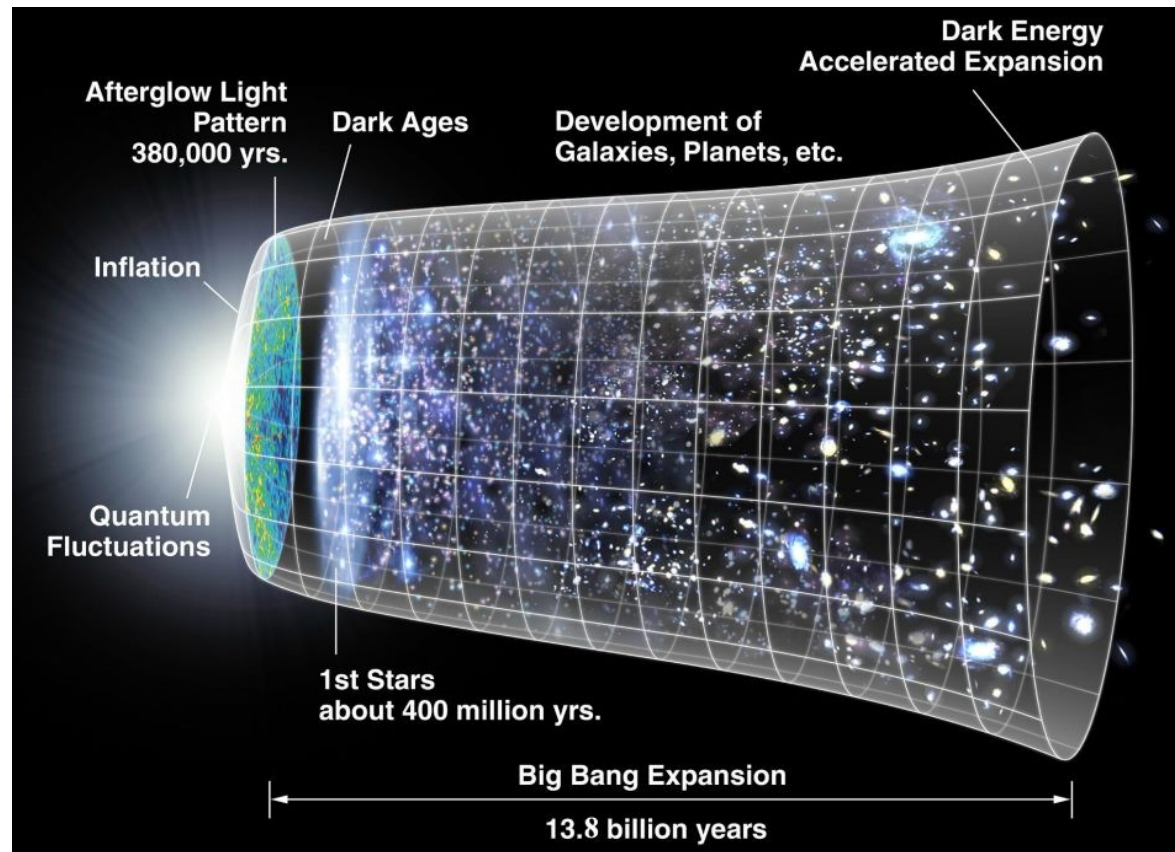
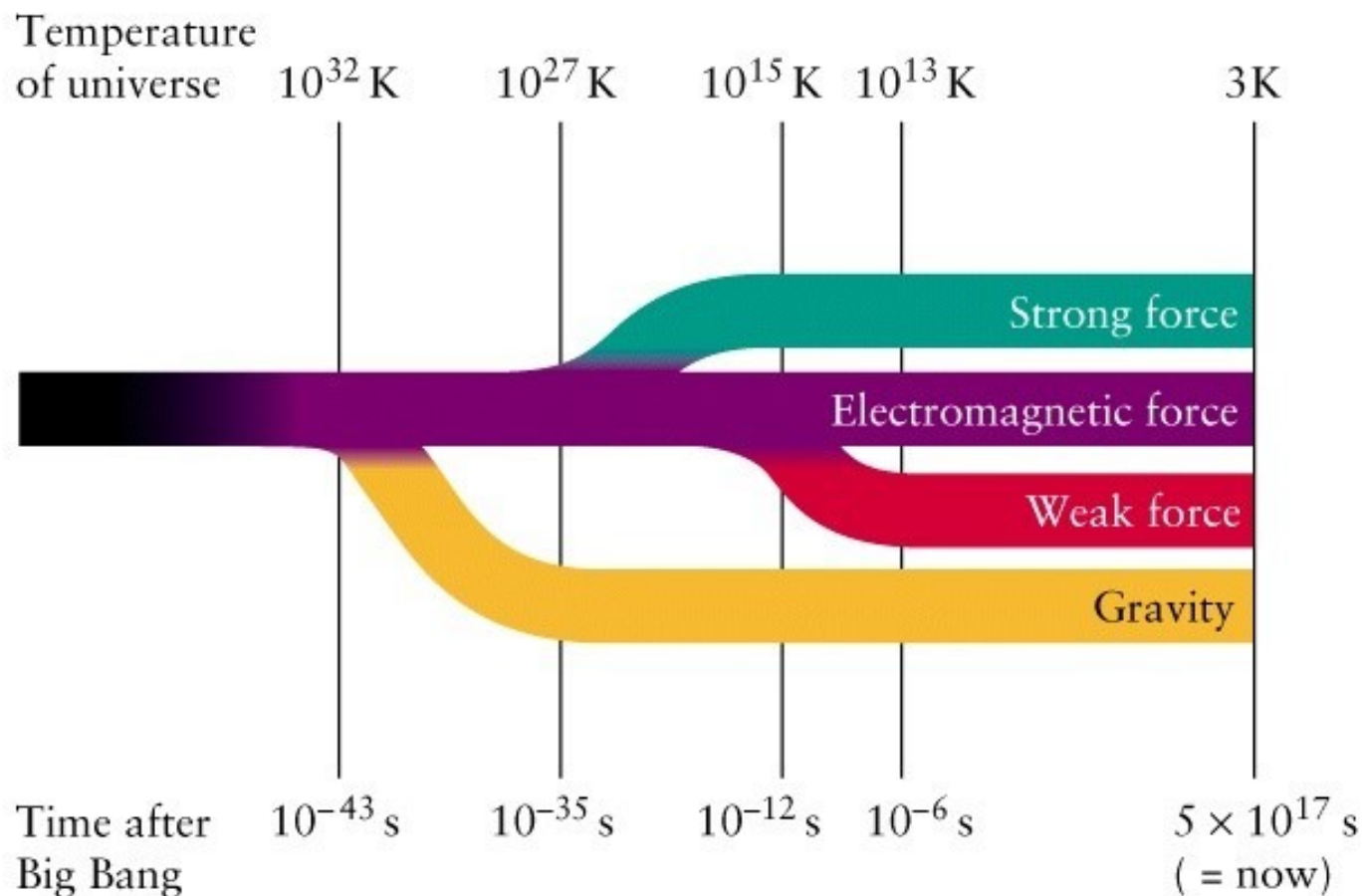


# Atoms and Solids



# Fundamental interactions



# Fundamental interactions

interaction	range	relative strength
1.Gravity	long	1
2.Weak nuclear	short	$10^{25}$
3.Electromagnetic	long	$10^{36}$
4.Strong nuclear	short	$10^{38}$

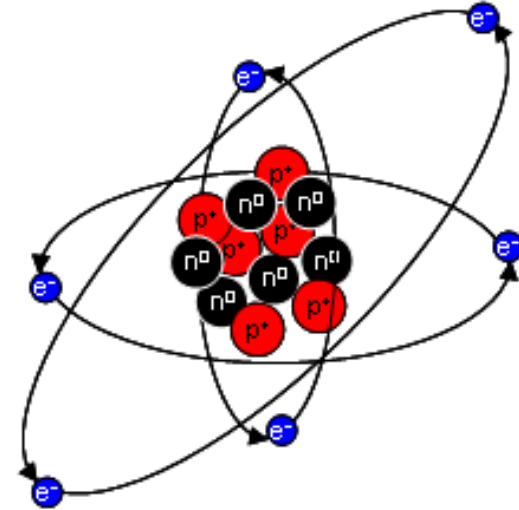
# Fundamental interactions

- |                    |                                        |
|--------------------|----------------------------------------|
| 1. Gravity         | acts on all objects                    |
| 2. Weak nuclear    | causes unstable atomic nuclei to decay |
| 3. Electromagnetic | between charged objects                |
| 4. Strong nuclear  | binds protons and neutrons together    |

- Smallest charge found free in nature:  $e=1.6 \times 10^{-19} \text{ C}$
- All charges must be  $Q = \pm Ne$  (N integer)  $\rightarrow$  quantization of the charge
- The total charge of the Universe is unchanged  $\rightarrow$  conservation of the charge

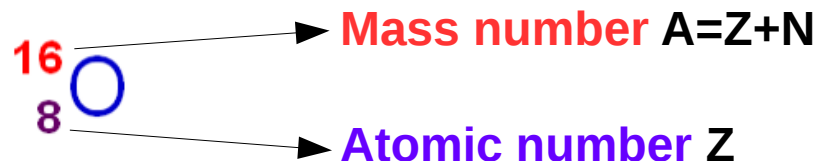
# Subatomic particles

	mass (kg)	Electric charge (C)
<b>proton</b>	$1.67 \times 10^{-27}$	$1.602 \times 10^{-19}$
<b>neutron</b>	$1.675 \times 10^{-27}$	0
<b>electron</b>	$9.11 \times 10^{-31}$	$- 1.602 \times 10^{-19}$



