Atomic Structure and Atomic Radiation

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Kyoung-Jae Chung

Department of Nuclear Engineering

Seoul National University

Modern units and prefixes

- With only a few exceptions, units used in nuclear science and engineering are those defined by the SI system of metric units.

Base SI units:

Physical quantity	Unit name	Symbol
length	meter	m
mass	kilogram	kg
time	second	s
electric current	ampere	A
thermodynamic temperature	kelvin	K
luminous intensity	candela	cd
quantity of substance	mole	mol

Examples of Derived SI units:

Physical quantity	Unit name	Symbol	Formula
force	newton	N	kg m s^{-2}
work, energy, quantity of heat	joule	J	N m
power	watt	W	J s^{-1}
electric charge	coulomb	C	A s
electric potential difference	volt	V	W A^{-1}
electric resistance	ohm	Ω	V A^{-1}
magnetic flux	weber	Wb	V s
magnetic flux density	tesla	T	Wb m^{-2}
frequency	hertz	Hz	s^{-1}
radioactive decay rate	bequerel	Bq	s^{-1}
pressure	pascal	Pa	N m^{-2}
velocity			m s^{-1}
mass density			kg m^{-3}
area			m^2
volume			m^3
molar energy			J mol^{-1}
electric charge density			C m^{-3}

Supplementary Units:

Physical quantity	Unit name	Symbol
plane angle	radian	rad
solid angle	steradian	sr

Factor	Prefix	Symbol
10^{24}	yotta	Y
10^{21}	zetta	Z
10^{18}	exa	E
10^{15}	peta	P
10^{12}	tera	T
10^{9}	giga	G
10^{6}	mega	M
10^{3}	kilo	k
10^{2}	hecto	h
10^{1}	deca	da
10^{-1}	deci	d
10^{-2}	centi	c
10^{-3}	milli	m
10^{-6}	micro	μ
10^{-9}	nano	n
10^{-12}	pico	p
10^{-15}	femto	f
10^{-18}	atto	a
10^{-21}	zepto	z
10^{-24}	yocto	y

Values of some important physical constants

Constant	Symbol	Value
Speed of light (in vacuum)	c	$2.997\,924\,58 \times 10^{8}$ m s^{-1}*
Electron charge	e	$1.602\,176\,6208(98) \times 10^{-19}$ C
Atomic mass constant	u	$1.660\,539\,040(20) \times 10^{-27}$ kg (931.4940954(57) MeV/c^2)
Electron rest mass	m_e	$9.109\,383\,56(11) \times 10^{-31}$ kg (0.510 998 9461(3) MeV/c^2) ($5.485\,799\,090\,70(16) \times 10^{-4}$ u)
Proton rest mass	m_p	$1.672\,621\,898(21) \times 10^{-27}$ kg (938.2720813(58) MeV/c^2) (1.007 276 466 879(91) u)
Neutron rest mass	m_n	$1.674\,927\,471(21) \times 10^{-27}$ kg (939.565 4133(58) MeV/c^2) (1.008 664 915 88(49) u)
Planck's constant	h	$6.626\,070\,040(81) \times 10^{-34}$ J s ($4.135\,667\,662(25) \times 10^{-15}$ eV s)
Avogadro's constant	N_a	$6.022\,140\,857(74) \times 10^{23}$ mol^{-1}
Boltzmann constant	k	$1.380\,648\,52(79) \times 10^{-23}$ J K^{-1} ($8.617\,3303(50) \times 10^{-5}$ eV K^{-1})
Ideal gas constant (STP)	R	8.314 4598(48) J mol^{-1} K^{-1}
Electric constant	ϵ_o	$8.854\,187\,817\ldots \times 10^{-12}$ F m^{-1}*
Magnetic constant	μ_o	$4\pi \times 10^{-7}$ N A^{-2}* $= 12.566\,370\,614\ldots \times 10^{-7}$ N A^{-2}

* indicates exact values.

