INTERSTELLAR MEDIUM

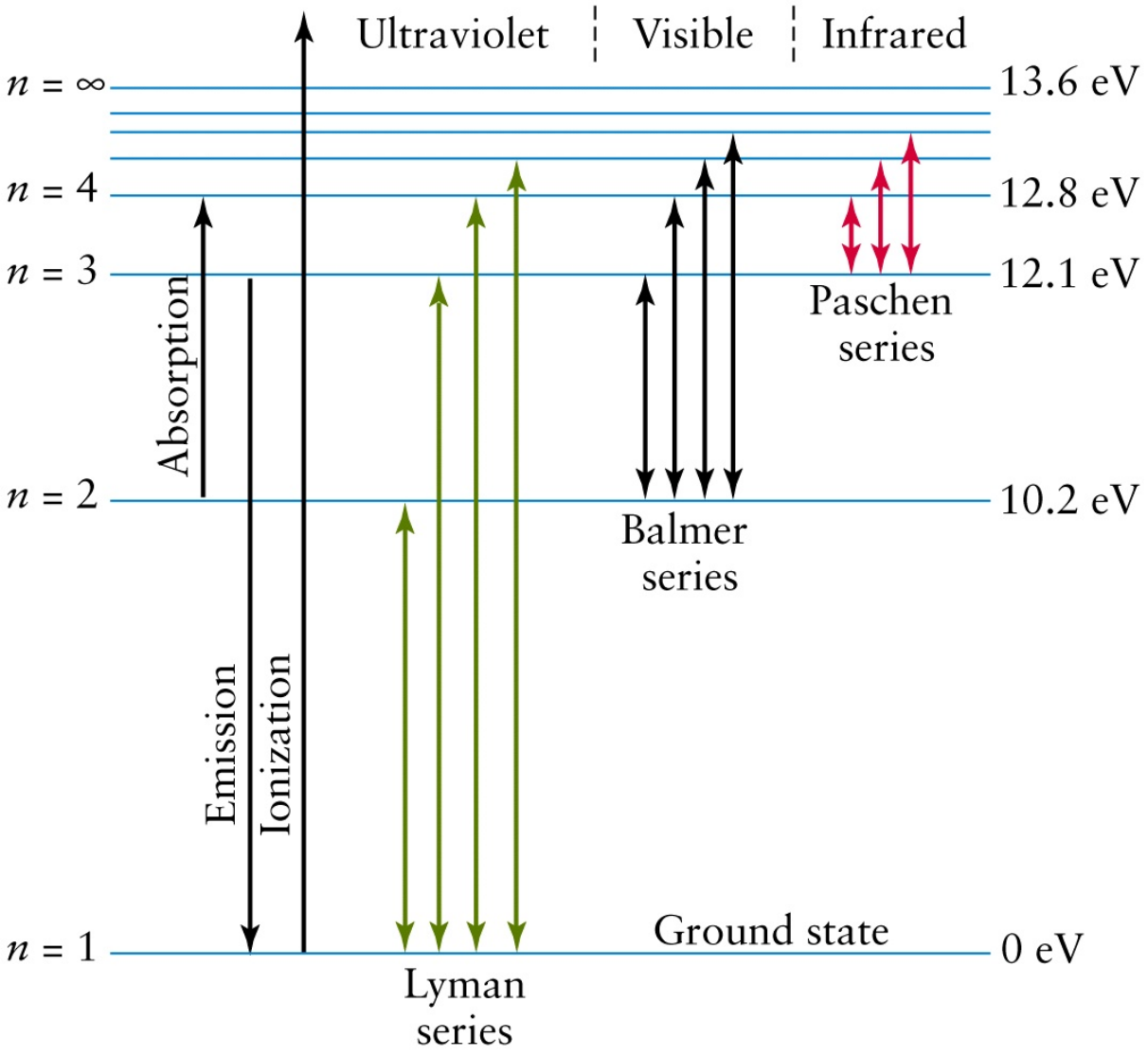
- Stefano Bovino -

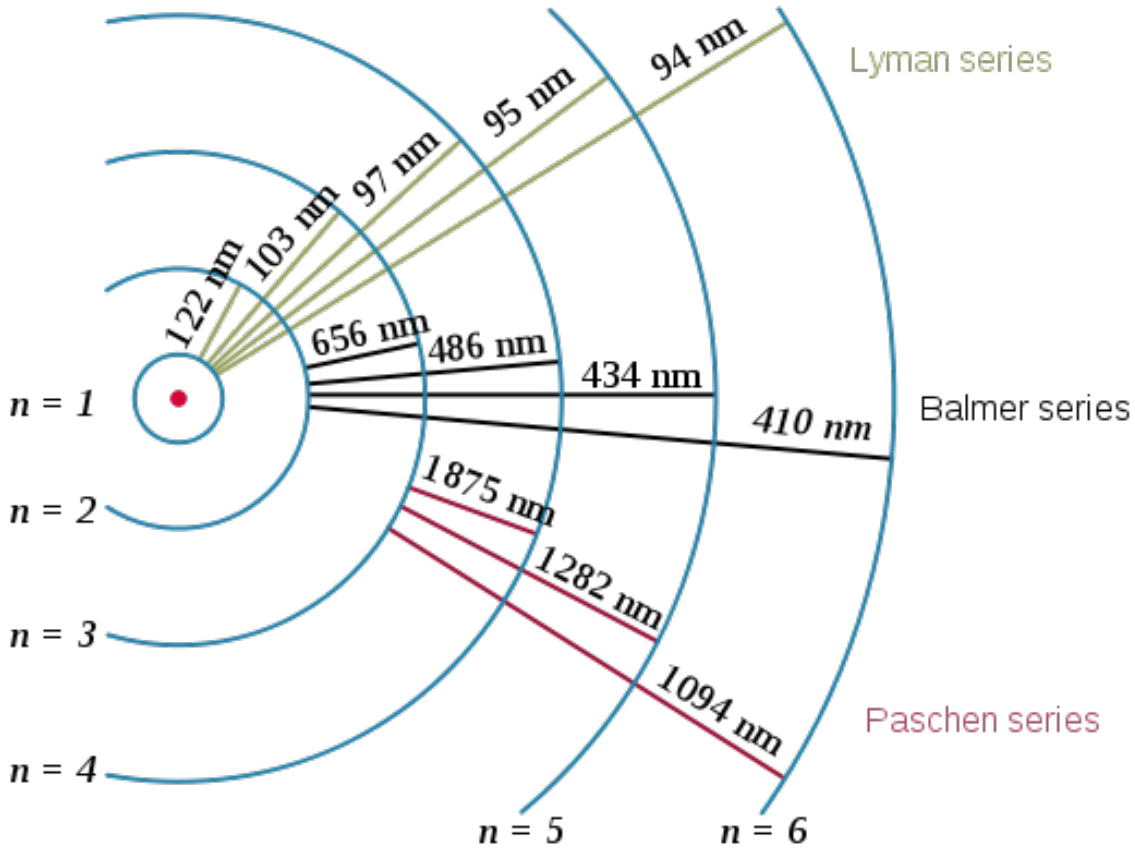
Atomic Structure

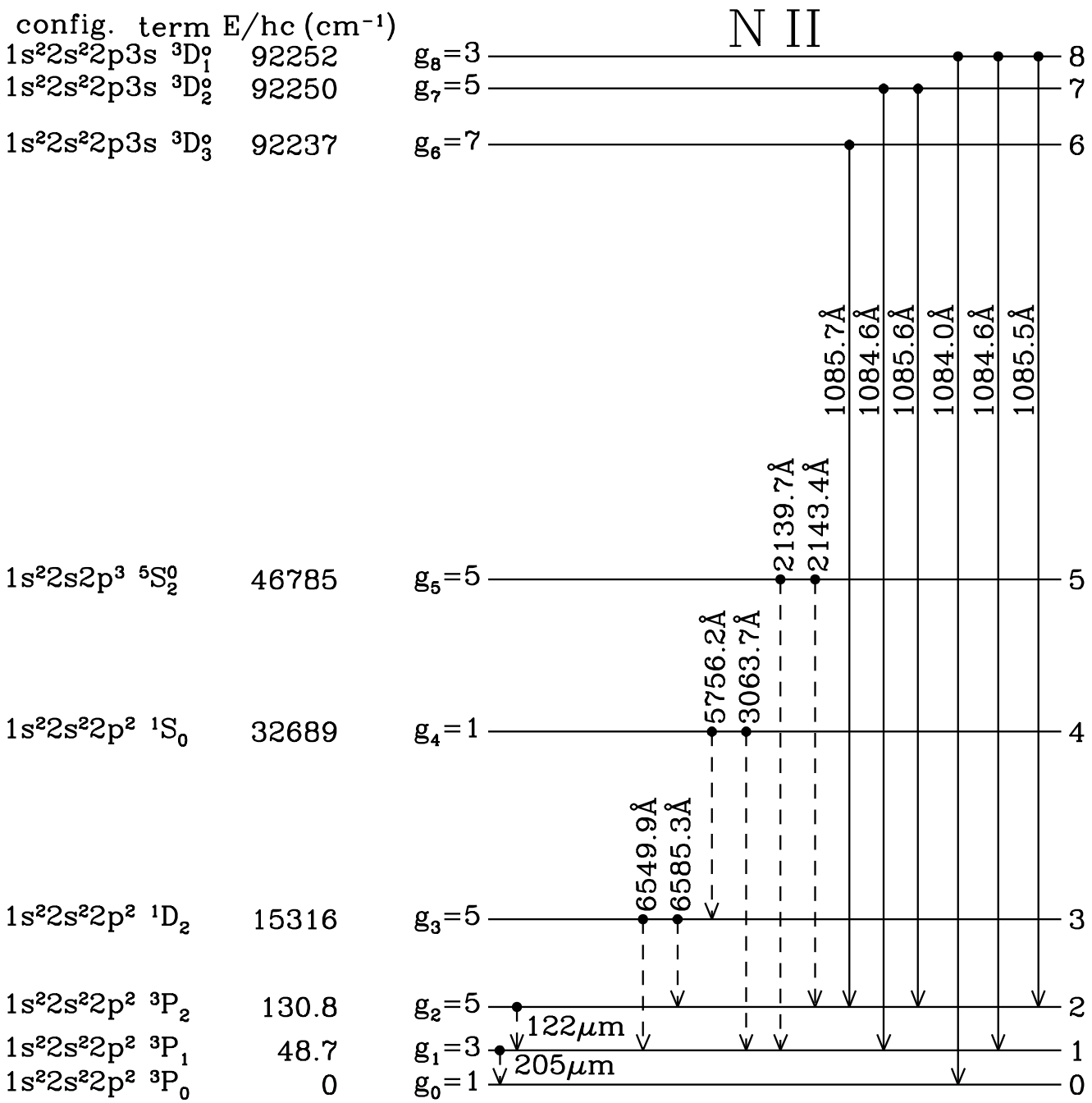
Collisions

Govern many key processes in the ISM

- Distribute energy
- Ionize the medium (collisional ionization)
- Recombination (radiative recombination)
- Excitation and loss of energy via de-excitation
- Govern chemistry (reactions)
- Gas-dust interaction and grain-grain


Ultraviolet
Visible
Infrared
n = ∞
n = 4
n = 3
n = 2
n = 1
13.6 eV
12.8 eV
12.1 eV
10.2 eV
0 eV
Absorption
Emission
Ionization
Paschen series
Balmer series
Lyman series
Ground state