- Atoms are normally in a neutral state. Number of protons **Z** is fixed → defines the element
- Number of neutrons **N** can vary → isotopes
- When electrons are removed the atom is ionised
- Elements are symbolised with their **mass number** and **atomic number**

Example:



# Foundation of atomic theory

Non continuity of matter proposed by

- Anaxagoras (c. 510-428 BC)
- Empedocles (c. 490-430 BC)
- Leucippus (~450 BC)
- **Democritus** (460-370 BC)



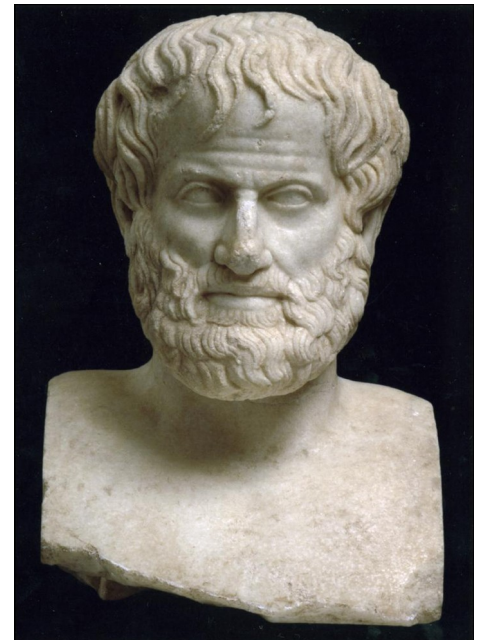
"ἔτεῃ δὲ ἄτομα καὶ κενόν"

"There are only atoms and void"

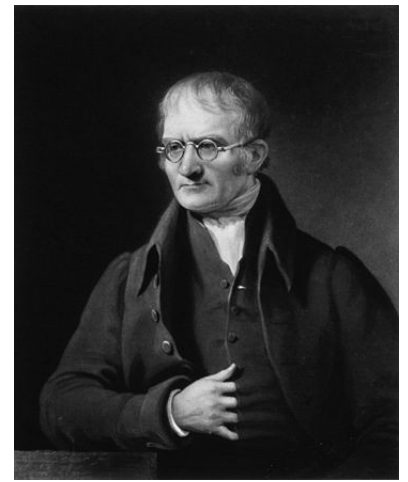
# Foundation of atomic theory

But **Aristotle** (384–322 BC) asserted that matter is continuous and consists of the 4 classical elements + aether:

- Earth → solids
- Air → gas
- Water → liquids
- Fire → plasma, heat
- Aether → heavenly bodies

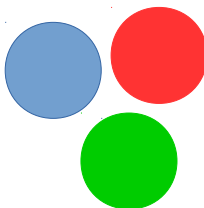
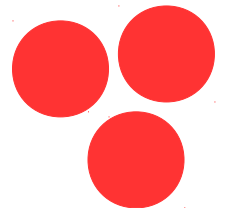
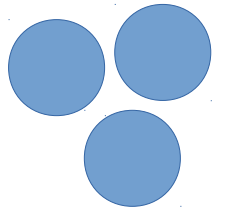


# Dalton model



John Dalton (1808) assumed that all elements are made of atoms.

- Atoms are indivisible particles
- For a given element all atoms are identical
- For different elements atoms are different
- Compounds are formed by combining atoms



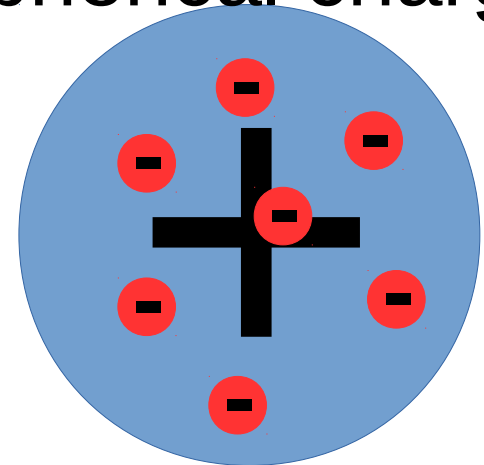




# J. J. Thomson's atomic model

Nobel Prize in Physics 1906  
Prize share: 1/1

- Atom is divisible! Spherical symmetry  $R \sim 10^{-10}$  m
- Electrons in fixed positions with negative charge and small mass (plum pudding model)
- Electrically neutral  $\rightarrow$  positive spherical charge

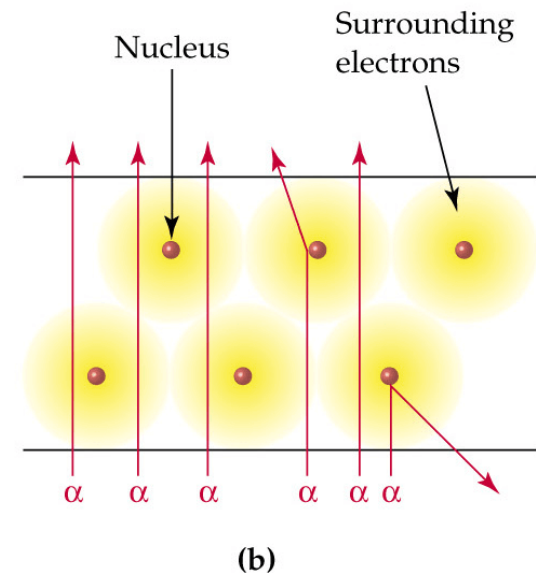
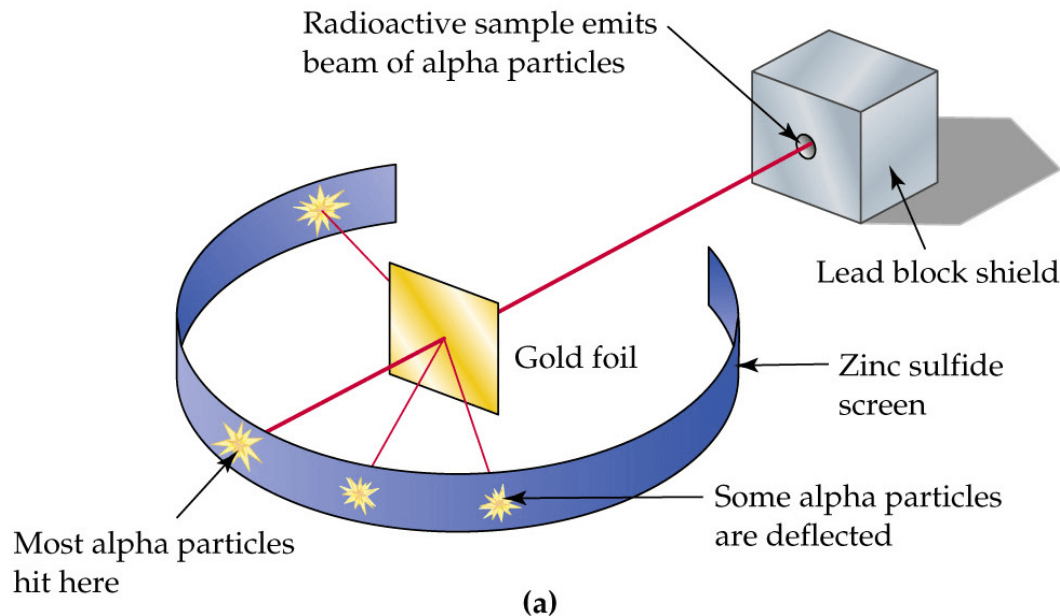


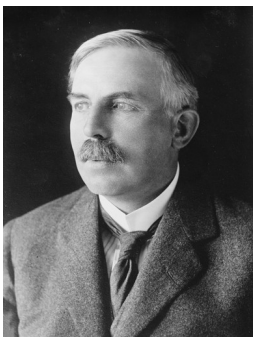
- $N_e = (\text{atomic weight})/2$
- Light emission  $\rightarrow$  oscillation of e around their equilibrium position

