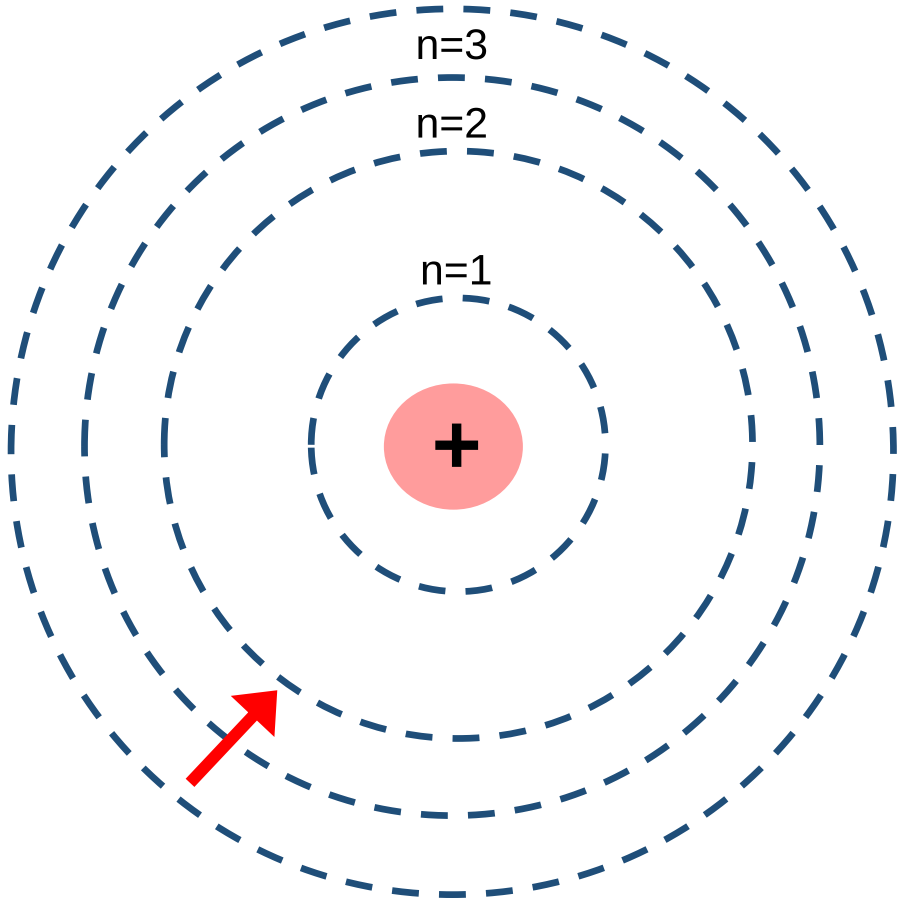
Energy



Bohr's Model of Hydrogen atom (or any 1-electron species)

Emission. If an electron goes from a higher to a lower energy level, the atom *emits* a photon whose energy equals the difference between the two levels.

Energy



Bohr's Model

How can this concept of orbits explain what the scientists were observing? How can it explain the discrete atomic spectra?

Applying Bohr's Model

Using Rydberg's equation and relating the wavelength of the spectral lines to the energy (using $E = hc/\lambda$) , Bohr calculated the energy corresponding to an orbit

Energy of an electron in orbit "n"

$$E = -2.18 \times 10^{-18}\left(\frac{Z^2}{n^2}\right)$$

Z is the atomic number;
Hydrogen it is 1, Helium it is 2, Lithium it is 3

Difference in energy between two levels

$$\Delta E = E_{\text{final}} - E_{\text{initial}}$$

Important takeaways:
In an atom
-Energy of each orbit is *quantized (depends on n)*
-The energy difference between two orbits for an atom is always a discrete value and results in a discrete spectral lines