Lyman series
94 nm
95 nm
97 nm
103 nm
122 nm
Balmer series
410 nm
434 nm
486 nm
656 nm
Paschen series
1094 nm
1282 nm
1875 nm
n = 1
n = 2
n = 3
n = 4
n = 5
n = 6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config. term E/hc (cm⁻¹)
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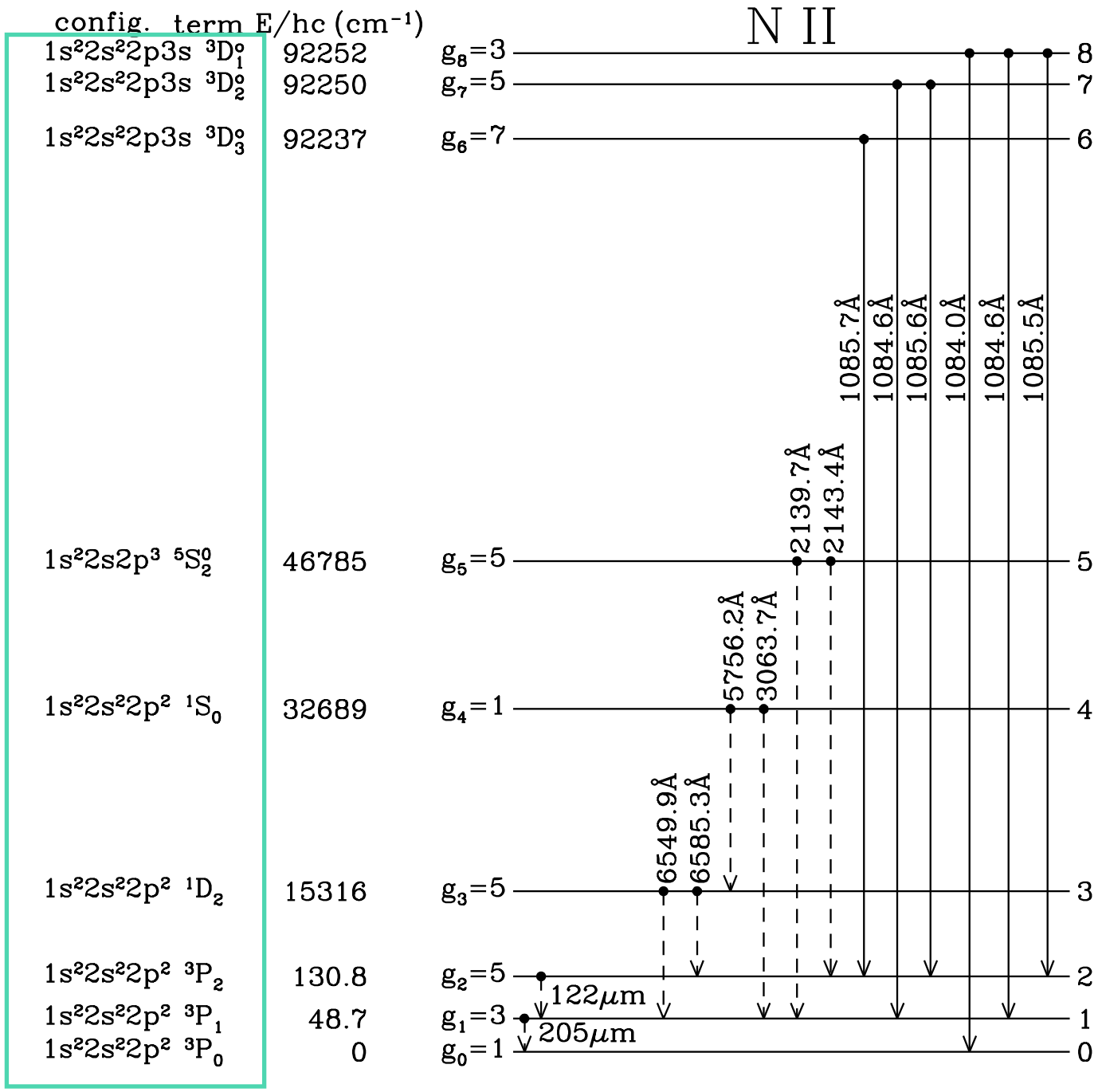
1s²2s²2p3s ³D°₂ 92250
1s²2s²2p3s ³D°₃ 92237
1s²2s2p³ ⁵S°₂ 46785
1s²2s²2p² ¹S₀ 32689
1s²2s²2p² ¹D₂ 15316
1s²2s²2p² ³P₂ 130.8
1s²2s²2p² ³P₁ 48.7
1s²2s²2p² ³P₀ 0
g₈=3
g₇=5
g₆=7
g₅=5
g₄=1
g₃=5
g₂=5
g₁=3
g₀=1
8
7
6
5
4
3
2
1
0
1085.7Å
1084.6Å
1085.6Å
1084.0Å
1084.6Å
1085.5Å
2139.7Å
2143.4Å
5756.2Å
3063.7Å
6549.9Å
6585.3Å
122μm
205μm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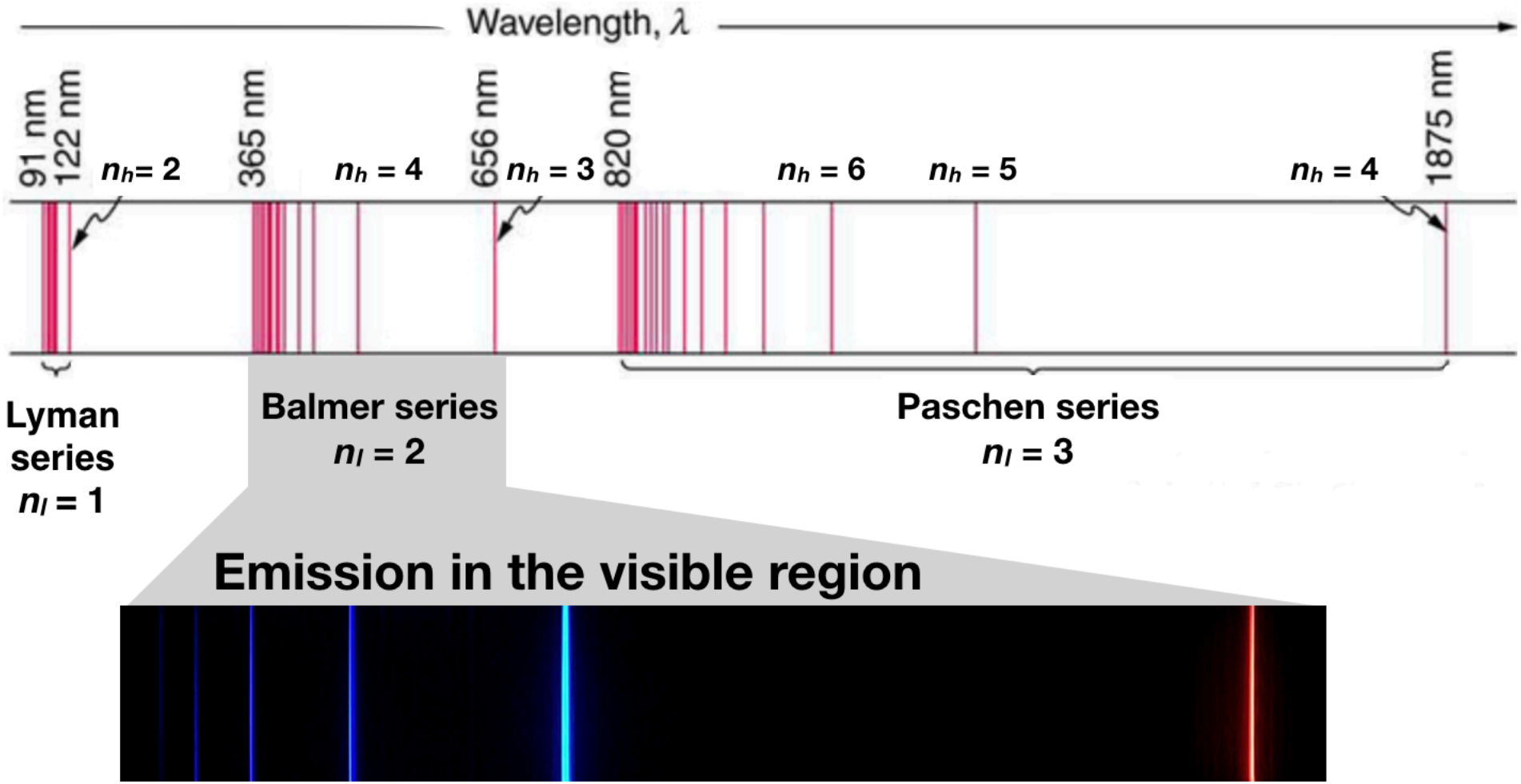
g₈=3
g₇=5
g₆=7
g₅=5
g₄=1
g₃=5
g₂=5
g₁=3
g₀=1
8
7
6
5
4
3
2
1
0
1085.7Å
1084.6Å
1085.6Å
1084.0Å
1084.6Å
1085.5Å
2139.7Å
2143.4Å
5756.2Å
3063.7Å
6549.9Å
6585.3Å
122μm
205μm

Failure of classical physics

- Black body radiation
- Photoelectric effect: electrons ejected from metals when irradiated
- Compton effect: electrons-photons scattering
- Atomic spectra

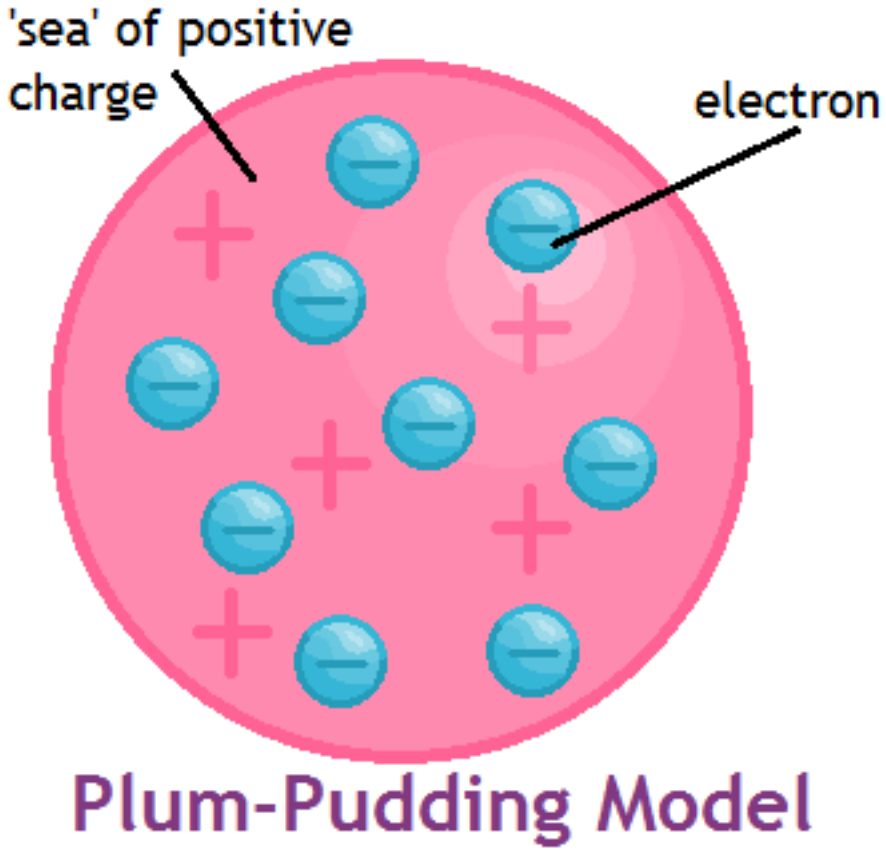
Balmer 1885

- Radiation from atoms produced discrete features



J.J. Thomson plum pudding model (1897)

He discovered the electron, still atoms are neutral so the pudding model!