# J. J. Thomson's atomic model

Failure: could not explain the scattering of  $\alpha$ -particles in gold foil

- Rutherford's experiment (by Geiger and Marsden)**

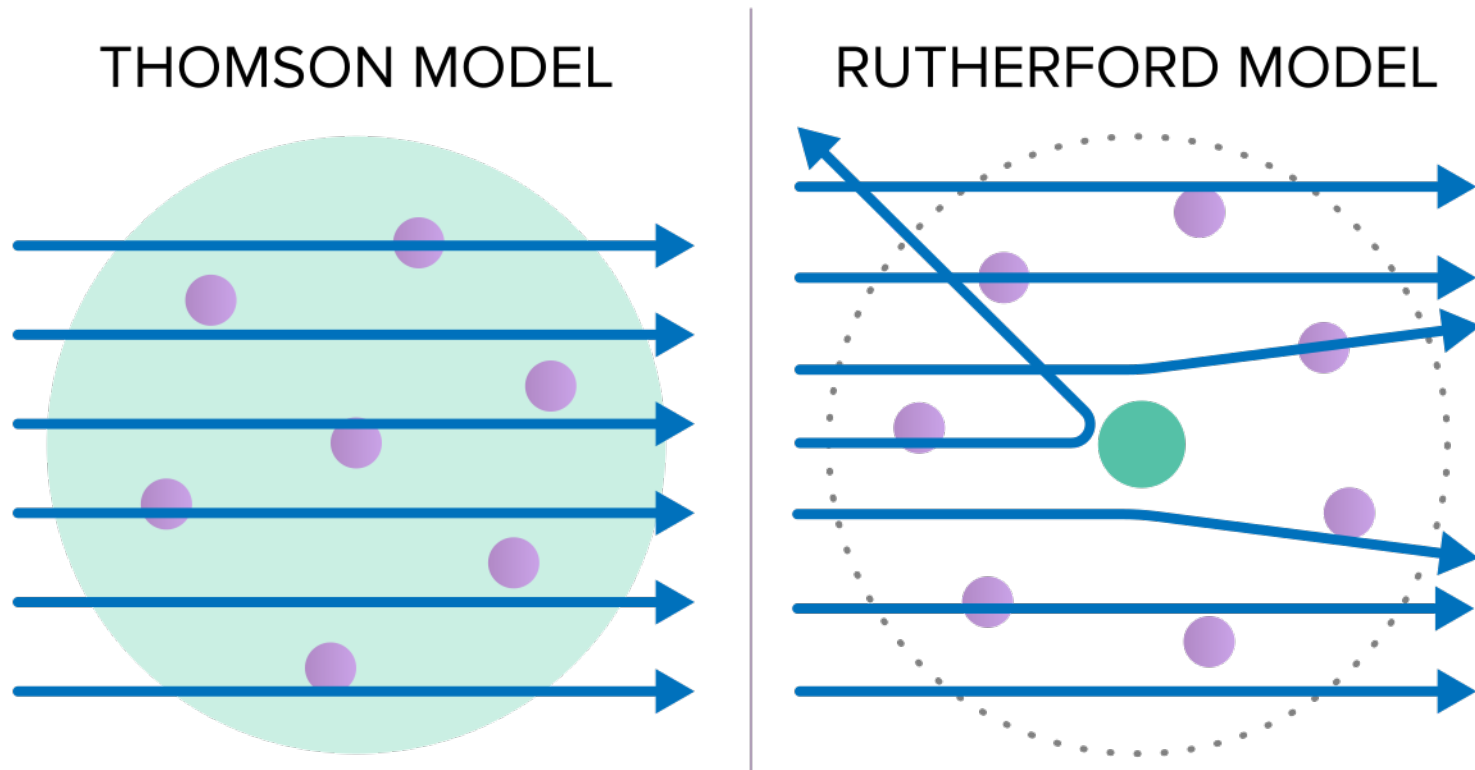




# Rutherford's atomic model

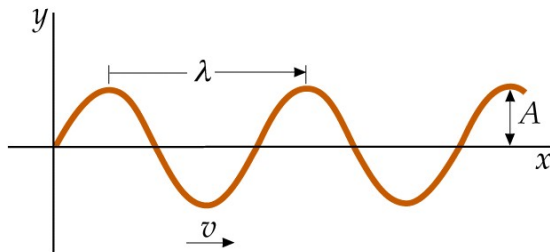
Nobel Prize in Chemistry 1908  
Prize share: 1/1

- A positive nucleus with e orbiting in circle
- Scattering of  $\alpha$ -particles from the gold (Au) nucleus is due to Coulomb force ( $F = kZ_1Z_2e^2/r^2$ )

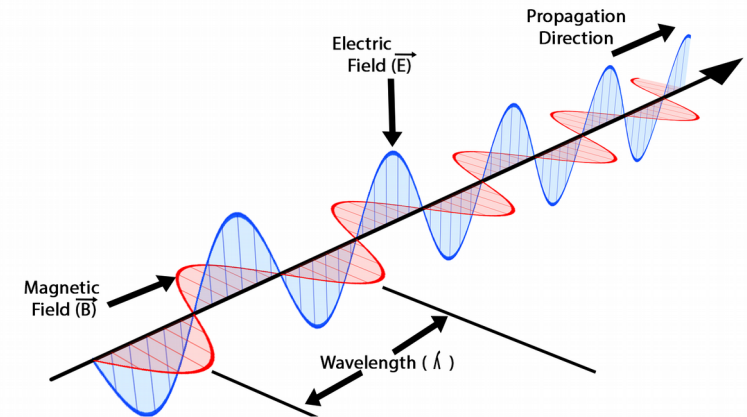


# Electromagnetic waves

- **Maxwell** unified existing laws of electricity and magnetism
- Light is an electromagnetic wave (coupled oscillating electric and magnetic field) that travels with speed  $c=2.998 \times 10^8$  m/s in vacuum