Applying Bohr's Model

Explaining Hydrogen spectra

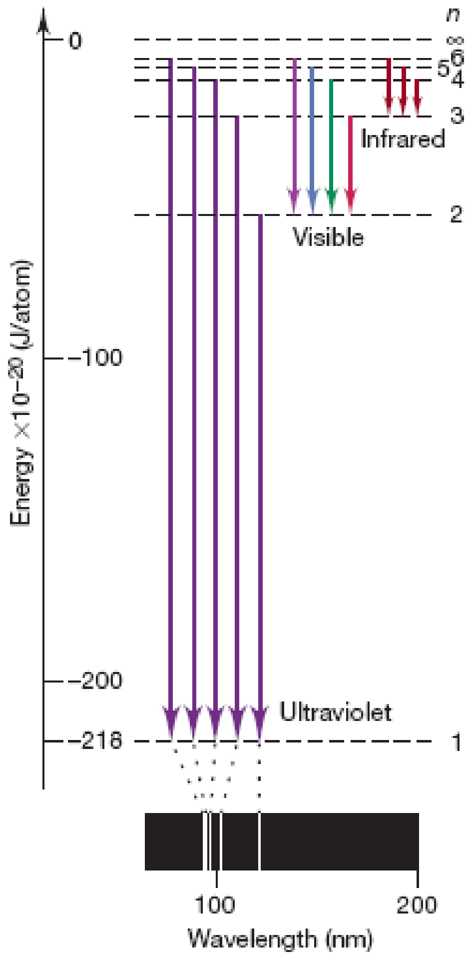


Figure 6.12
Chemistry: The Molecular Nature of Matter and Change
Silberberg, 2e

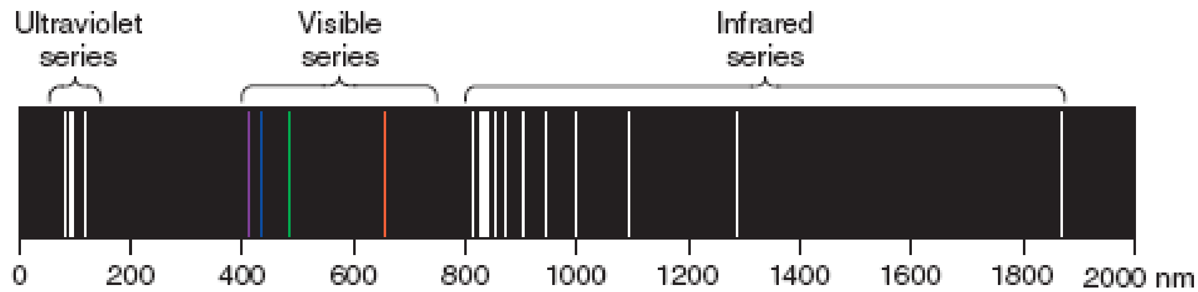
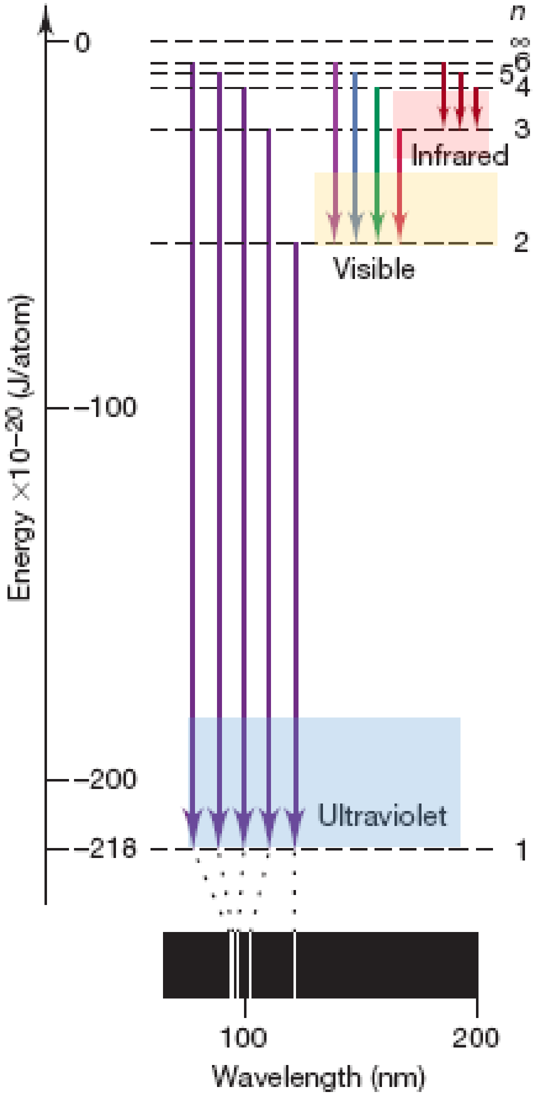


Figure 6.10
Chemistry: The Molecular Nature of Matter and Change
Silberberg, 2e

Bohr's model explains the data for 1-electron species well

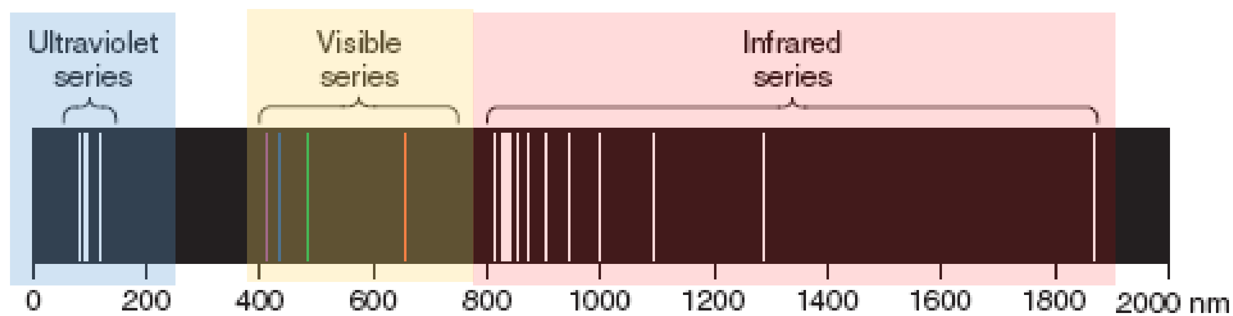
Applying Bohr's Model of the atom

Explaining the Hydrogen spectra



What does the energy emission tell us about the different orbits?

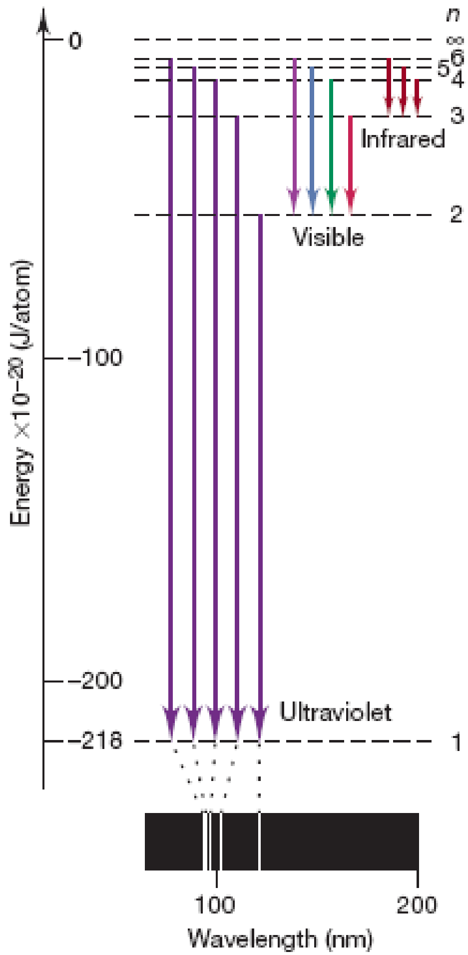
Any emission to n=1 falls in the UV region
Any emission to n=2 falls in Visible range
Any emission to n=3 falls in the IR range



Energy difference between n=1 and n=2 is the largest
Followed by that between n=2 and n=3, so on and so forth……

Applying Bohr's Model

Explaining Hydrogen spectra



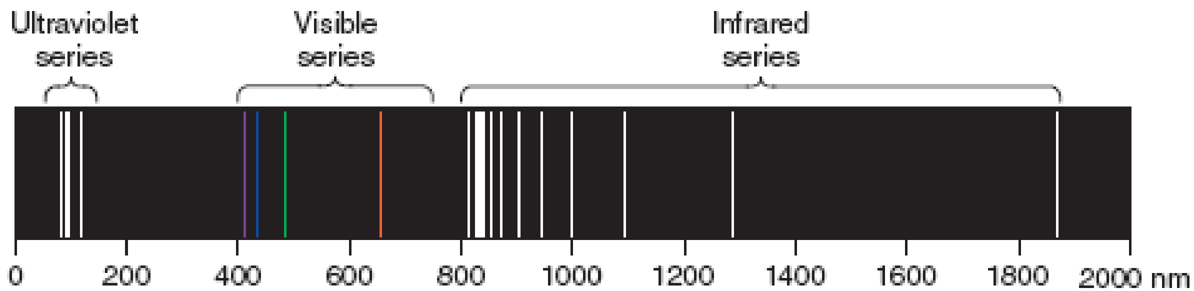


Figure 6.10
Chemistry: The Molecular Nature of Matter and Change
Silberberg, 2e

Bohr's model explains the data for 1-electron species well

CANNOT BE USED FOR MULTI-ELECTRON SPECIES

Figure 6.12
Chemistry: The Molecular Nature of Matter and Change
Silberberg, 2e

Matter and energy are more similar than you think!