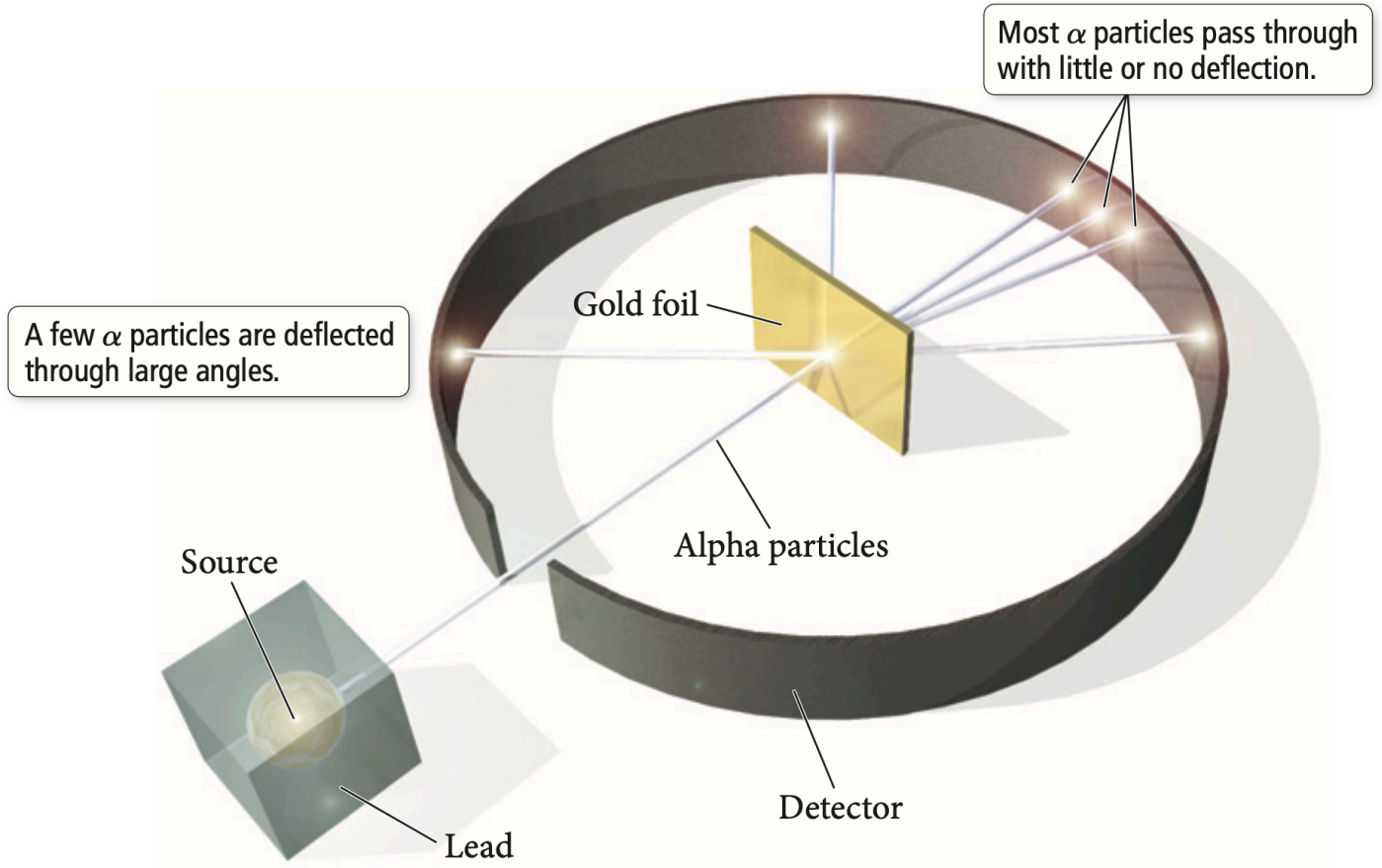
Structure of the Atom ~1900

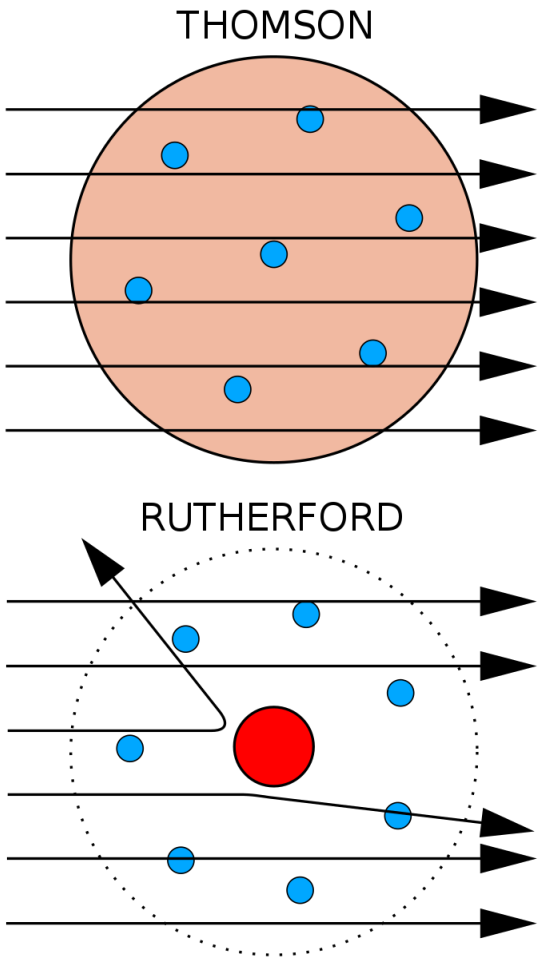
- Atom is electrically neutral
- Negative charge carried by electrons
- Electron has very small mass (Millikan exp)
- Bulk of the atom is positive

How the charges are distributed?

Rutherford's model

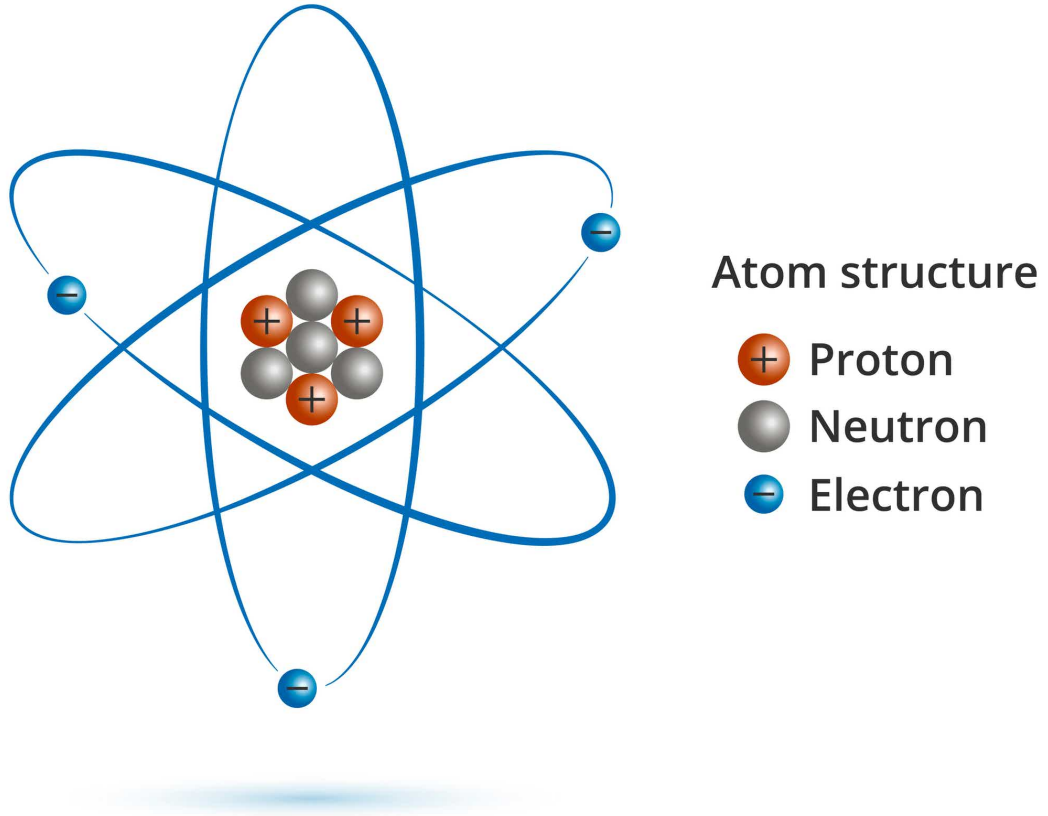
- 1909: Rutherford experiment with alpha-particles (positively charged)





Rutherford's failure

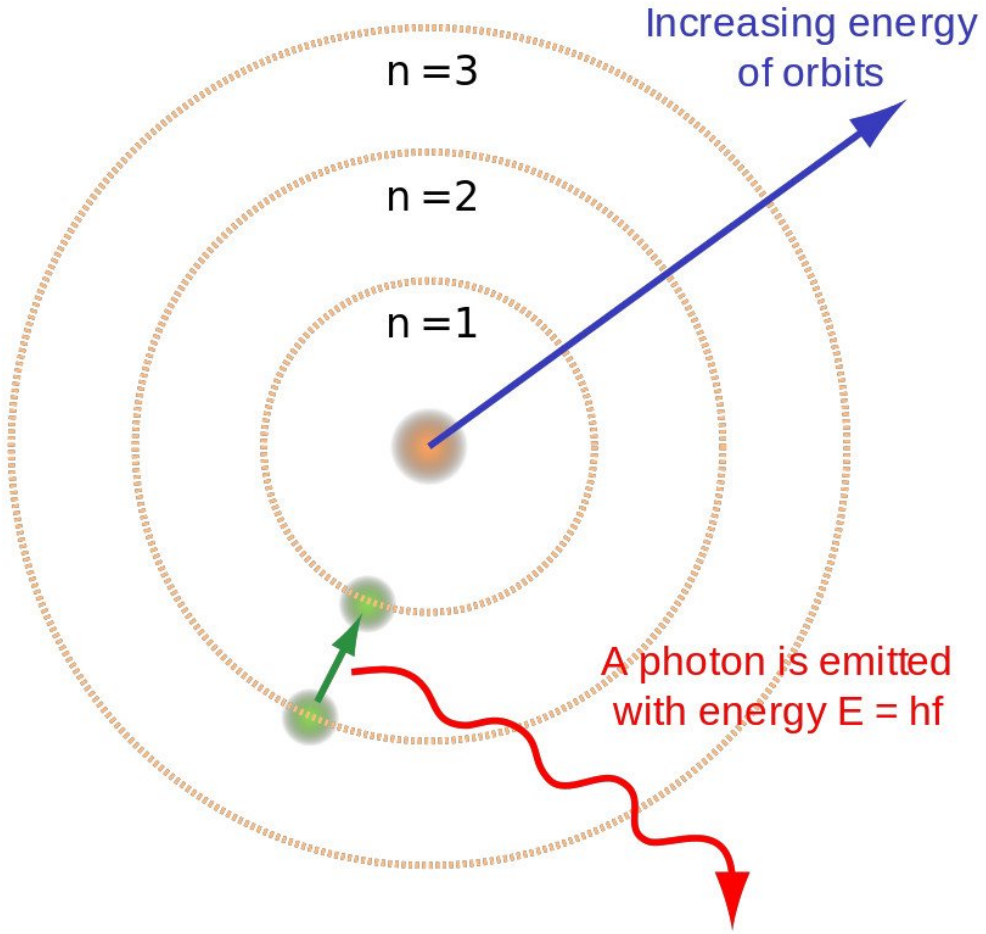
- 1909: Rutherford electrons move in the Coulomb field of the nucleus in orbits
- Limits:
  - Orbiting electron will accelerate
  - Accelerating particles emit radiation (classical EM)
  - Loss of energy in 10^{-10} s
  - Catastrophic collapse



Bohr's model (1)

- 1913: Niels Bohr starting from Rutherford's idea

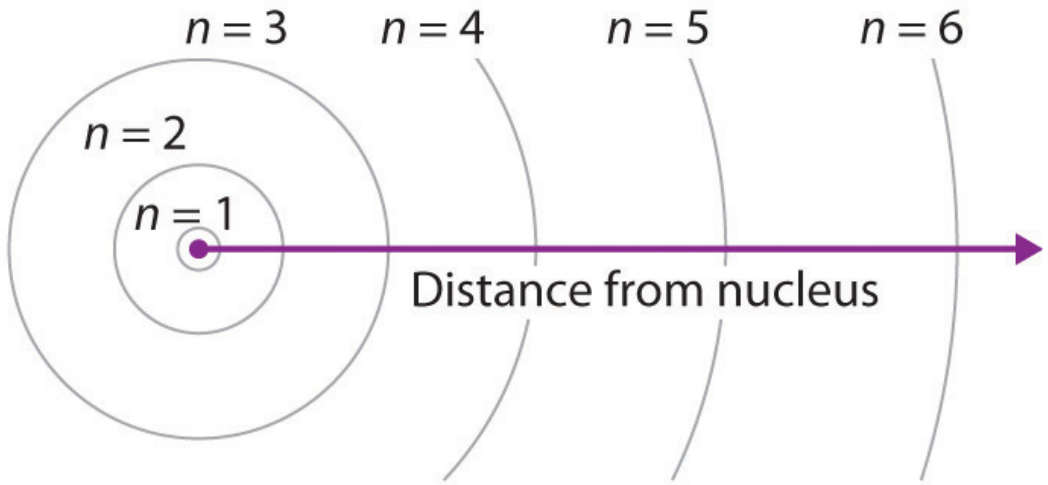
- Introduced:
  - Quantization of energy (Planck)
  - Atoms can only exist in certain energetic levels
  - Electrons in stable orbits do not emit radiation
  - Radiation is only emitted in a transition between different orbits