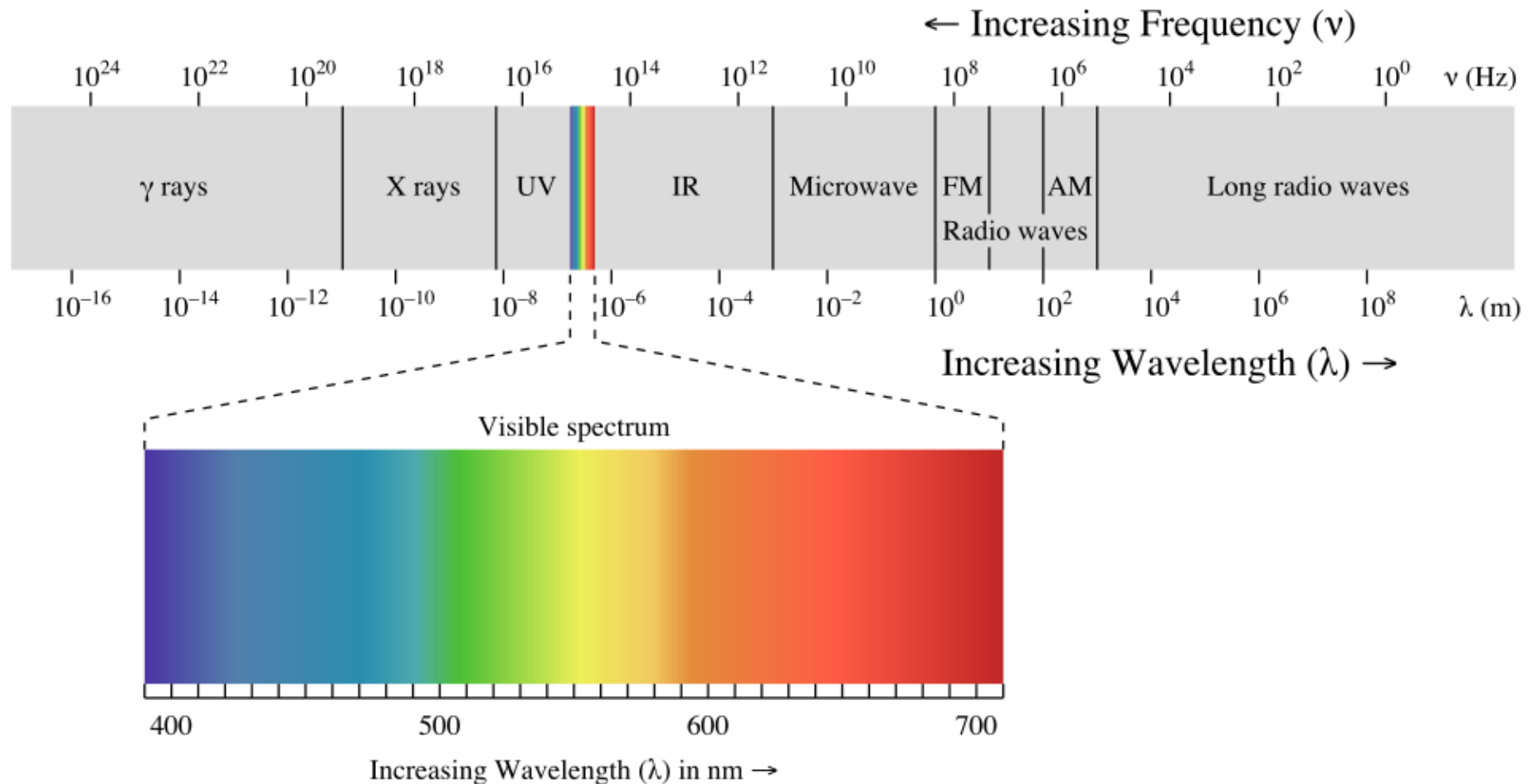
Electromagnetic Wave



## Wave properties:

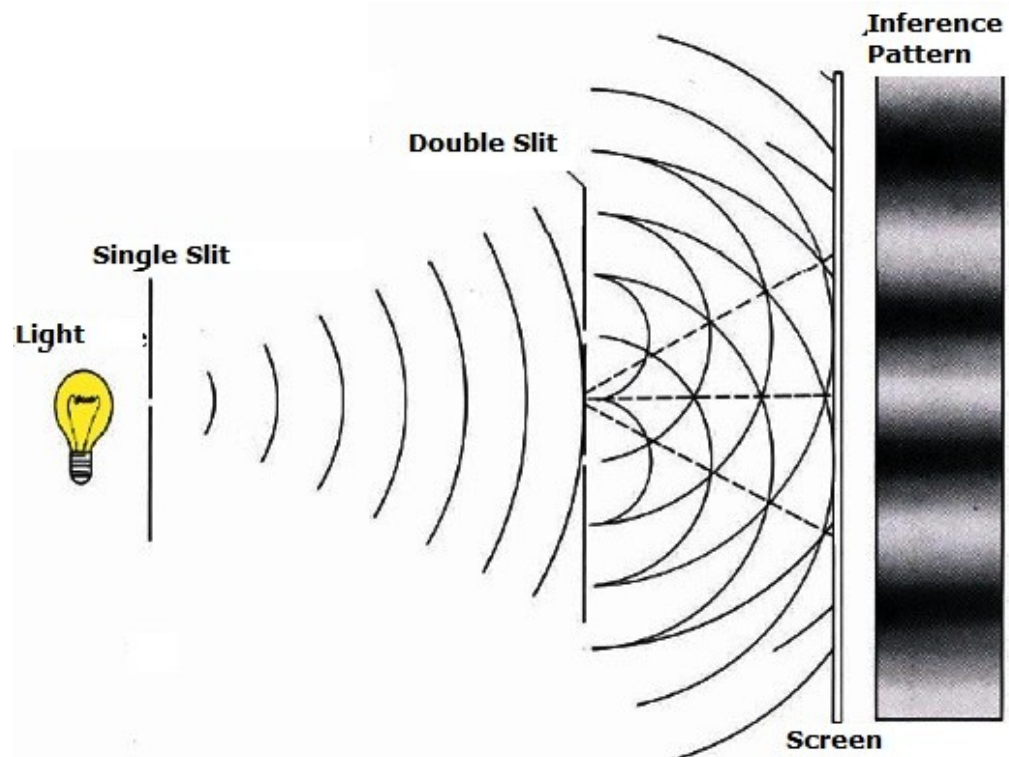
- **Amplitude  $A$ :** maximum displacement
- **Period  $T$ :** Time to make a complete oscillation ( $T=1/\nu$ )
- **Wavelength  $\lambda$ :** distance between two consecutive maxima
- **Energy:**  $E \propto A^2$
- **constant speed:**  $c=\lambda\nu$

# Electromagnetic spectrum



# Wave nature of light

- **Thomas Young** demonstrated the wave nature of light with the double slit experiment (1801). Maxwell later developed the electromagnetic theory (1865).



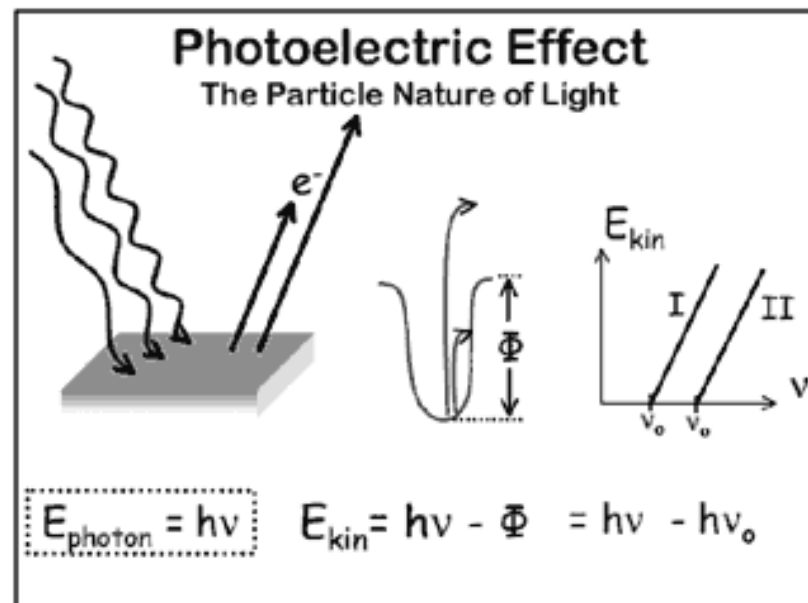
# Particle nature of light

- **Albert Einstein** explained the photoelectric effect (1905) assuming light is a particle, a photon of energy  $E=h\nu$

Planck's constant  $h=6.626 \times 10^{-34} \text{ J s}$



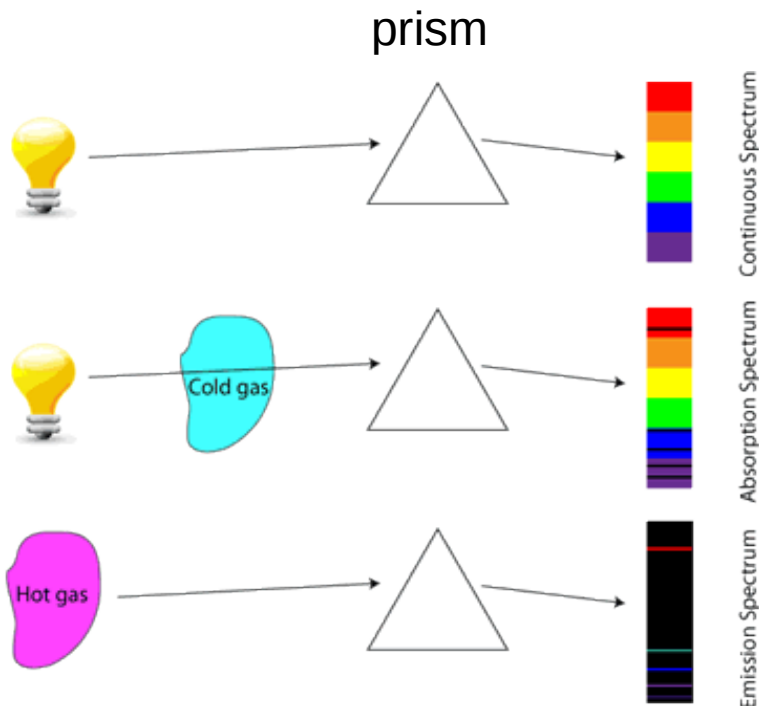
Nobel Prize in Physics 1921  
Prize share: 1/1



UC Berkeley's Digital Chem1A

# Atomic spectra

- Kirchhoff and Bunsen discovered that every atom has a characteristic spectrum.
- Balmer suggested an empirical formula for the wavelength



$$\frac{1}{\lambda} = R_H \left( \frac{1}{2^2} - \frac{1}{n^2} \right) \quad n = 3, 4, 5, \dots$$