Light has wave-like properties
e.g Diffraction

Light has particle-like properties
e.g Photoelectric Effect

Matter has particle-like properties

Can matter also have wave-like properties?

Wavelength of matter

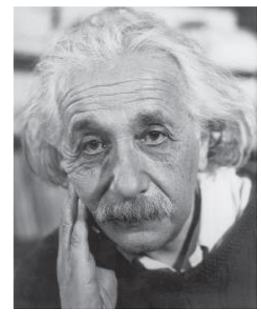
For Light

$$E = hc/\lambda$$

Energy of a photon related to wavelength

$$p = E/c$$

p: Momentum of a photon



Can electrons have a wavelength too?

Louie de Broglie

If electrons have a wavelength – that implies that all matter has a wavelength!

Momentum = mass x velocity

$$p = m \times u$$

Wavelength of matter

Louie de Broglie hypothesized that all matter can have wave-like properties

$$\lambda = h/p$$

$$\downarrow \; p = m \times u$$

$$\lambda = h/mu$$

For Light

$$E = hc/\lambda$$

Energy of a photon related to wavelength

$$p = E/c$$

p: Momentum of a photon

For Matter

$$\lambda = hc/E$$

$$E = cp$$

$$\lambda = hc/cp$$

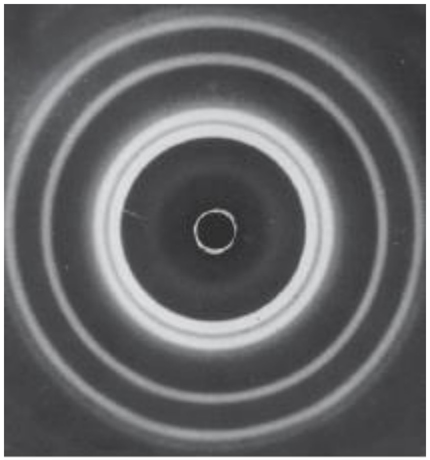
$$\lambda = h/p$$

p (momentum) = mass x velocity

Experiments show that matter has wave-like nature!.....

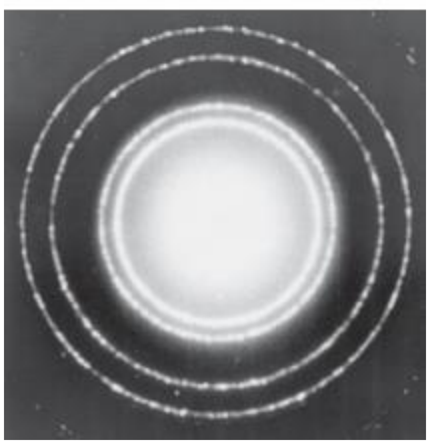
de Broglie’s hypothesis was confirmed by experiments by Davisson and Germer