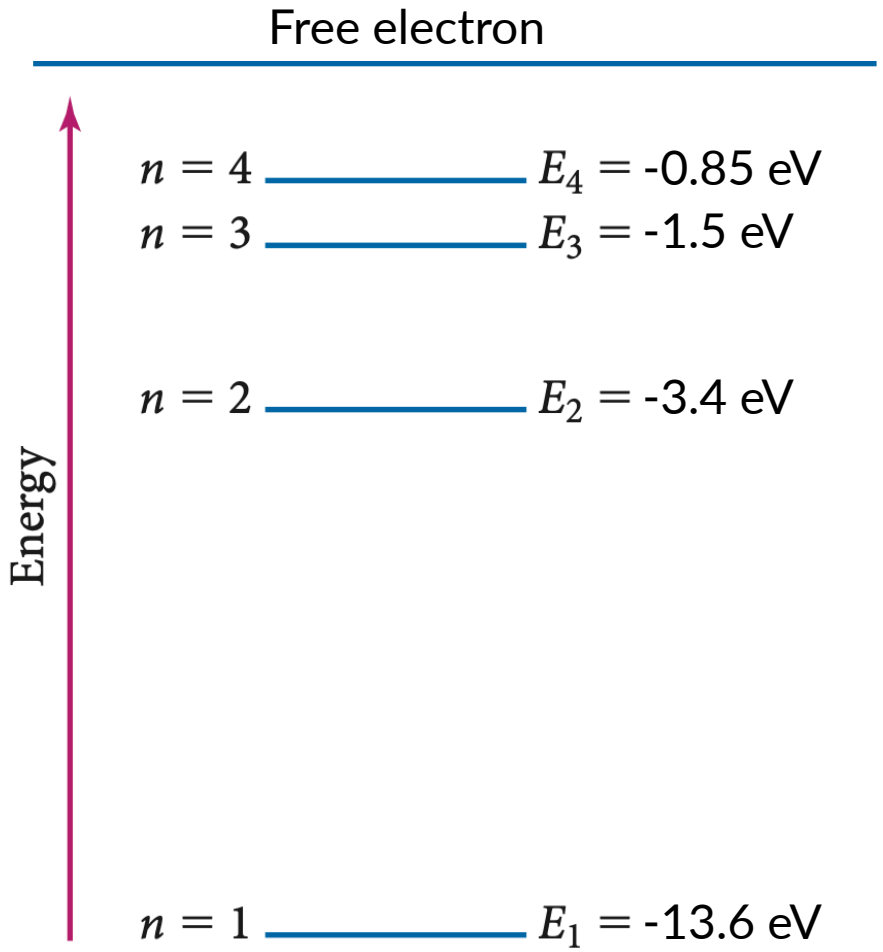


Bohr's model (2)

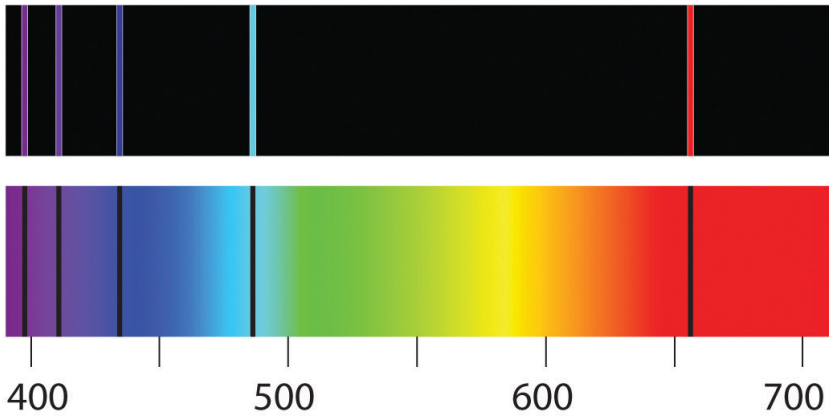
- Second postulate: The angular momentum of an electron moving in a circular orbit is also quantized
- He determined the allowed energy levels

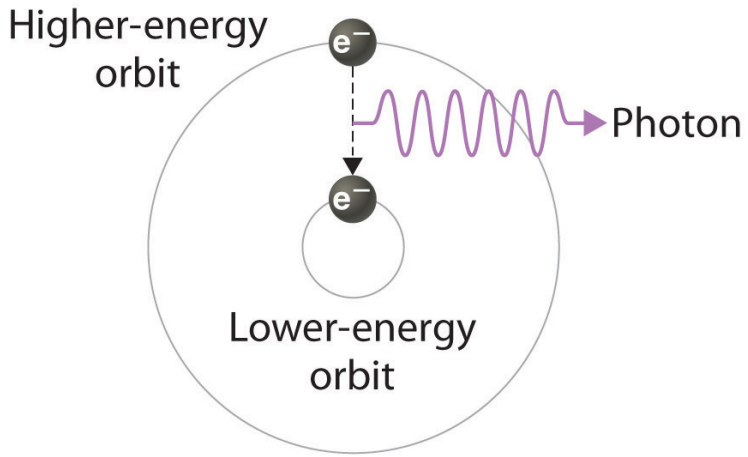
$$E_n = -13.6\frac{Z^2}{n^2}\text{eV}$$

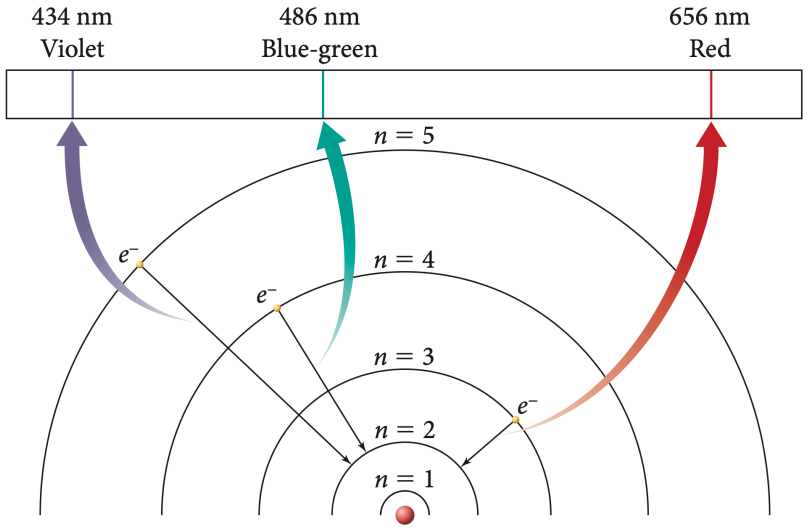


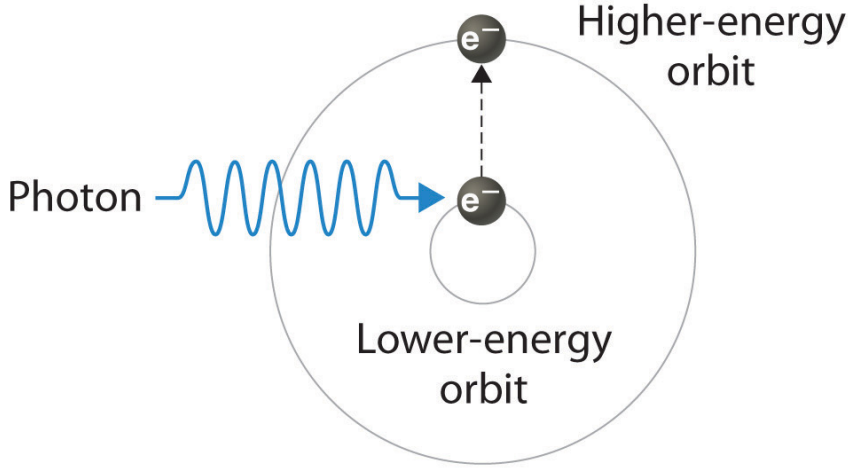


Bohr's model (H-spectrum)









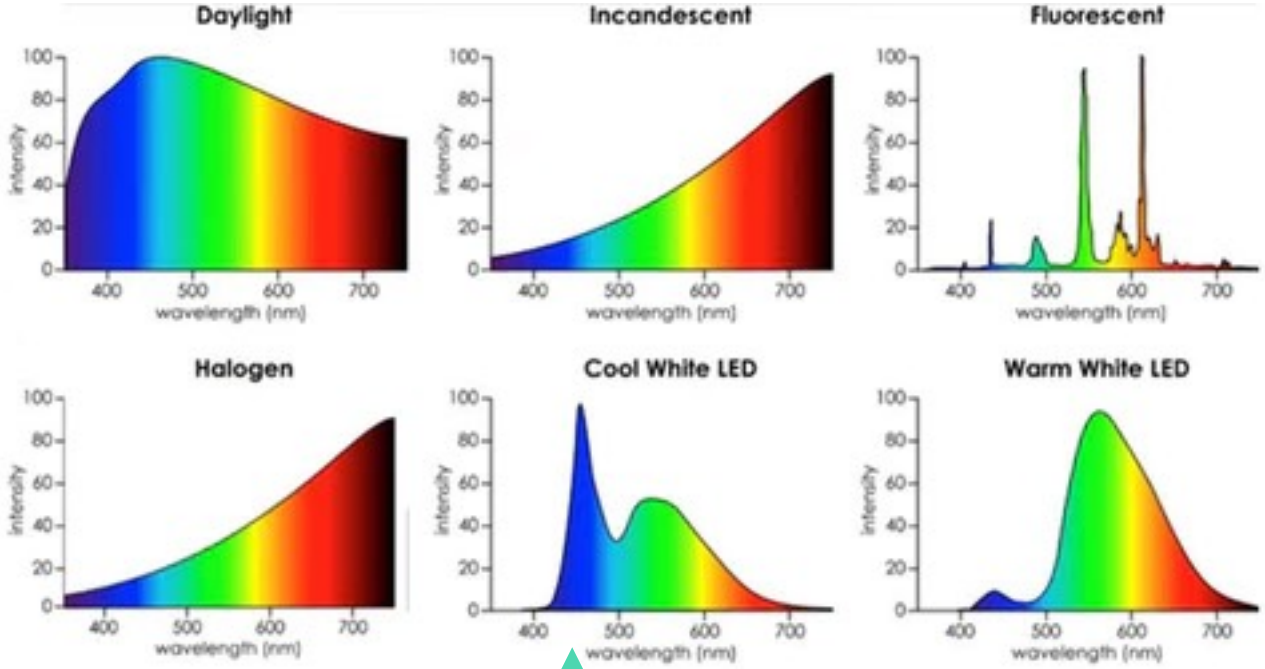
Bohr’s model limits

Ionization Energy: Energy needed to remove an electron from an atom

The free electron don’t feel the potential of the nucleus anymore.

Hydrogen EXAMPLE, Z=1

Bohr's model limits



Let's have a look at this 450 nm peak

Li^{2+} if you calculate

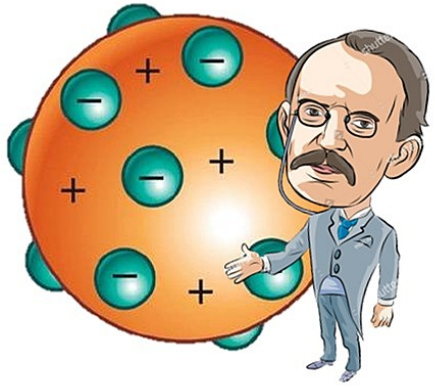
Bohr's model limits

- Limits:
  - Assumption of circular orbits
  - **Valid only for single-electron systems**
  - Only applied to the Balmer lines
  - Heisenberg: p and x cannot be known at the same time!