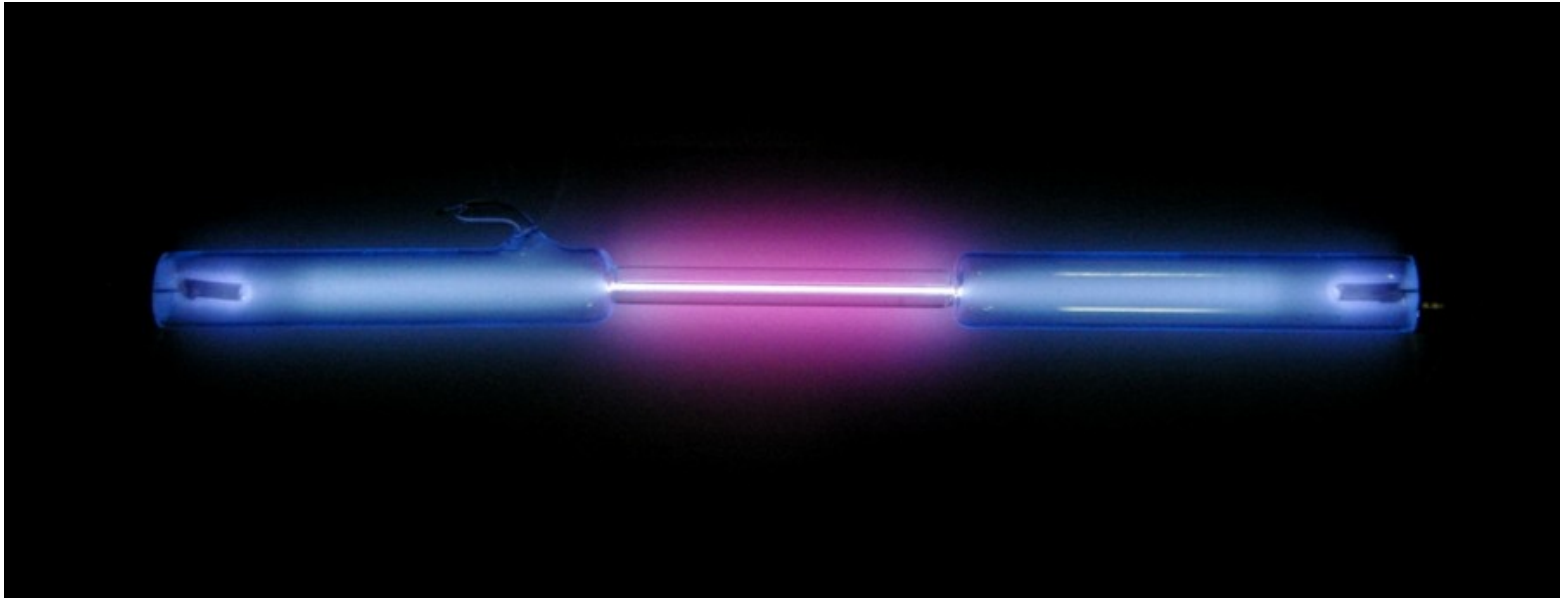
$R_H$ : Rydberg constant

$$R_H = 1.0973731568527 \times 10^7 \text{ m}^{-1}$$



# Failures of Rutherford's model

- Could not explain the atomic spectra of gases



Hydrogen emission spectrum

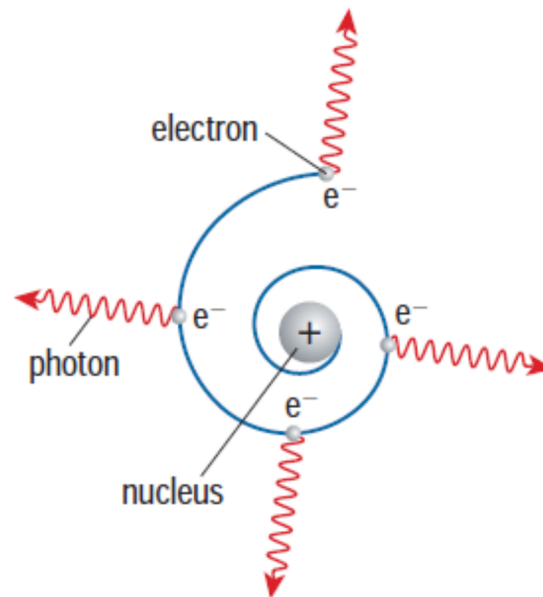


Hydrogen absorption spectrum



# Failures of Rutherford's model

- According to Maxwell's theory an e accelerating around the nucleus would emit electromagnetic radiation and loose energy  $\rightarrow$  collapse of the atom in  $\sim 10^{-12}$  s





# Bohr's model

Nobel Prize in Physics 1922  
Prize share: 1/1

- **Niels Bohr** developed a semiclassical model (1913) to explain the emission spectra of the H atom.
- An electron of charge  $-e$  orbiting the nucleus

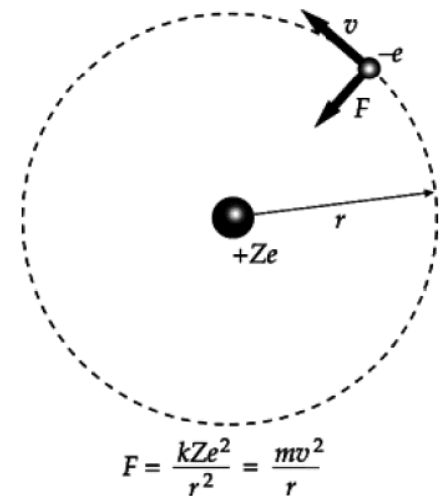
potential energy

$$U = \frac{kq_1q_2}{r} = \frac{k(Ze)(-e)}{r} = -\frac{kZe^2}{r}$$

$$F = \frac{kZe^2}{r^2} = m \frac{v^2}{r}$$

$$K = \frac{1}{2}mv^2 = \frac{1}{2} \frac{kZe^2}{r}$$

$$E = K + U = -\frac{1}{2} \frac{kZe^2}{r}$$



# Bohr's model

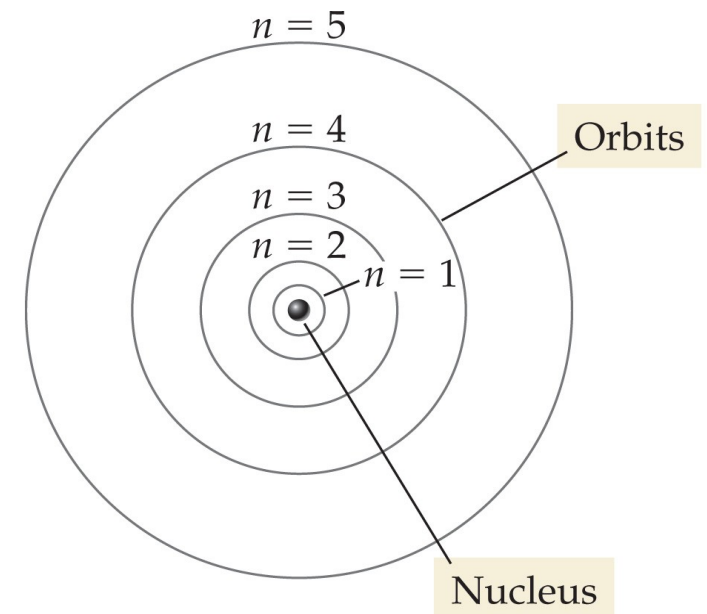
- From classical electromagnetic theory (Maxwell) such an atom would be unstable. If  $e$  accelerates  $\rightarrow$  it should radiate electromagnetic energy of frequency  $\nu=1/T$

Bohr's postulates:

- The electron in the hydrogen atom can move only in certain nonradiating, circular orbits called stationary states. The angular momentum of the  $e$  in a stable orbit is*

$$L = mvr = n\hbar \quad n = 1, 2, 3, \dots$$
$$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34} \text{ Js}$$

$$E_n = -\frac{me^4}{2\hbar^2} \frac{1}{n^2} = -\frac{13.6}{n^2}$$

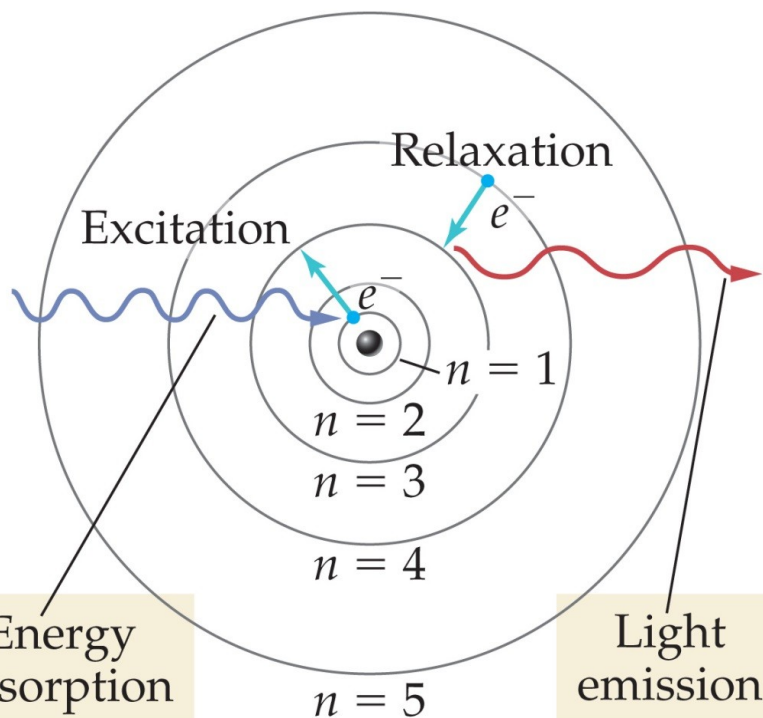


# Bohr's model

Bohr's postulates:

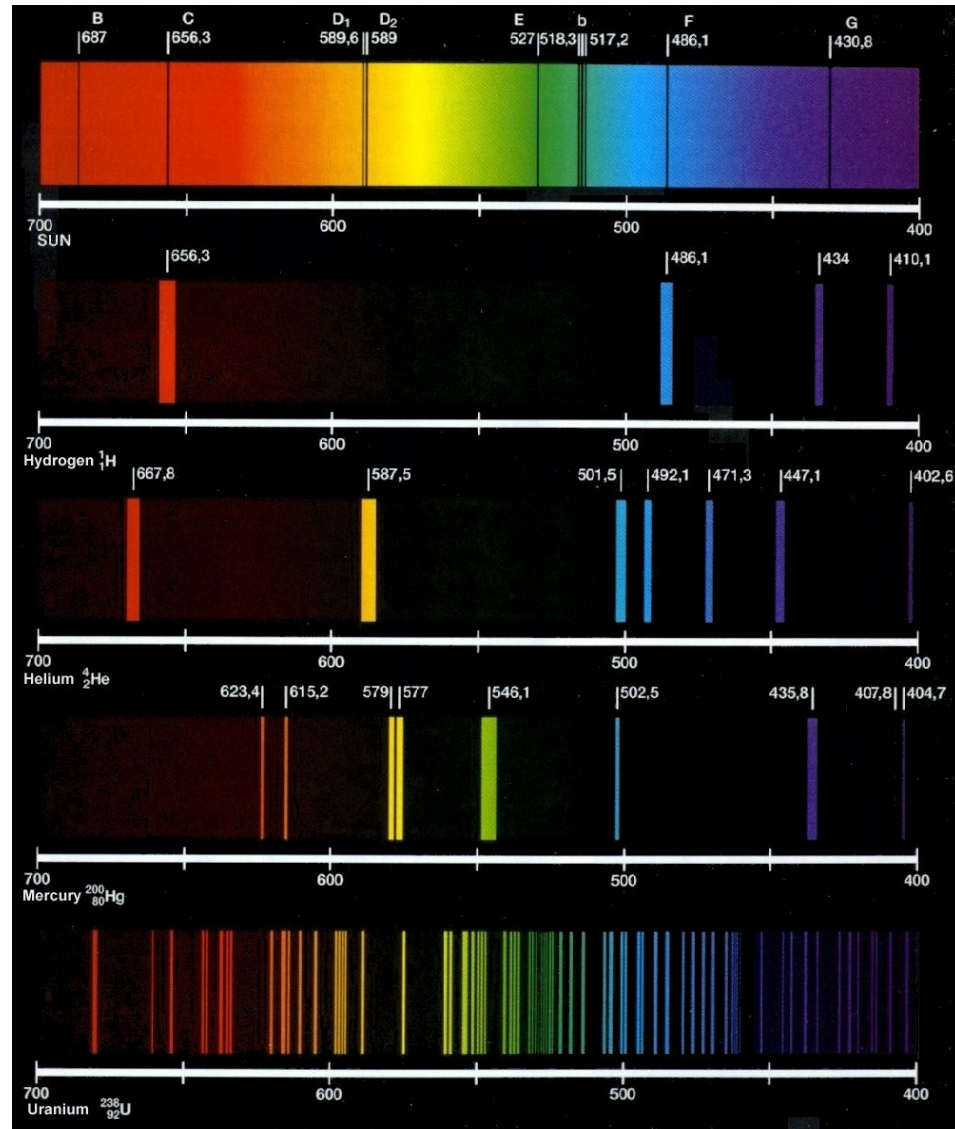
2) *The frequency of the emitted radiation during a transition is given by* 
$$\nu = \frac{E_i - E_f}{h}$$