Electrons indeed had wave-like properties



Diffraction pattern of aluminum using X Rays

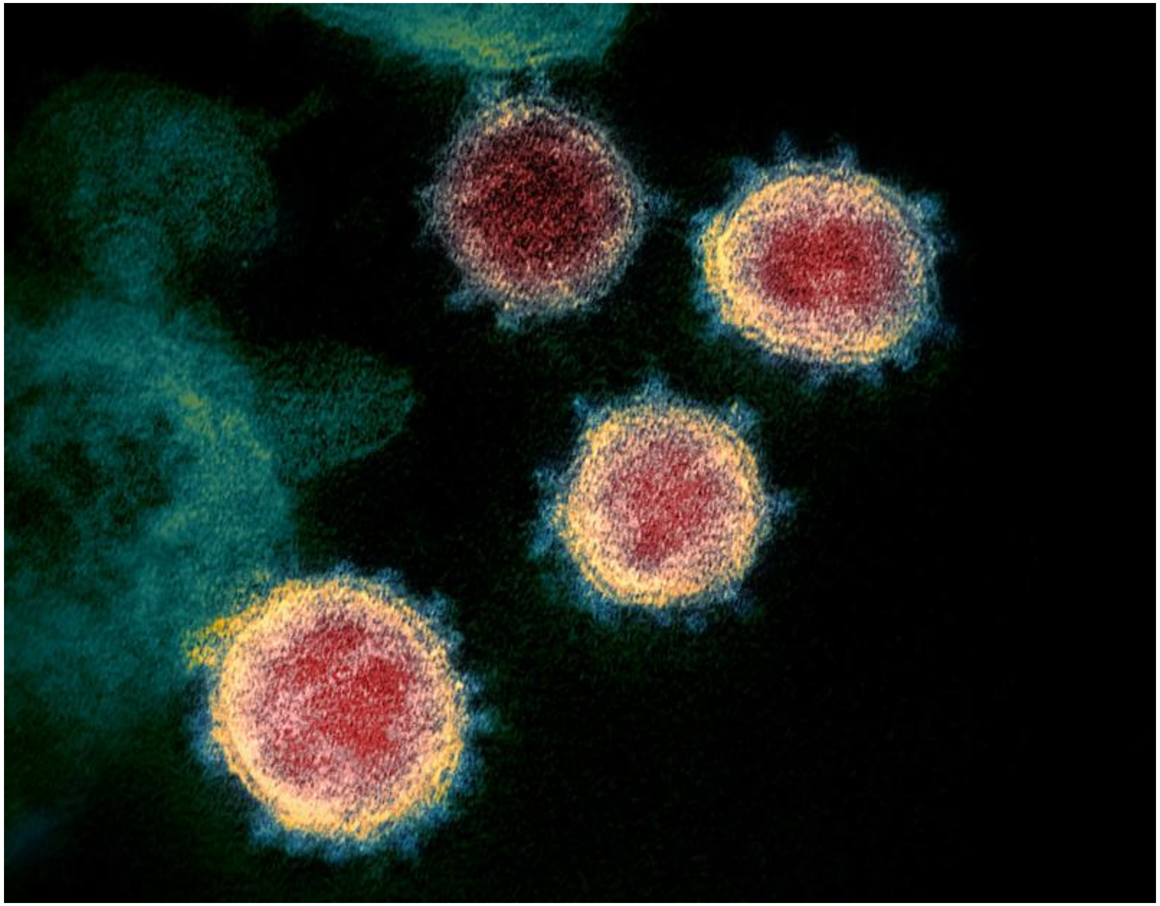
Light with wave-like properties



Diffraction pattern of aluminum using electrons

Electrons (which make up all matter) with wave-like properties

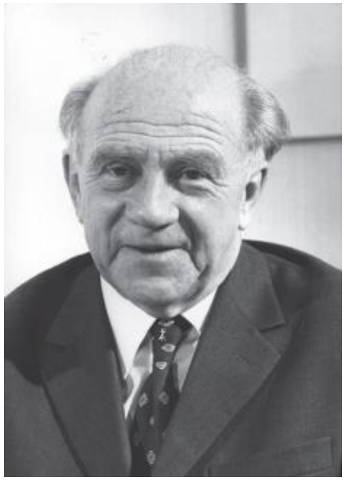
Electron Microscopy



Electron microscopy image of SARS-Cov2 Virus

Image Courtesy – NIAID RML
https://www.flickr.com/photos/niaid/albums/72157712914621487/with/49534865371/

Determining position and momentum of a particle



Heisenberg

Heisenberg's Uncertainty Principle

uncertainty in position

$$\Delta x \,.\, \Delta p \geq h/4\pi$$

uncertainty in momentum

Precision of positon and momentum have an inverse relation i.e if the position of a particle can be determined more precisely, then the momentum of the particle is predicted less precisely. You cannot determine both the position and the momentum of a particle precisely.

Matter and energy are more similar than you think!

Light has wave-like properties
e.g Diffraction

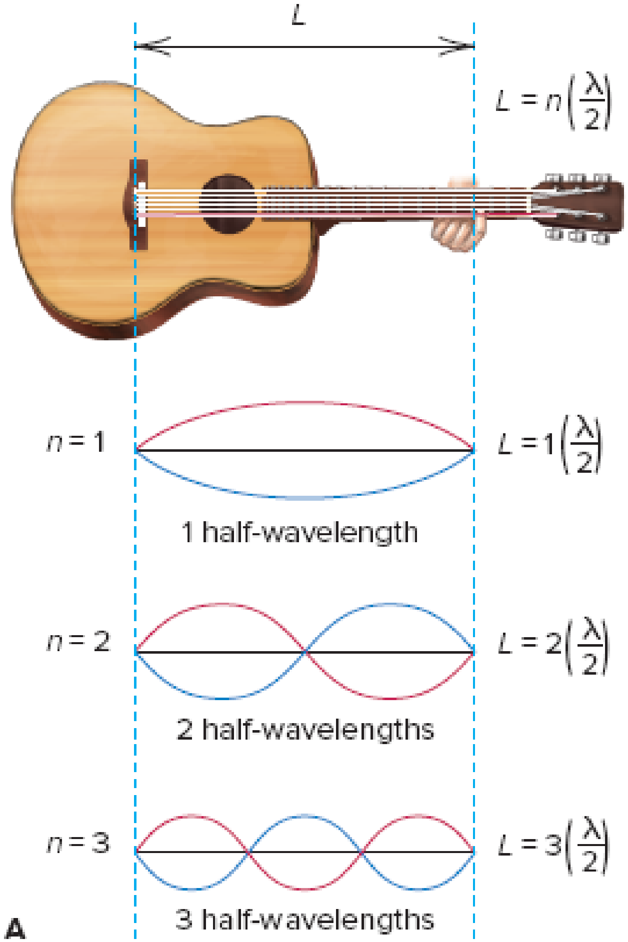
Light has particle-like properties
e.g Photoelectric Effect

Matter has particle-like properties

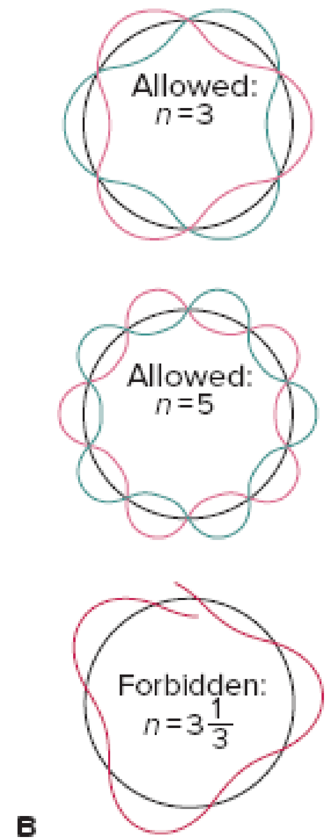
Matter has wave-like properties

Need something other than wave-theory to explain this wave-particle duality of light and matter

Wavelength of matter



If electrons have wavelike motion in orbits of fixed radii, they would have only certain allowable frequencies and energies



Vibrations of a guitar string – since the two ends are fixed, only certain vibrations are allowed (standing wave)

Quantum Mechanics

Atom can be described in terms of specific quantities of energy depending upon the allowed frequencies of its electrons' wave-like function
Described electron distribution as a *standing wave* and provided solutions for it

Erwin Schrödinger
1887-1961

Schrödinger Equation

$$\hat{H}\psi = E\psi$$

$\hat{H}$: Hamiltonian Operator
E: Binding Energy
Ψ: Wave Function

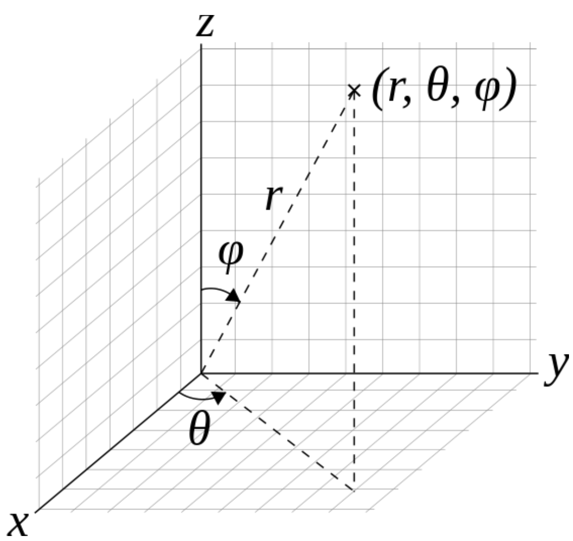
Wave Function (Ψ; pronounced "sai")

A mathematical function that relates the location of an electron at a given point in space to its energy

Wavefunctions

A mathematical function that relates the location of an electron at a given point in space to its energy.