Bohr contributed to the development of quantum mechanics
His approach is known as "old quantum mechanics"

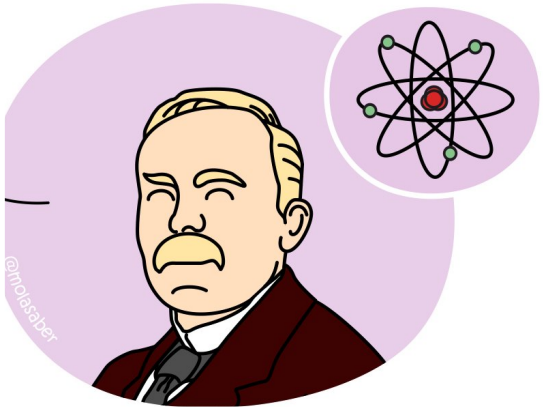
J.J. Thomson

NEW THEORY NEEDED



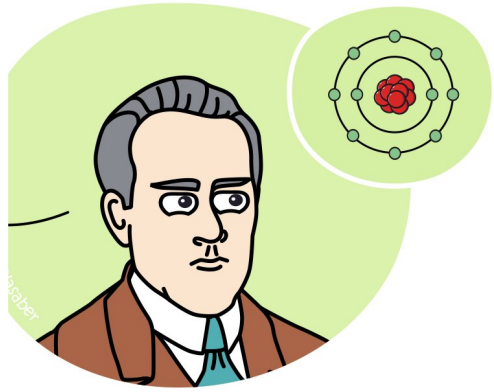
Protons&Electrons

Ernest Rutherford



Nucleus

Niels Bohr



Electron shells

The new quantum mechanics

Duality

- Every object in the universe has both particle-like and wave-like behavior

Quantum states are discrete

- Everything in quantum physics comes in discrete amounts

Probability

- The only thing quantum mechanics can predict is the probability
- This is given by the wave function square (Born interpretation)

Measurement determines reality

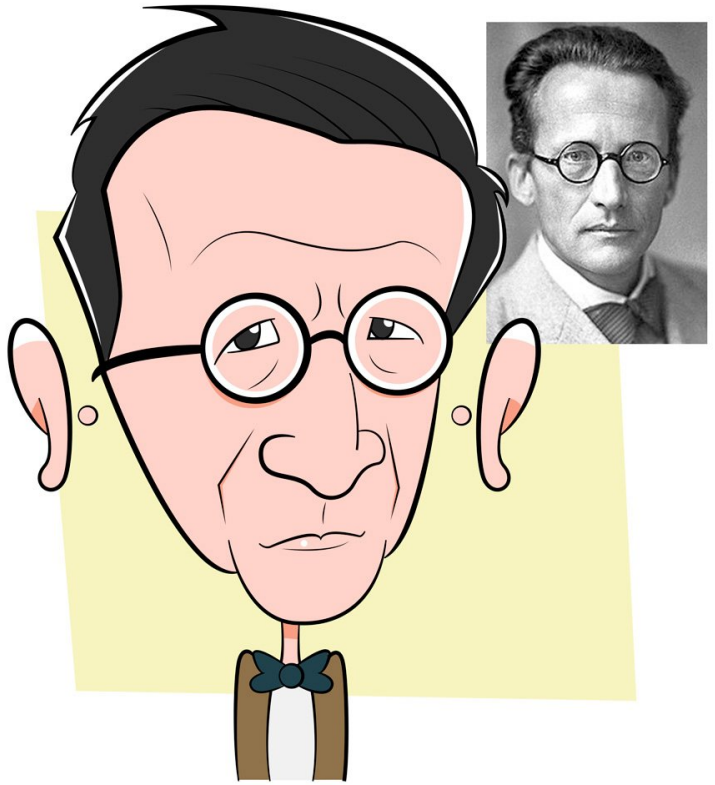
- State is indeterminate until measurement

Schrödinger equation

- De Broglie
    - Duality of light (particle-wave)

- Time independent (wave equation)

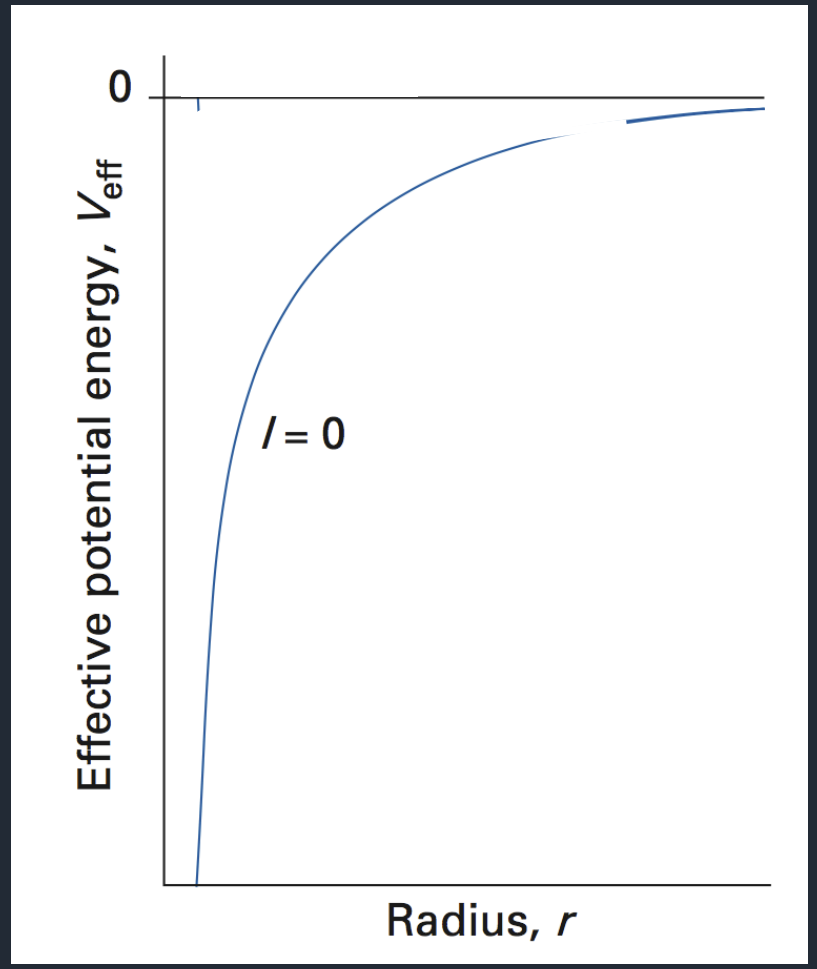
$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+V(x)\psi=E\psi$$



Solution of hydrogen atom

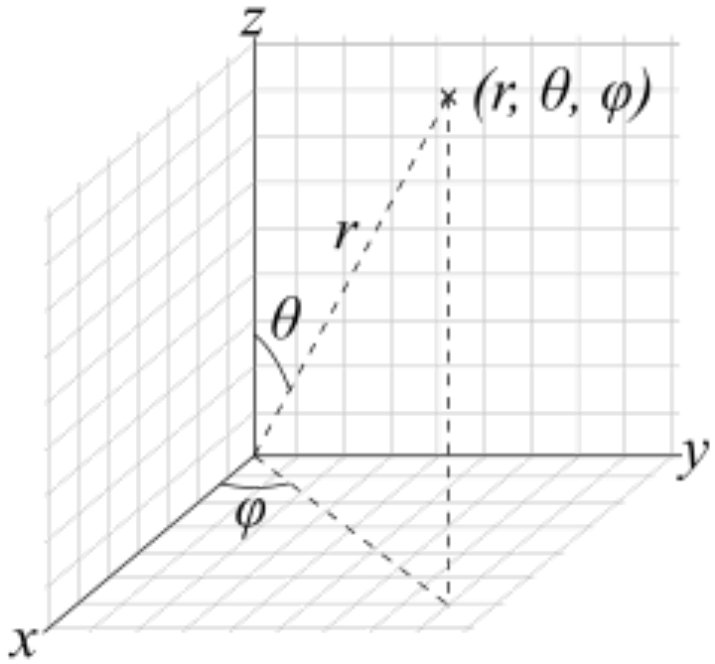
$$-\frac{Ze^2}{4\pi\varepsilon_0 r}$$

Attractive coulomb potential energy



Solution of hydrogen atom

- We solve S.E. in spherical coordinates
- Separation of variables



$$\Psi(r,\theta,\phi) = R(r)P(\theta)F(\phi)$$

Quantum numbers

- Three quantum numbers are used to describe the motion of the electron
- These determine the electron configuration of an atom
- And its most probable location

- n, l, m_l
- Designate shells, subshells, and orbitals (direction)

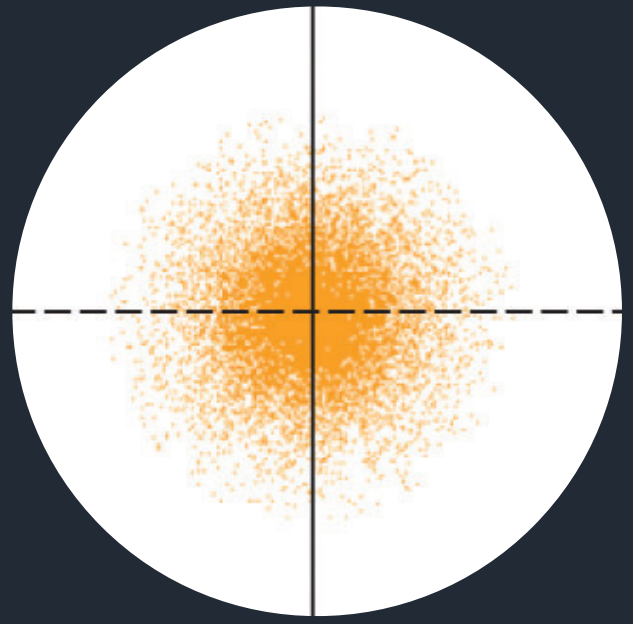
Quantum numbers (radial)

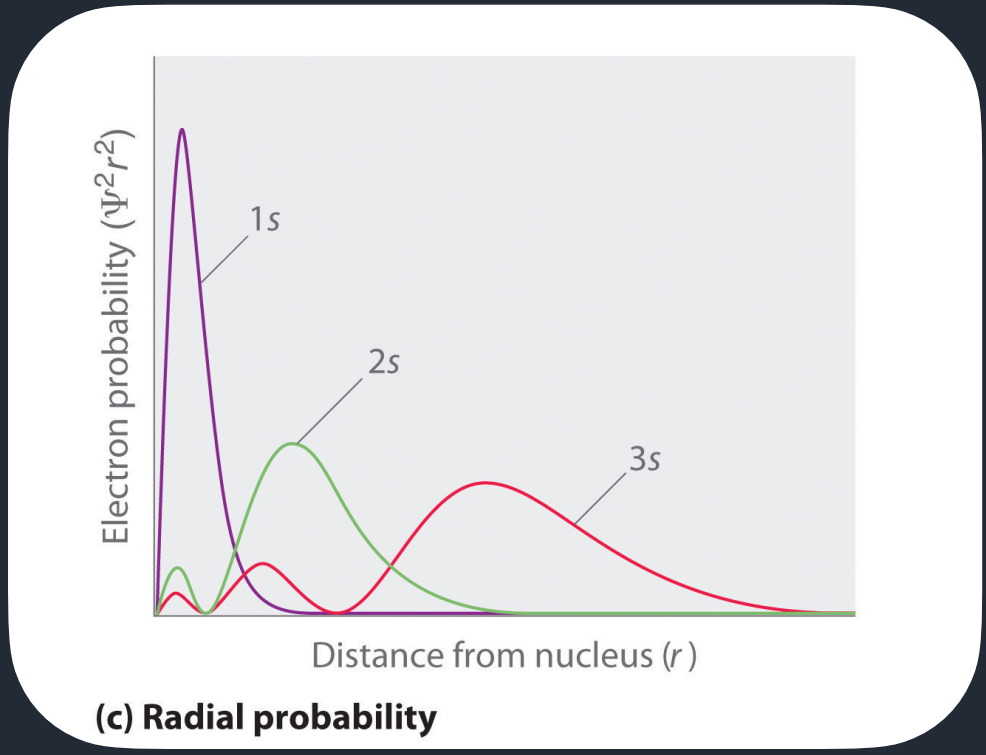
- n ⟶ principal quantum number
- Specifies the energy of the orbital and the shell
- Assume values n = 1, 2, 3…

$$E_n = -\left(\frac{Z^2 \mu e^4}{32\pi^2 \varepsilon_0^2 \hbar^2}\right)\frac{1}{n^2} \qquad n = 1, 2, \ldots$$

Solution of hydrogen atom (radial)