$$E_n = -\frac{me^4}{2\hbar^2} \frac{1}{n^2} = -\frac{13.6}{n^2}$$



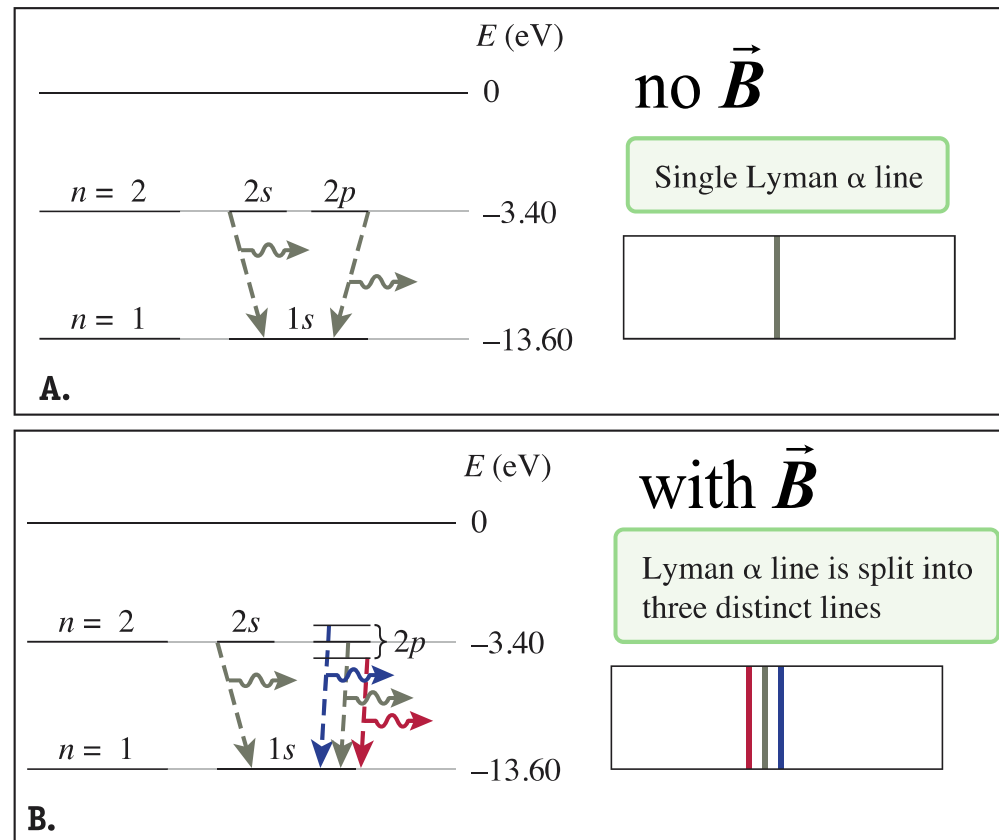
Principal quantum number	Unbound states ( $E > 0$ ) are not quantized.	$E$ (eV)	
$n = \infty$		0	
$n = 7$			
$n = 6$			
$n = 5$	H $\delta$ H $\gamma$	-0.544	
$n = 4$	H $\beta$ Brackett series	-0.850	
$n = 3$	H $\alpha$ Paschen series	-1.51	
$n = 2$	Balmer series	-3.40	
$n = 1$	Lyman series	-13.6	

- Can only explain the emission spectrum of hydrogen, not of complex atoms



# Bohr's model shortcomings

- Could not explain the fine structure of H and Zeeman effect (split of spectral lines of some atoms into three when a magnetic field is applied )



# De Broglie: the wave-like electron

- **Louis de Broglie** described the electron as a wave → wave-particle duality

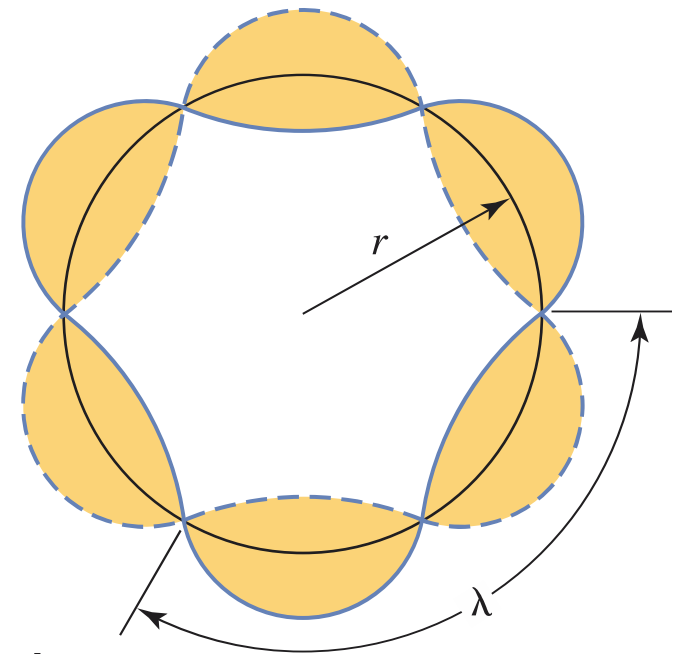


Nobel Prize in Physics 1929  
Prize share: 1/1

$$\lambda = \frac{h}{p} = \frac{h}{m_e v}$$

$$m_e v = \frac{L}{r} = \frac{n(h/2\pi)}{r}$$

$$\lambda = \frac{h}{nh} 2\pi r = \frac{2\pi r}{n}$$





# Heisenberg uncertainty principle

**Werner Karl Heisenberg** determined that it is fundamentally impossible to know precisely both the velocity and position of a particle at the same time



$$\Delta x (m \Delta v) \geq \frac{h}{4 \pi}$$

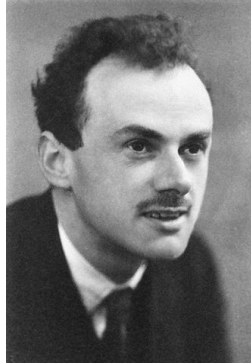
Nobel Prize in Physics 1932  
Prize share: 1/1



# Schrödinger equation

- Schrödinger  
Nobel Prize in Physics 1933  
Prize share: 1/2

- Dirac  
Nobel Prize in Physics 1933  
Prize share: 1/2



**Erwin Schrödinger** formulated the wave equation:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x) \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

$\Psi$  is the electron wavefunction

The probability density to find the electron in a small length  $dx$  at position  $x$  and time  $t$   $P(x,t) = |\Psi(x,t)|^2$

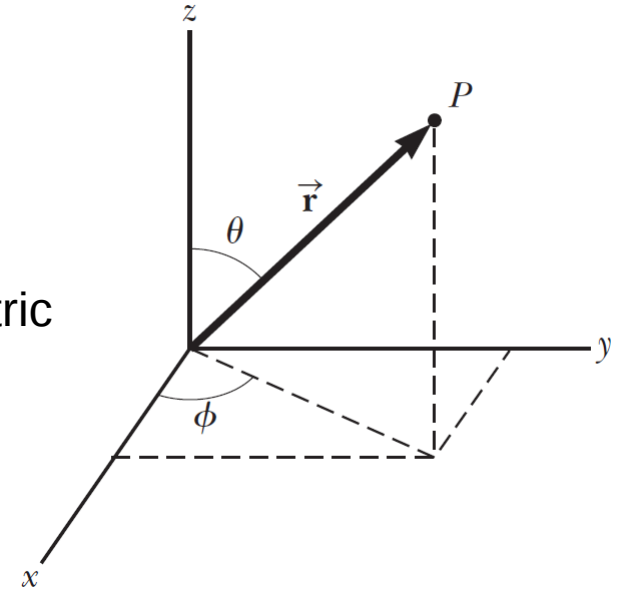
This equation asserts that an electron in an atom cannot be considered as a particle having an orbit with a definite radius. Instead, there is a probability of an electron being at certain spatial positions → electron cloud