Contains a radial (r) and angular component (θ, φ)



$$\Psi_{n,\, l,\, m}\,(r,\, \theta,\, \varphi) = R(r) \times Y_{l,\, m}\,(\theta,\, \varphi)$$

Each wavefunction is defined by characteristic **quantum numbers** (n, l, m)

The square of the wave function Ψ^2 gives us the **probability of finding an electron** at a given point

Orbitals : Mathematically derived regions of space with different *probabilities* of containing an electron.

QUANTUM NUMBERS (describing orbitals)

1. Principal Quantum Number (n)

1. Positive integer (1,2,3….)
2. Indicates the relative size of the orbital – relative distance
3. Specifies the energy level (higher n indicated higher energy)

2. Angular Quantum Number (*l*)

1. Positive Integer (0 to n-1)
2. Shape of the orbital
3. The value of n limits *l*

if n=1, *l* can only have the value 0; if n=2, *l* can have the values 0 and 1

When l =0 (s orbital); l=1 (p orbital); l=2 (d orbital); l=3 (f orbital)

3. Magnetic Quantum Number (m_l)

1. Integer (-*l* to +*l*)
2. Orientation of the orbital around the nucleus
3. The value of l limits m_l; For l=1, values of m_l can be -1,0, and 1

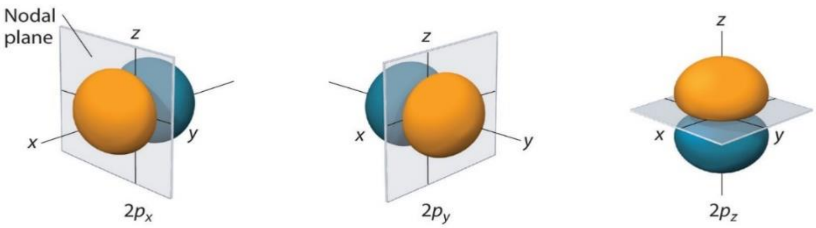
Orbitals

Lowest possible value of the principal quantum number : n=1

IMAGE COURTESY: UCDAVIS CHEMWIKI, CC BY-NC-SA 3.0 US

When n= 1, only possible value of *l* = 0
as *l* is a +ve integer from 0 to (n-1)

An orbital with *l* = 0; s orbital – This is called the 1s orbital
When l = 0; only 1 possible value of m_l = 0 (one orientation of the orbital, symmetric)



Next possible value: n=2

IMAGE COURTESY: UCDAVIS CHEMWIKI, CC BY-NC-SA 3.0 US

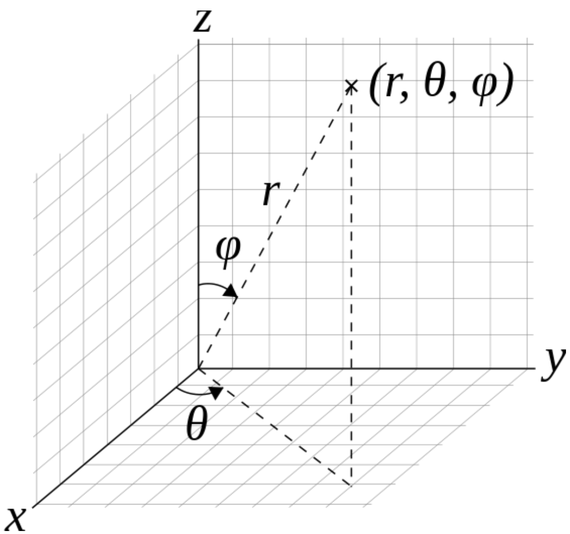
When n= 2, two possible values of *l* = 0 and 1

An orbital with *l* = 0; s orbital – 2s orbital (spherical – larger n so larger than 1s)
An orbital with *l* = 1; p orbital – 2p orbital (dumbbell shaped)
When l = 1; three possible values of m_l =-1, 0, +1 (three orientations of the orbital, $2p_x$, $2p_y$, and $2p_z$)

Wavefunctions

A mathematical function that relates the location of an electron at a given point in space to its energy.

Contains a radial (r) and angular component (θ, φ)



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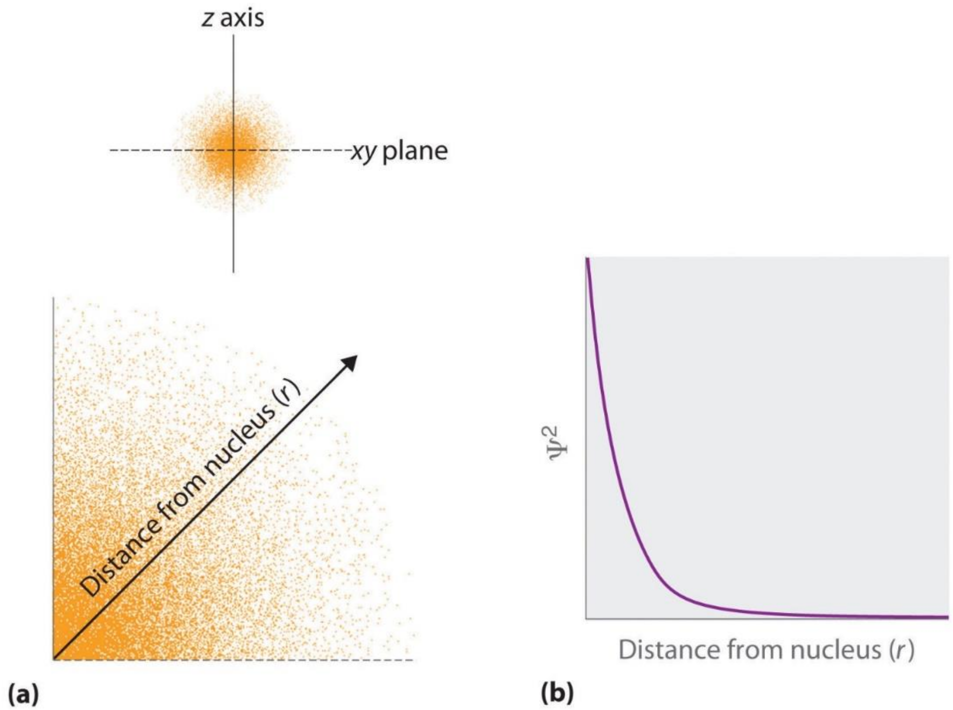
Orbitals : Mathematically derived regions of space with different *probabilities* of containing an electron.