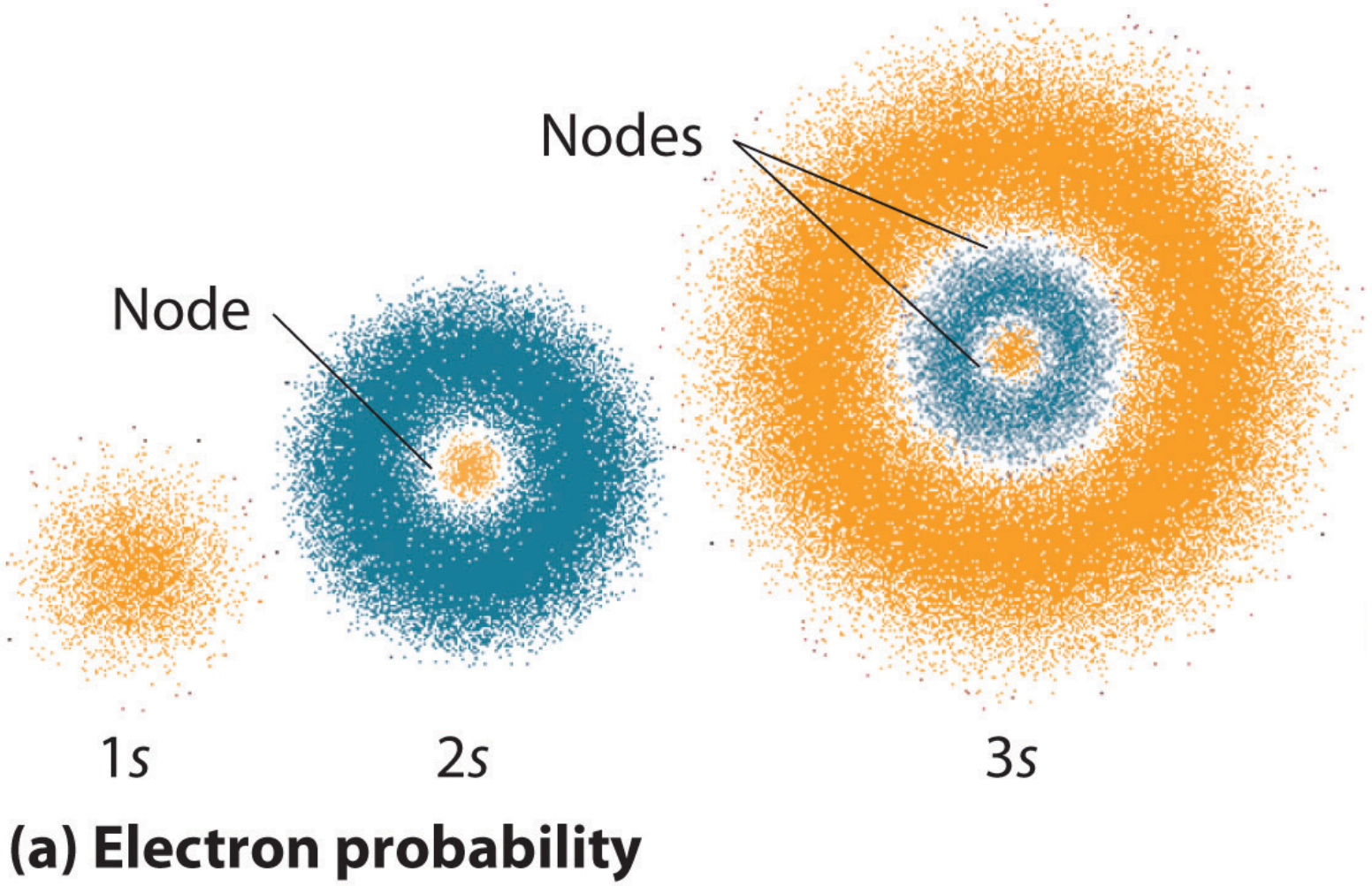
Solutions of the radial equation are associated Laguerre functions





Now we have a probability!
n -> principal quantum #

Solution of hydrogen atom (radial)



(a) Electron probability

Quantum numbers (angular part in theta)

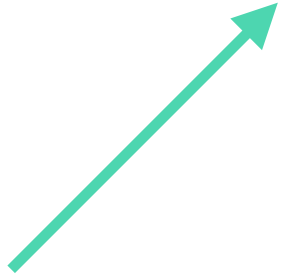
- l → orbital (angular momentum) quantum number
- Rate at which electrons circulate around the nucleus
- Defines the shape of the orbitals (NO ORBITS)
- Assume values l = 0, 1, 2, n-1
- Orbitals of a shell fall into l groups called “subshells”

0	1	2	3
s-orbital	p-orbital	d-orbital	f-orbital

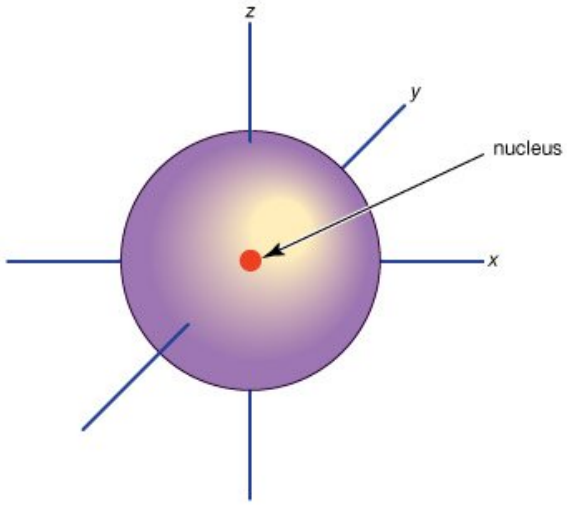
Solution of hydrogen atom (angular)

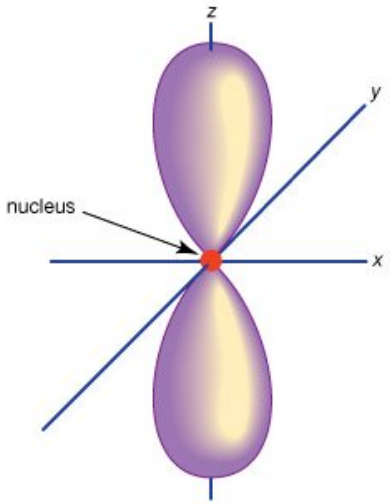
- Angular part (theta), another quantization!
- It describes the angular shape of the orbital.

0	1	2	3
s-orbital	**p**-orbital	**d**-orbital	**f**-orbital



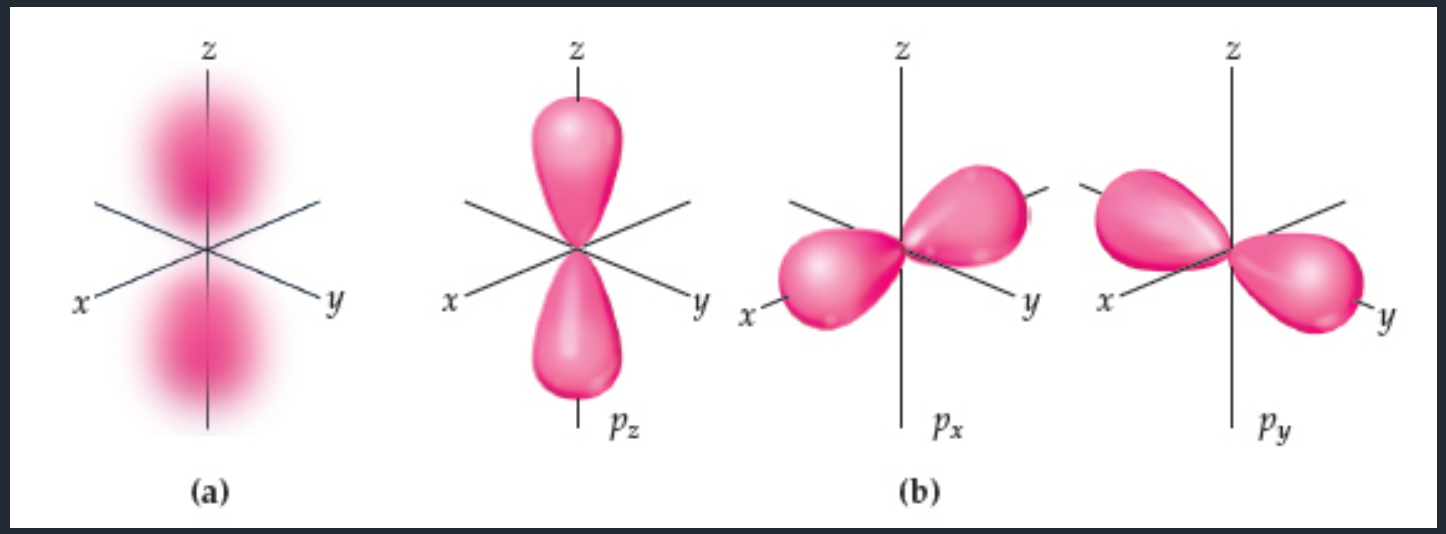
No angular dependence





Quantum numbers (angular in phi)

- m_l ⟶ magnetic quantum number
- Orientation of the angular momentum around the nucleus
- Different orbitals within a shell
- Assume values m_l = -l, l-1,+l
- 2l + 1 values of m_l for a given value of l



Hydrogen Electron Orbitals

Probability Density

$$\psi_{n\ell m}(r,\vartheta,\varphi) = \sqrt{\left(\frac{\rho}{r}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{-\rho/2} \rho^{\ell} L_{n-\ell-1}^{2\ell+1}(\rho) \cdot Y_{\ell}^{m}(\vartheta,\varphi)$$

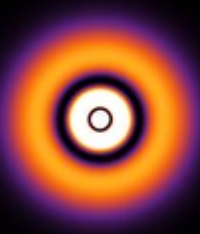
$$\rho = 2r/na_0$$

darksilverflame.deviantart.com


(2,0,0)


(2,1,0)


(2,1,1)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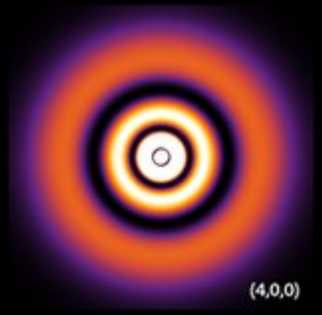
(3,2,1)


(3,2,2)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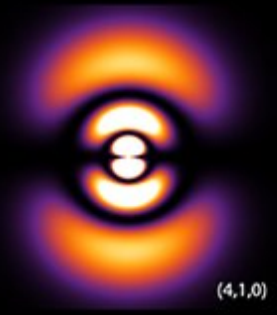
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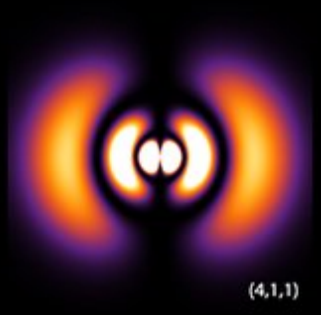
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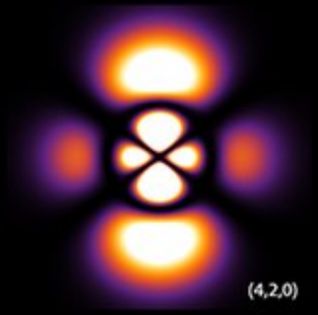
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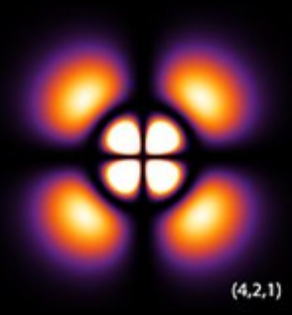
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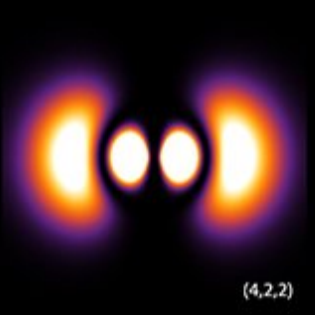
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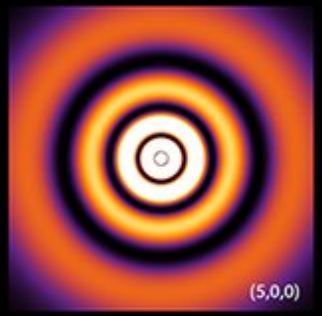
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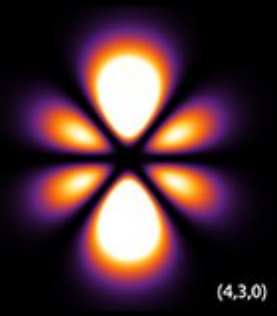
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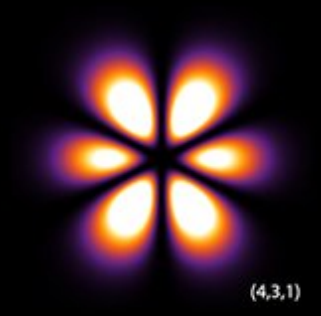
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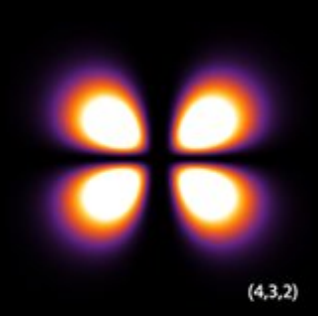
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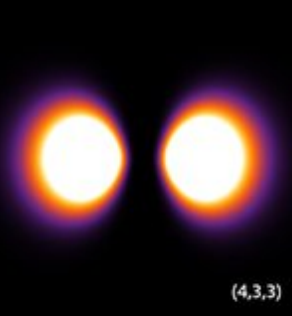
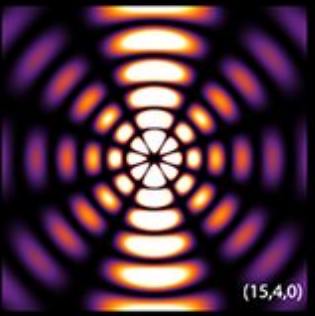

(4,3,3)


(15,4,0)