# Time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U \Psi = E \Psi$$

$$U(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

Potential energy is spherically symmetric for the Hydrogen atom



$$\Psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$$

Wave function with 3 quantum numbers  $n, l, m$

$$R(r)$$

Radial function

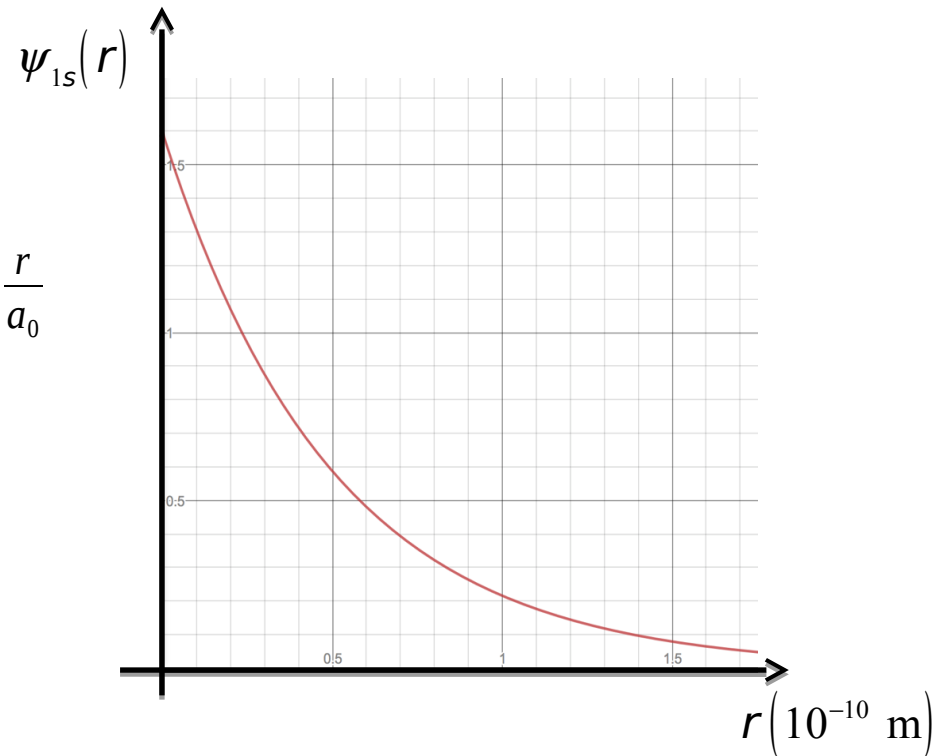
$$Y_l^m(\theta, \phi)$$

Spherical harmonics

$$\text{Radial Probability density: } P(r) = 4\pi r^2 |\psi|^2$$

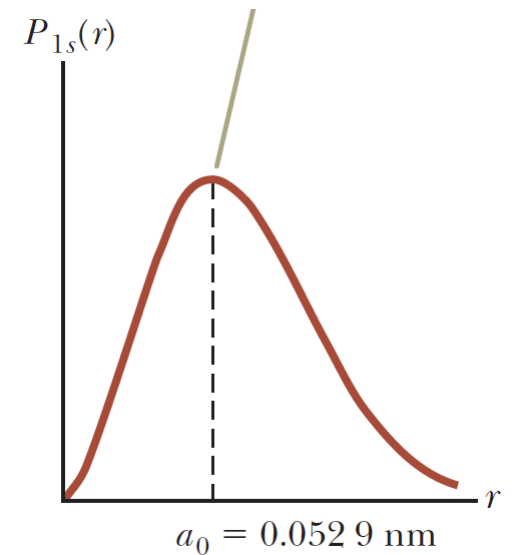
# Solutions for Hydrogen atom

1s Hydrogen wavefunction:  $\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$

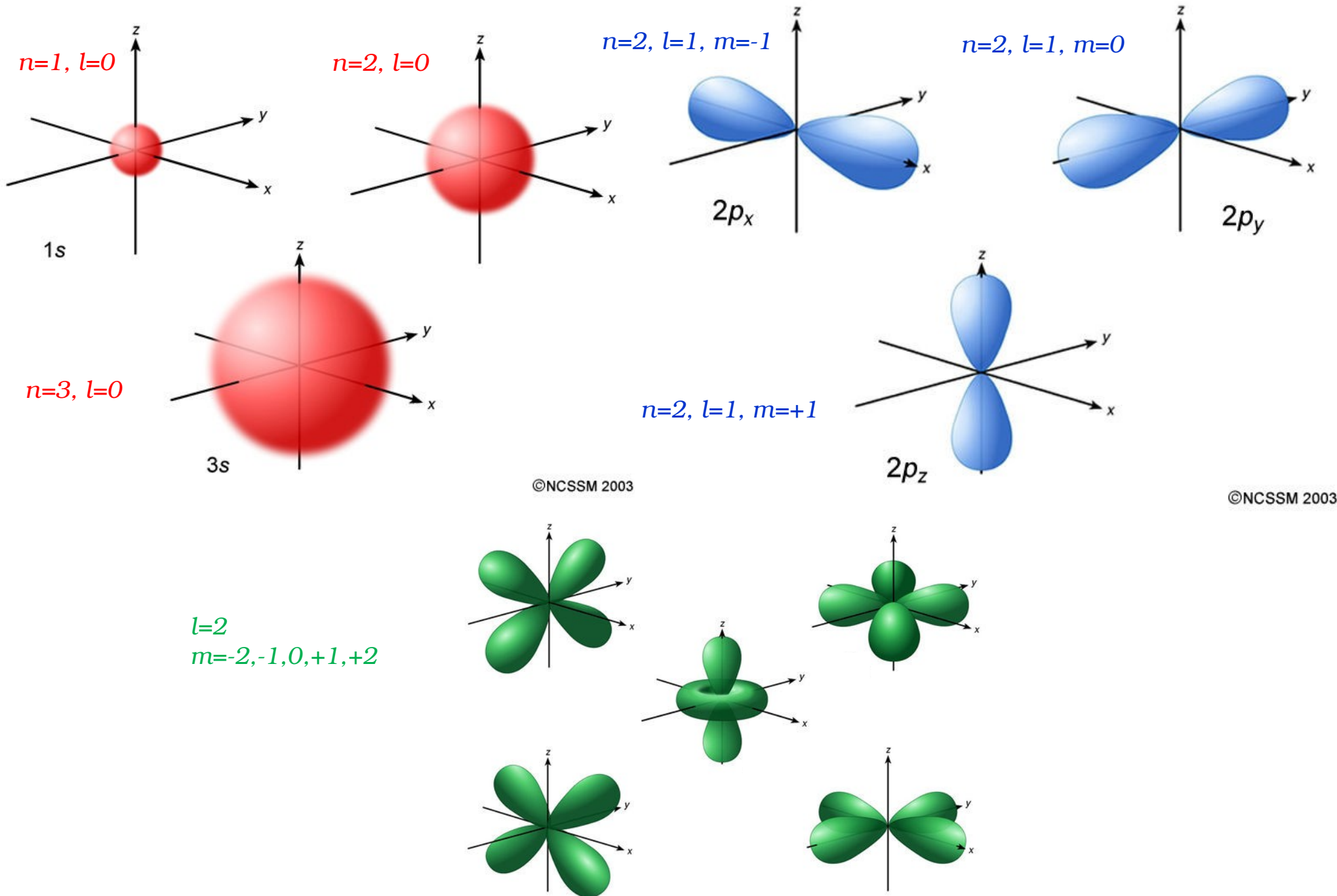


Probability maximum

1s Radial probability density:  $P_{1s}(r) = \left(\frac{4r^2}{a_0^3}\right) e^{-2r/a_0}$



# Atomic orbitals



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# Quantum numbers

The three coordinates that come from Schrödinger's wave equations are the principal ( $n$ ), angular ( $l$ ), and magnetic ( $m$ ) quantum numbers. These quantum numbers describe the size, shape, and orientation in space of the orbitals on an atom.

**$n$ : Principal quantum number**  
values:  $n = 1, 2, 3, \dots$   
(also called K, L, M, N, ...)



- related to “*the radii of the orbits*”.
- Determines the size
- Energy states with the same  $n$  form a *shell*.

**$l$ : Orbital quantum number**  
values:  $l = 0, \dots, n-1$   
(also called s, p, d, f, g, ...)



- related to the angular momentum.
- Determine the shapes
- Energy states with the same  $l$  form a *subshell*.

**$m$ : Magnetic quantum number**  
values:  $m = -l, \dots, l$



- Is related to the spatial orientation.
- Determines the orientation
- Energy does not depend on  $m$  unless there is an external magnetic field.

**ALSO a fourth quantum number  $s$ : spin quantum number**  
values:  $s = -1/2, 1/2$

# The Pauli exclusion principle

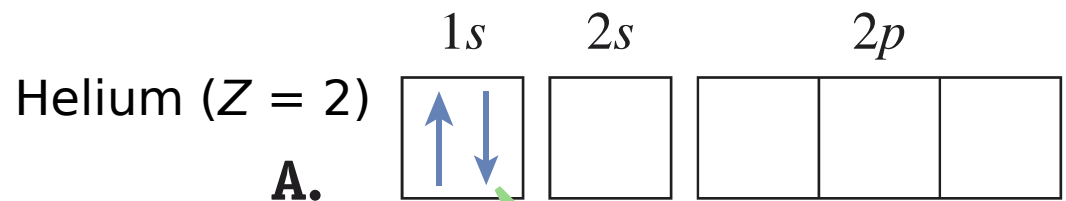
In 1925, Wolfgang Pauli discovered a rule, known as the Pauli exclusion principle, for determining the number of electrons in filled shells of an atom.