Probability Density (1s orbital)

Based on this probability density we can obtain a three dimensional representation of the orbital



Probability of Finding the Electron in the Ground State of the Hydrogen Atom at Different Points in Space. (a) The density of the dots shows electron probability. (b) Plot of Ψ^2 versus r

The density of the dots shows electron probability. The electron probability density is highest at $r = 0$

But how do we physically interpret it?

Probability Density and Radial Probability (1s orbital)

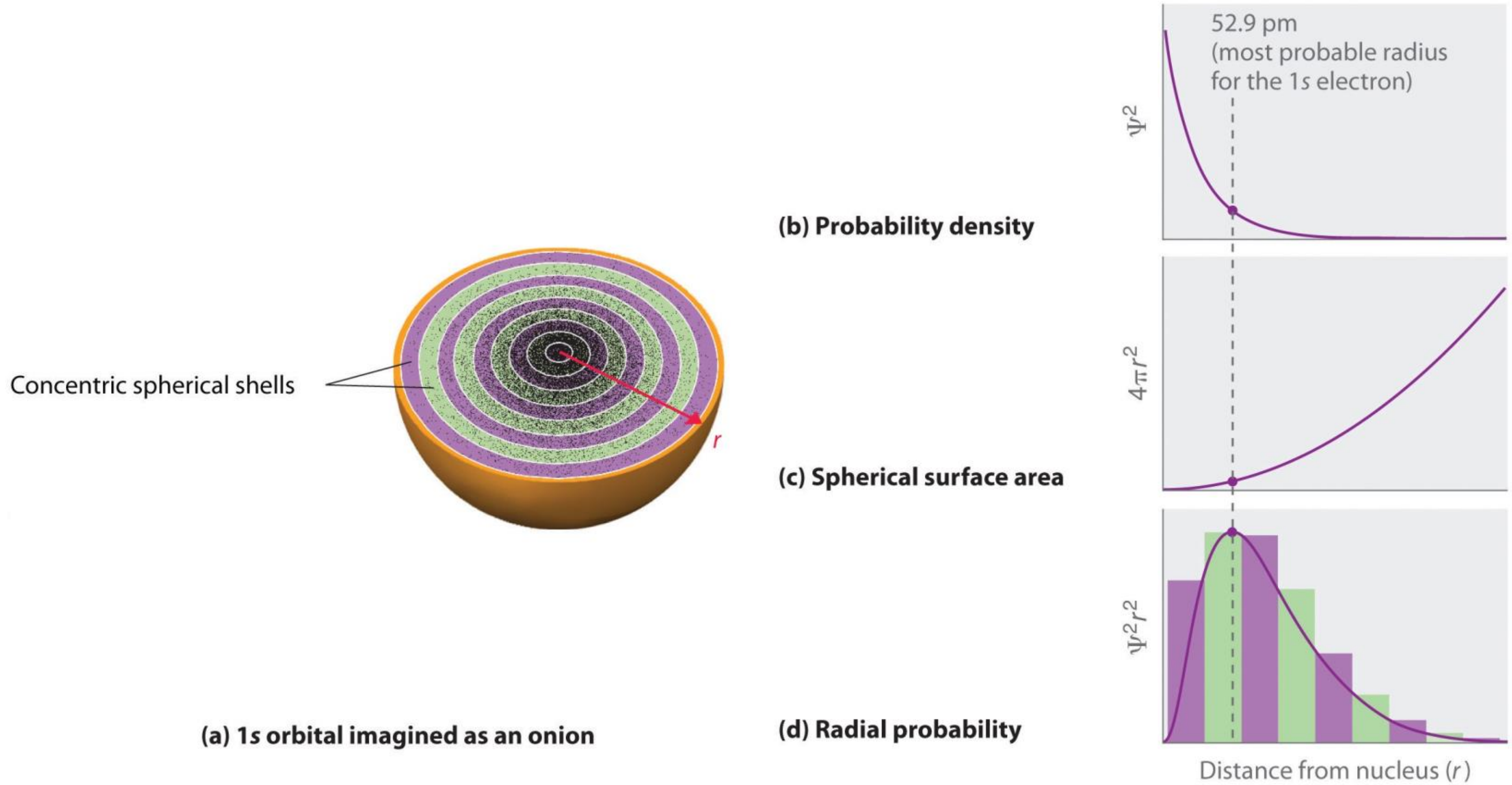
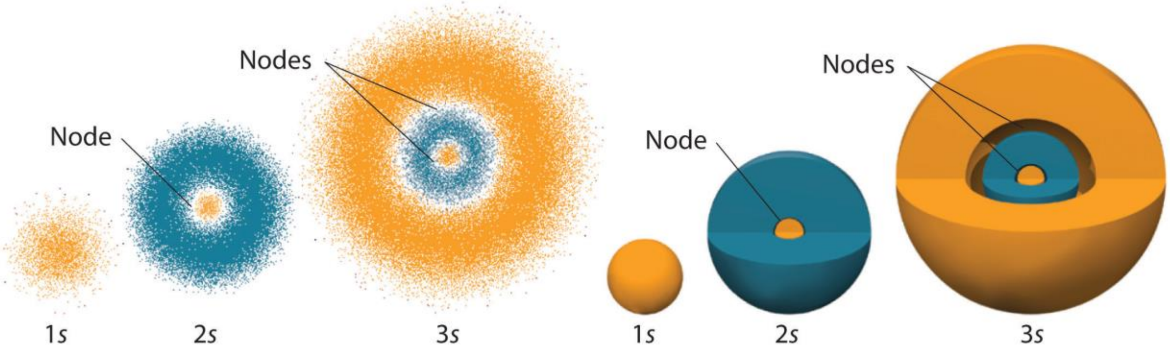