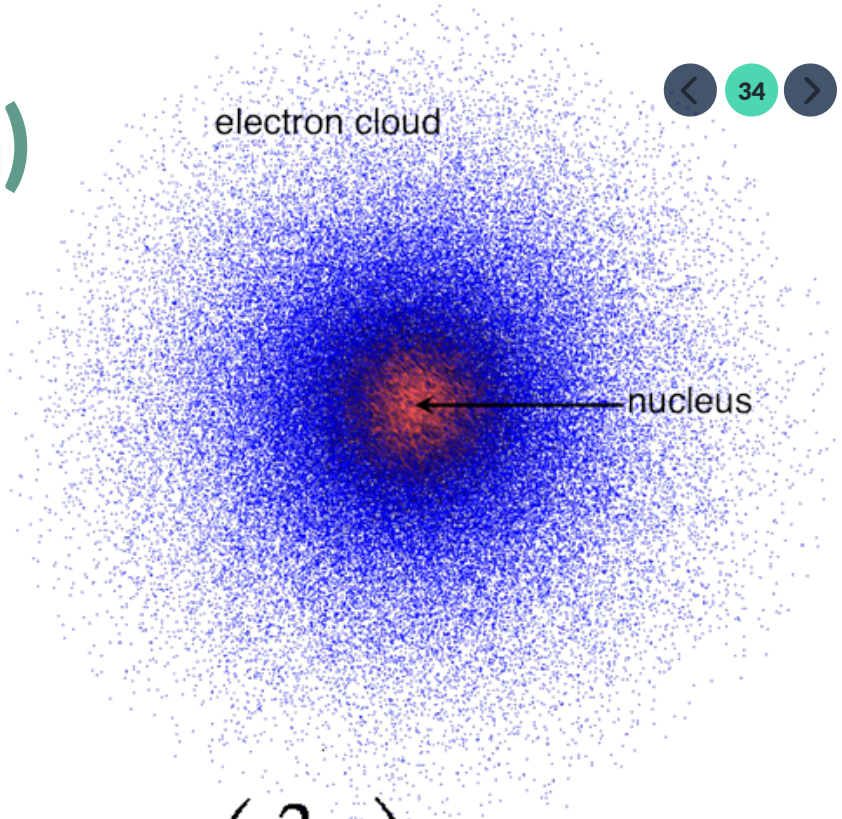
Atomic structure in a nutshell

- Electrons behave both as particles and waves (De Broglie)
- Quantisation of energy (Planck, Bohr)
- Wave function and energy of an atom (solution of S.E.)
- Wavefunction square represent a probability (Born)

How electrons are arranged in an atom?

- Location/Energy is determined by a set of three quantum numbers (?)

Hydrogen atom (single electron)



$$R_{nl}(r) = -\left\{\frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2}\left(\frac{2}{na_0}\right)^{l+3/2} r^l e^{-r/na_0} L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)$$

Radial

$$Y_l^m(\theta,\phi) = \left[\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)e^{im\phi}$$

Angular

H-alpha line (n=3-> n=2)

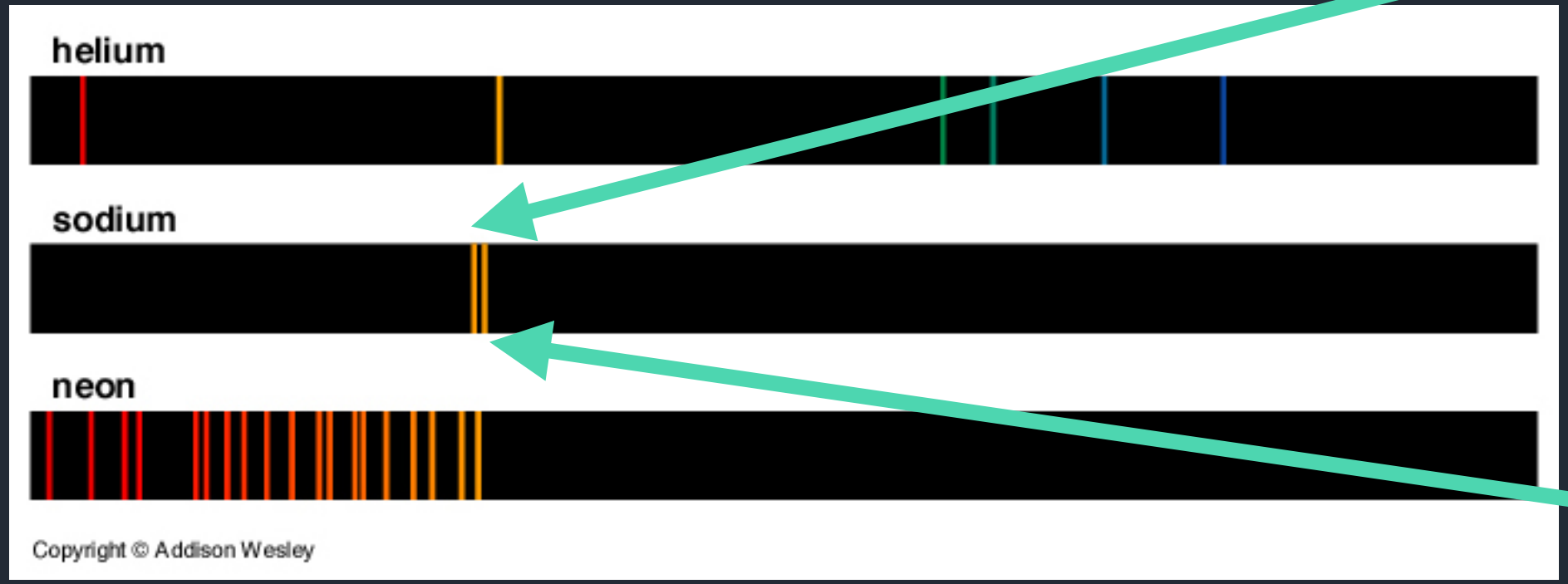
Balmer represents the strongest line

UV radiation ionize H which then recombines

Produce a cascade between the levels (electron jumps through levels)

Schrödinger equation could not explain a few phenomena

He predicted one line for Sodium @ 590 nm



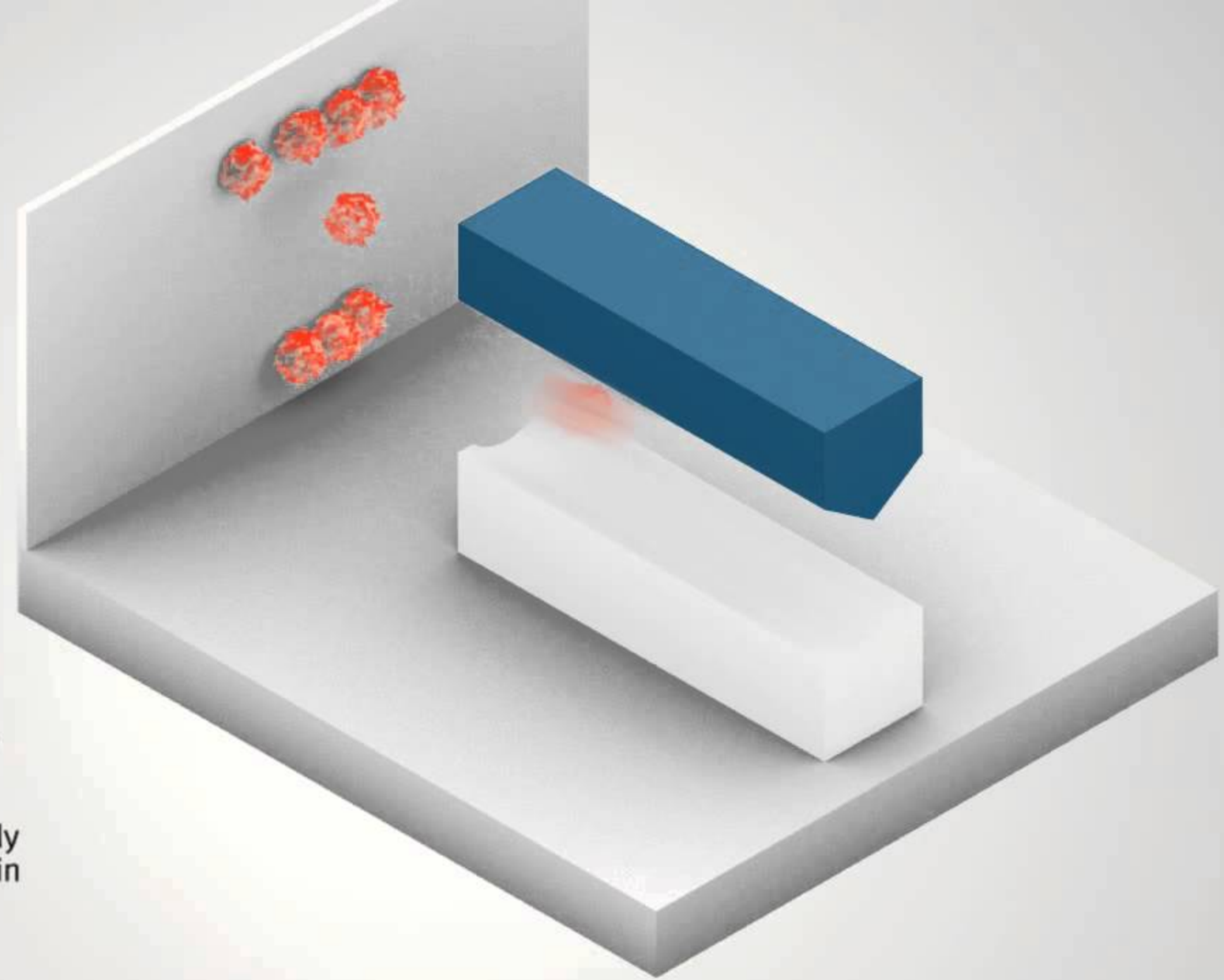
588.99 nm

589.59 nm

THE SPIN, A QUANTUM MAGNET

- classical magnets
- quantum spins

When quantum electrons are sent through this magnetic setup, they are deflected. But they reach the screen only upward or downward, never in the middle.