It states that two or more indistinguishable or identical particles with spin one-half can not be in the same quantum state.

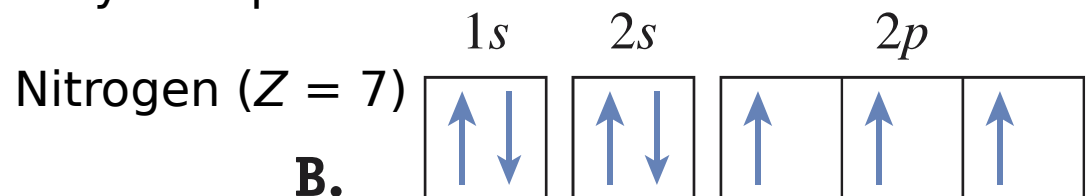


Nobel Prize in Physics 1945  
Prize share: 1/1

Hund's rule: Every orbital in a subshell is singly occupied before any are doubly occupied



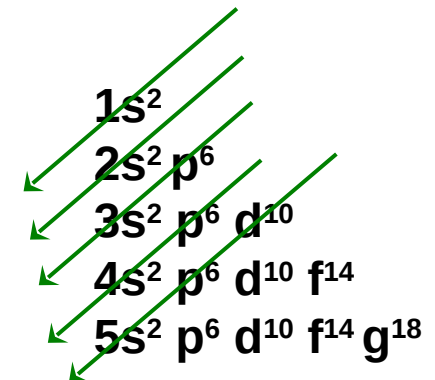
Each electron is represented by an arrow, pointing up or down according to its spin.



# How to write electron configurations

- maximum number of electrons that can fit in an energy level is:  $2n^2$
- Aufbau principle: Orbitals with lower energy filled first
- Pauli's exclusion principle: Two electrons cannot have the same 4 quantum numbers → each orbital (defined by  $n$ ,  $l$  and  $m$ ) can only have two electrons, corresponding to  $s=1/2$  and  $s=-1/2$ .
- Hund's rule: As energy does not normally depend on  $m$ , there can be several orbitals with the same energy (degenerate). These orbitals are filled so that there is one electron on each level (all with the same spin) before more electrons fill that level (maximum multiplicity).
- Madelung rule: The states crossed by the same arrow have same  $n + l$  value. The arrow direction indicates the order of filling states.

This rule has exceptions...





# How to write electron configurations

The "Worksheet"

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

	1s	2s	2p	Electron configuration
H	$\uparrow$			$1s^1$
He	$\uparrow\downarrow$			$1s^2$
Li	$\uparrow\downarrow$	$\uparrow$		$1s^2 2s^1$
Be	$\uparrow\downarrow$	$\uparrow\downarrow$		$1s^2 2s^2$
B	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$1s^2 2s^2 2p^1$
C	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\uparrow$	$1s^2 2s^2 2p^2$
N	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\uparrow\uparrow$	$1s^2 2s^2 2p^3$
O	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow\uparrow\uparrow$	$1s^2 2s^2 2p^4$
F	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow\uparrow\downarrow\uparrow$	$1s^2 2s^2 2p^5$
Ne	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$	$1s^2 2s^2 2p^6$

Examples

Put spin up electron here to obey Hund's rule

# The periodic table

- The electron configuration is related to where an element is located on the periodic table.

18 groups (columns) →

← 7 periods (rows) ↓

Period	Group	Element	Category
1	IA	1 H	Alkali metals
1	IIA	2 He	Noble gases
2	IIA	3 Li	Alkali metals
2	IIA	4 Be	Alkaline earth metals
2	IIIA	5 B	Alkali metals
2	IIIA	6 C	Nonmetals
2	IIIA	7 N	Nonmetals
2	IIIA	8 O	Nonmetals
2	IIIA	9 F	Nonmetals
2	IIIA	10 Ne	Noble gases
3	IIIA	11 Na	Alkali metals
3	IIIA	12 Mg	Alkaline earth metals
3	IIIA	13 Al	Alkali metals
3	IIIA	14 Si	Nonmetals
3	IIIA	15 P	Nonmetals
3	IIIA	16 S	Nonmetals
3	IIIA	17 Cl	Nonmetals
3	IIIA	18 Ar	Noble gases
4	IIIA	19 K	Alkali metals
4	IIIA	20 Ca	Alkaline earth metals
4	IIIA	21 Sc	Transition metals
4	IIIA	22 Ti	Transition metals
4	IIIA	23 V	Transition metals
4	IIIA	24 Cr	Transition metals
4	IIIA	25 Mn	Transition metals
4	IIIA	26 Fe	Transition metals
4	IIIA	27 Co	Transition metals
4	IIIA	28 Ni	Transition metals
4	IIIA	29 Cu	Transition metals
4	IIIA	30 Zn	Transition metals
4	IIIA	31 Ga	Alkali metals
4	IIIA	32 Ge	Nonmetals
4	IIIA	33 As	Nonmetals
4	IIIA	34 Se	Nonmetals
4	IIIA	35 Br	Nonmetals
4	IIIA	36 Kr	Noble gases
5	IIIA	37 Rb	Alkali metals
5	IIIA	38 Sr	Alkaline earth metals
5	IIIA	39 Y	Transition metals
5	IIIA	40 Zr	Transition metals
5	IIIA	41 Nb	Transition metals
5	IIIA	42 Mo	Transition metals
5	IIIA	43 Tc	Transition metals
5	IIIA	44 Ru	Transition metals
5	IIIA	45 Rh	Transition metals
5	IIIA	46 Pd	Transition metals
5	IIIA	47 Ag	Transition metals
5	IIIA	48 Cd	Transition metals
5	IIIA	49 In	Alkali metals
5	IIIA	50 Sn	Nonmetals
5	IIIA	51 Sb	Nonmetals
5	IIIA	52 Te	Nonmetals
5	IIIA	53 I	Nonmetals
5	IIIA	54 Xe	Noble gases
6	IIIA	55 Cs	Alkali metals
6	IIIA	56 Ba	Alkaline earth metals
6	IIIA	57 La	Lanthanide series
6	IIIA	58 Ce	Lanthanide series
6	IIIA	59 Pr	Lanthanide series
6	IIIA	60 Nd	Lanthanide series
6	IIIA	61 Pm	Lanthanide series
6	IIIA	62 Sm	Lanthanide series
6	IIIA	63 Eu	Lanthanide series
6	IIIA	64 Gd	Lanthanide series
6	IIIA	65 Tb	Lanthanide series
6	IIIA	66 Dy	Lanthanide series
6	IIIA	67 Ho	Lanthanide series
6	IIIA	68 Er	Lanthanide series
6	IIIA	69 Tm	Lanthanide series
6	IIIA	70 Yb	Lanthanide series
6	IIIA	71 Lu	Lanthanide series
6	IIIA	72 Hf	Transition metals
6	IIIA	73 Ta	Transition metals
6	IIIA	74 W	Transition metals
6	IIIA	75 Re	Transition metals
6	IIIA	76 Os	Transition metals
6	IIIA	77 Ir	Transition metals
6	IIIA	78 Pt	Transition metals
6	IIIA	79 Au	Transition metals
6	IIIA	80 Hg	Transition metals
6	IIIA	81 Tl	Alkali metals
6	IIIA	82 Pb	Nonmetals
6	IIIA	83 Bi	Nonmetals
6	IIIA	84 Po	Nonmetals
6	IIIA	85 At	Nonmetals
6	IIIA	86 Rn	Noble gases
7	IIIA	87 Fr	Alkali metals
7	IIIA	88 Ra	Alkaline earth metals
7	IIIA	89 Ac	Actinide series
7	IIIA	90 Th	Actinide series
7	IIIA	91 Pa	Actinide series
7	IIIA	92 U	Actinide series
7	IIIA	93 Np	Actinide series
7	IIIA	94 Pu	Actinide series
7	IIIA	95 Am	Actinide series
7	IIIA	96 Cm	Actinide series
7	IIIA	97 Bk	Actinide series
7	IIIA	98 Cf	Actinide series
7	IIIA	99 Es	Actinide series
7	IIIA	100 Fm	Actinide series
7	IIIA	101 Md	Actinide series
7	IIIA	102 No	Actinide series
7	IIIA	103 Lr	Actinide series
7	IIIA	104 Rf	Transition metals
7	IIIA	105 Db	Transition metals
7	IIIA	106 Sg	Transition metals
7	IIIA	107 Bh	Transition metals
7	IIIA	108 Hs	Transition metals
7	IIIA	109 Mt	Transition metals
7	IIIA	110 Ds	Transition metals
7	IIIA	111 Rg	Transition metals
7	IIIA	112 Uub	Transition metals
7	IIIA	113 Uut	Transition metals
7	IIIA	114 Uuq	Transition metals
7	IIIA	115 Uup	Transition metals
7	IIIA	116 Uuh	Transition metals
7	IIIA	117 Uus	Transition metals
7	IIIA	118 Uuo	Transition metals

In elements in period 3, the last shell filled with electrons (called valence shell) is  $n=3$ .

In elements in group IVA, the number of electrons on the valence shell is 4.