IMAGE COURTESY: UCDAVIS CHEMWIKI, CC BY-NC-SA 3.0 US

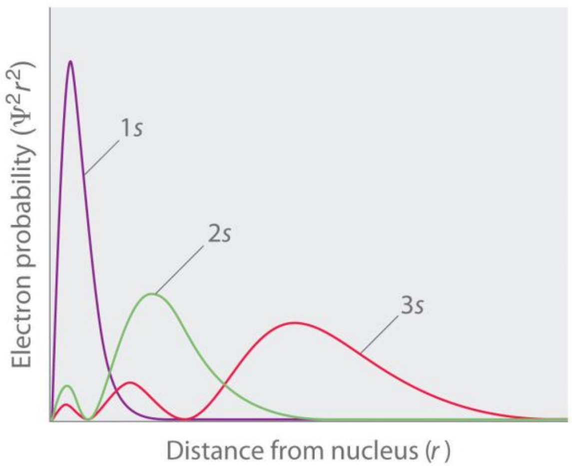
The probability density is multiplied by volume to obtain the probability of finding an electron at a certain distance from the nucleus

Shapes of Atomic Orbital (1s, 2s, 3s orbitals)



(a) Electron probability **(b) Contour probability**

IMAGE COURTESY: [UCDAVIS CHEMWIKI](), [CC BY-NC-SA 3.0 US]()



(c) Radial probability

1s orbital: 0 radial nodes
2s orbital: 1 radial node

What are nodes?

Regions where there is no probability of finding an electron

What is a radial node?

Depends on quantum numbers n and l

Radial node = n-1-l

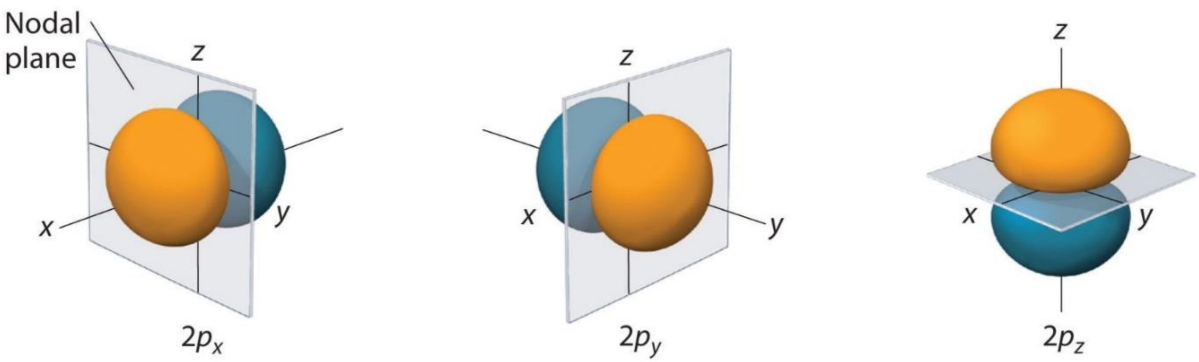
Shapes of Atomic Orbitals; p orbital

How many p orbitals will there be in a shell?

Which is the first shell to have p orbitals?

What are nodes?

Regions where there is no probability of finding an electron



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What is an angular node?

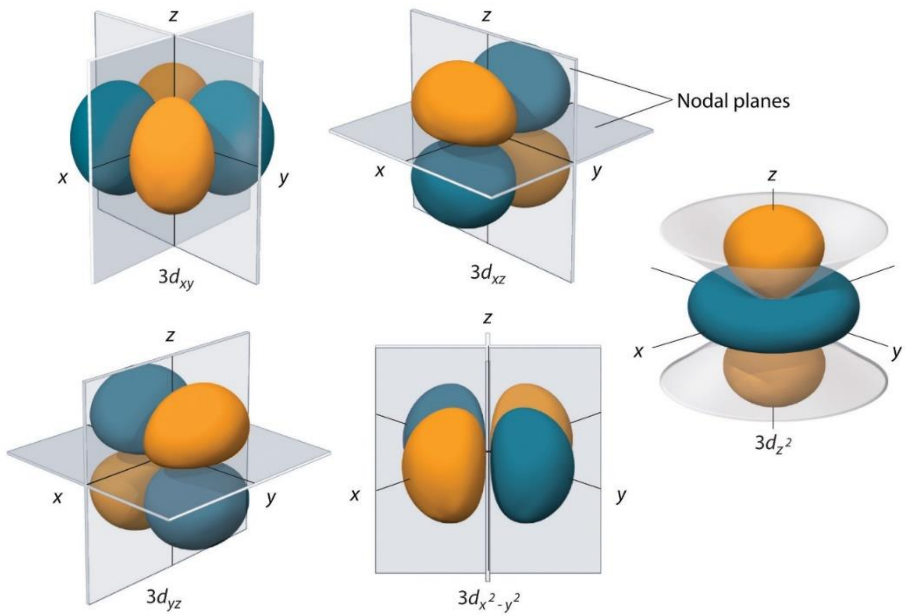
1s orbital: 0 angular nodes
2p orbital: 1 angular node

Depends on quantum number *l*
Angular node = *l*

What does the radial distribution of a 2p orbital look like?

Shapes of Atomic Orbitals; d orbital

How many d orbitals will there be in a shell?



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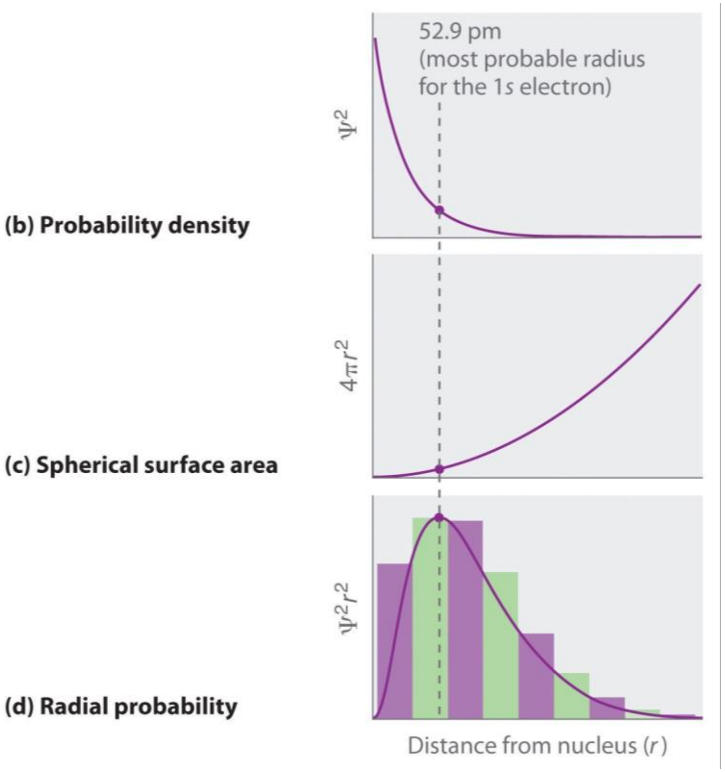
What does the radial distribution of a 3d orbital look like?