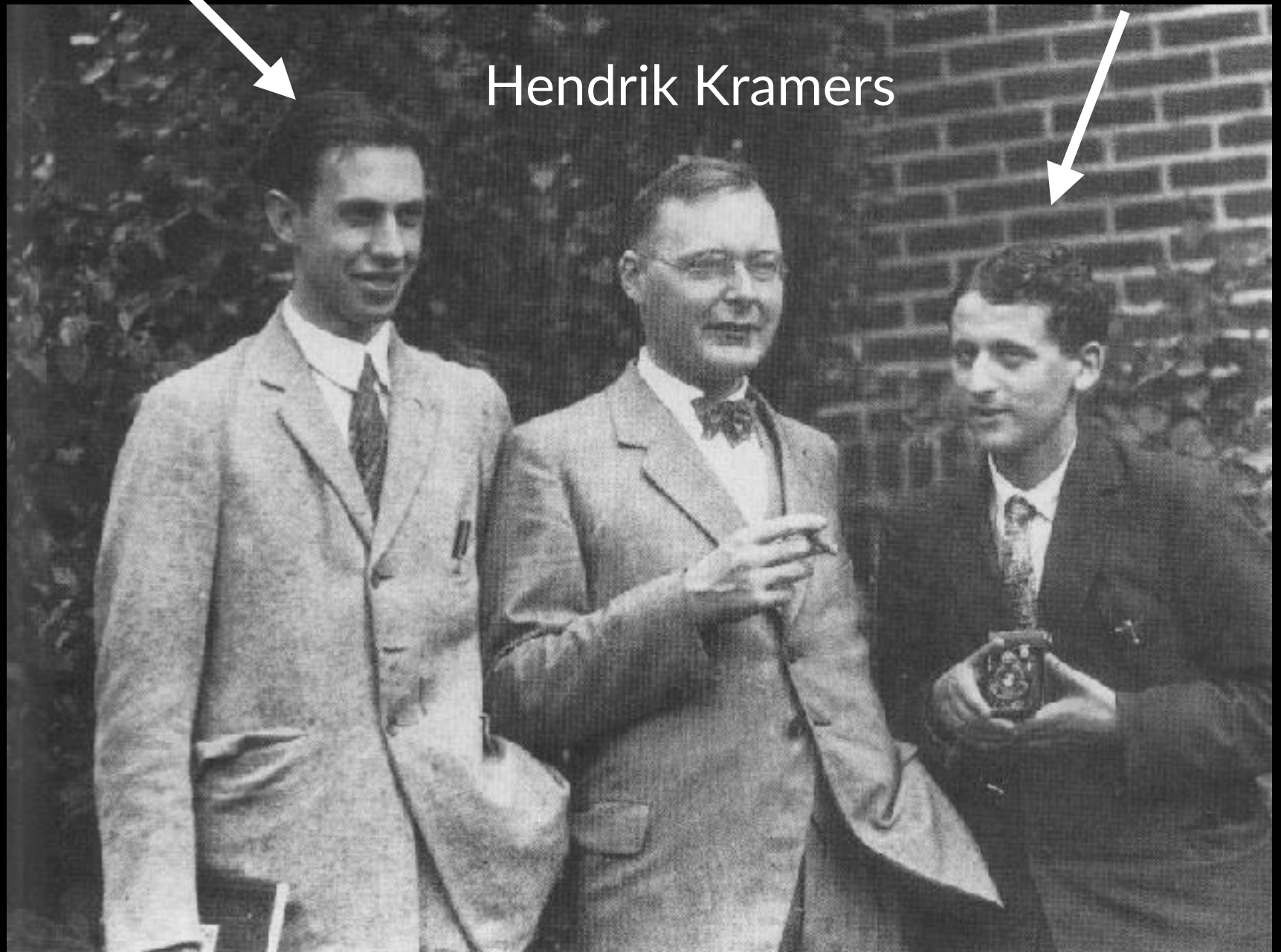


1925

George Uhlenbeck

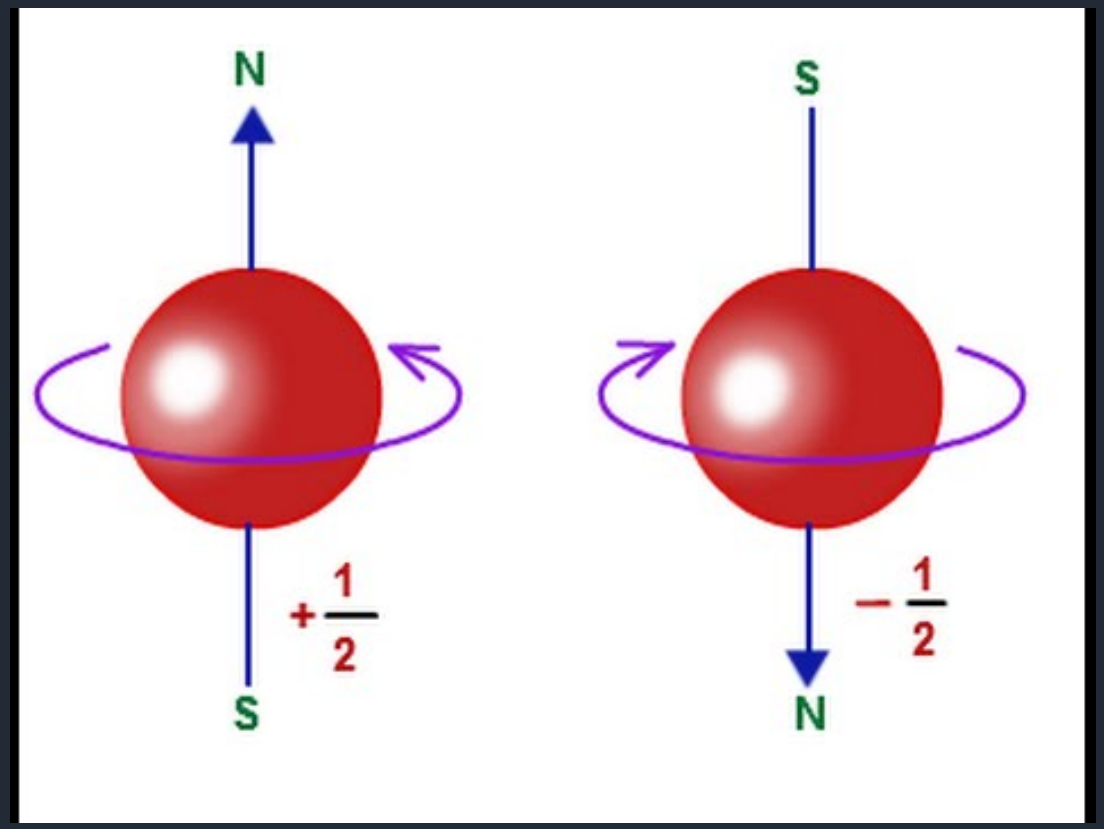
Hendrik Kramers

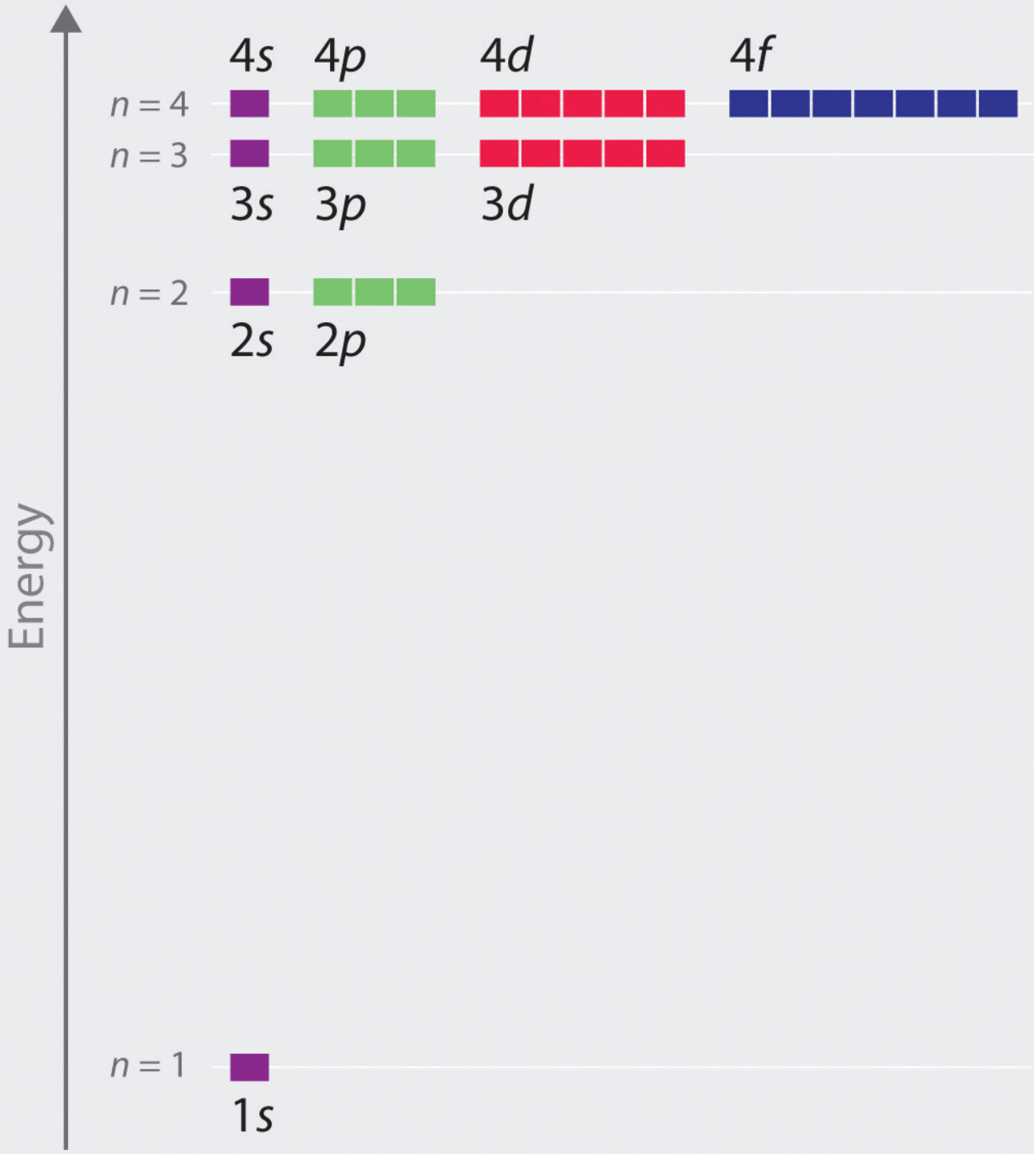
Samuel Goudsmith



The spin quantum number (4th)

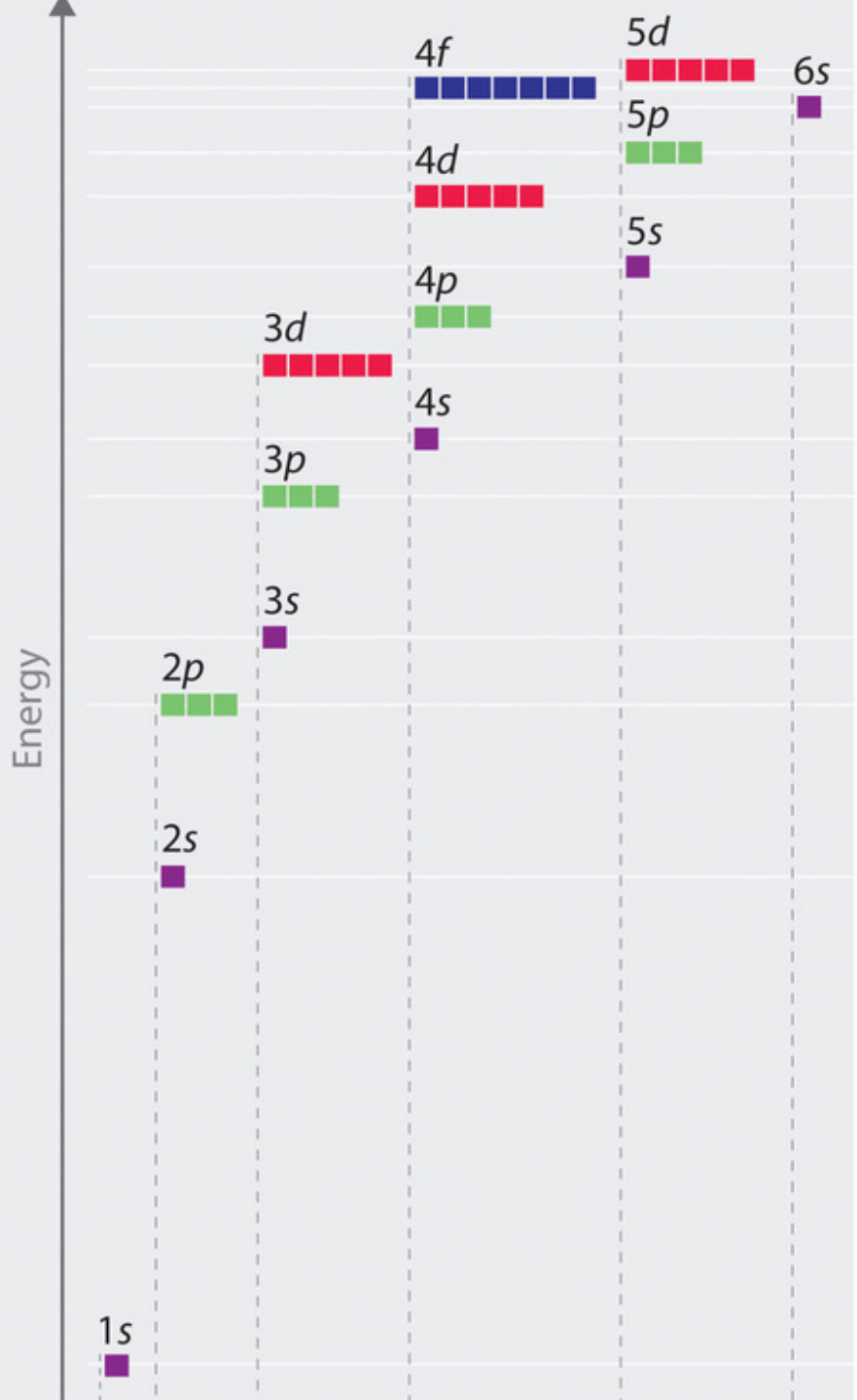
- s, m_s → spin magnetic quantum number (z-component)
- Intrinsic angular momentum of the electron
- Assume values m_s = -1/2, +1/2





BOHR MODEL Energy Levels
1 electron


Energy
4s
4p
4d
4f
n = 4
n = 3
3s
3p
3d
n = 2
2s
2p
n = 1
1s


Energy
4f
5d
6s
5p
4d
5s
4p
3d
4s
3p
3s
2p
2s
1s

BASICS TEXTBOOKS

Physics of Atoms and Molecules (Bransden&Joachain)

Physical Chemistry (McQuarrie & Simon)

Molecular Quantum Mechanics (Atkins & Friedman)