How many radial and angular nodes in a 3d orbital?

Why did Bohr's Model work for hydrogen atom?

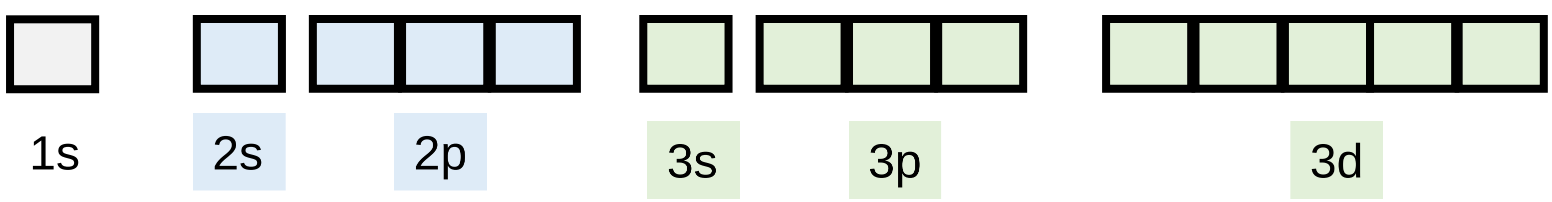
Bohr's model correctly predicted the radius of the H-atom – even though Bohr's atomic theory is incorrect. It cannot be applied to multi-electron species.
Why does it work for H?
Hydrogen is special – only one electron but there is more but there is more.....



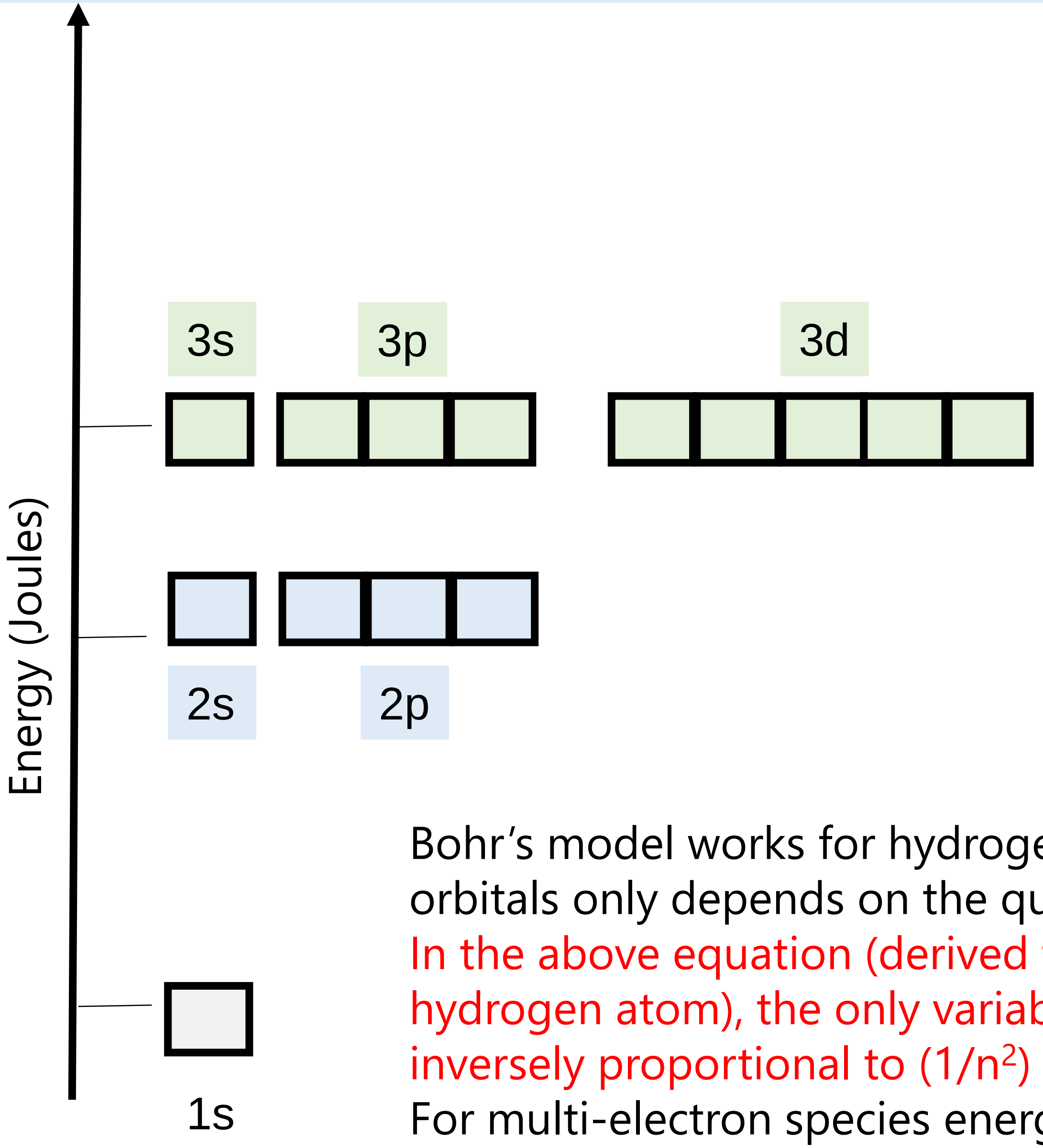
Why did Bohr's Model work for hydrogen atom?

Hydrogen is special – only one electron but there is more….

Can you draw the energy levels (energy of different orbitals based on increasing energy) for a H-atom?



Energy Levels of Hydrogen Atom



From Schrodinger Equation, we obtain the solution for the hydrogen atom

$$E_n = -\frac{m_e e^4}{8{\epsilon_0}^2 h^2 n^2}$$

Bohr's model works for hydrogen atom because the energy of the orbitals only depends on the quantum number n.

In the above equation (derived from applying quantum theory to hydrogen atom), the only variable to determine E_n is *n* (En is inversely proportional to $(1/n^2)$)

For multi-electron species energy of orbitals depends on more than one quantum numbers so Bohr model cannot be applied.