Source: `http://physics.nist.gov/cuu/index.html`

Relativistic particle momentum

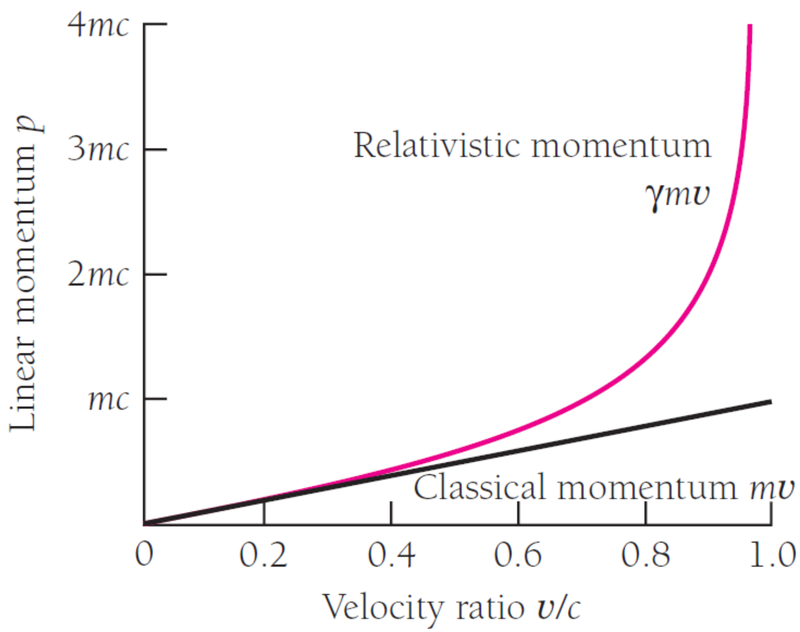
- The special theory of relativity states that the inertia of a particle observed in a frame of reference depends on the magnitude of its speed in that frame.

$$\gamma = \frac{1}{\sqrt{1-(v/c)^2}} = \frac{1}{\sqrt{1-\beta^2}}$$

Lorentz factor

- The inertia of a particle is proportional to γ. The apparent mass is γm.
- The particle momentum, a vector quantity, equals $\boldsymbol{p} = \gamma m \boldsymbol{v}$.
- The equation of motion:

$$\frac{d\boldsymbol{p}}{dt} = \frac{d(\gamma m\boldsymbol{v})}{dt} = \boldsymbol{F}$$



Relativistic particle energy

- The kinetic energy equals the total energy minus the rest energy:

$$E = \gamma mc^2 \qquad\qquad T = (\gamma - 1)mc^2$$

- Newtonian dynamics describes the motion of low-energy particles when $T \ll mc^2$.

$$T = \frac{1}{2}mv^2$$

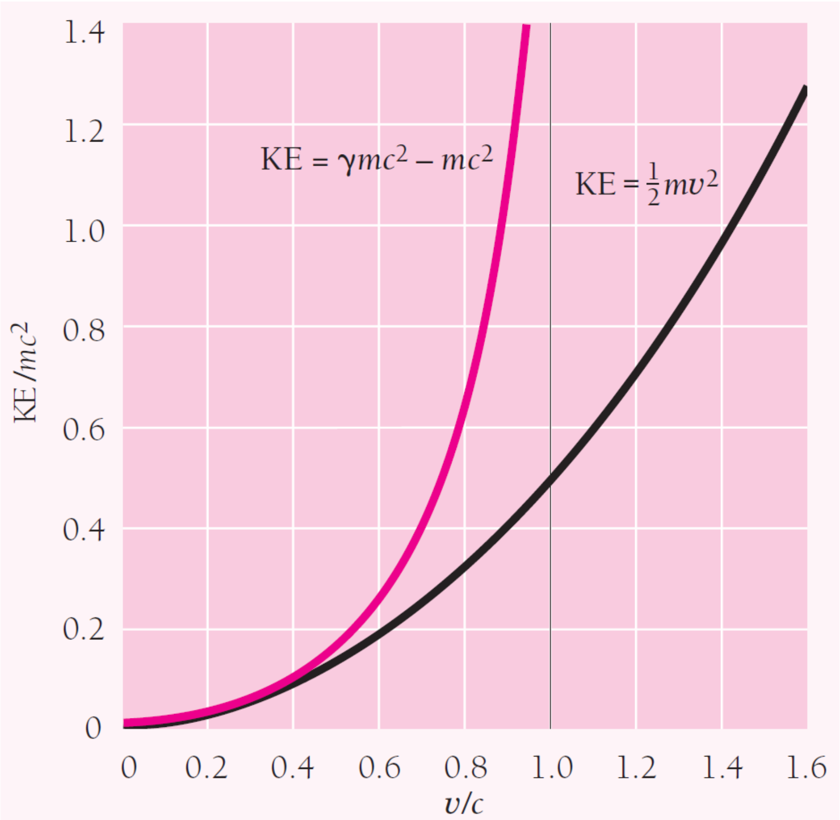
$$(1+x)^{-1/2} \approx 1 - \frac{1}{2}x + \cdots$$

- Energy and momentum

$$E^2 = (mc^2)^2 + p^2c^2$$

- For massless particles

$$E = pc$$



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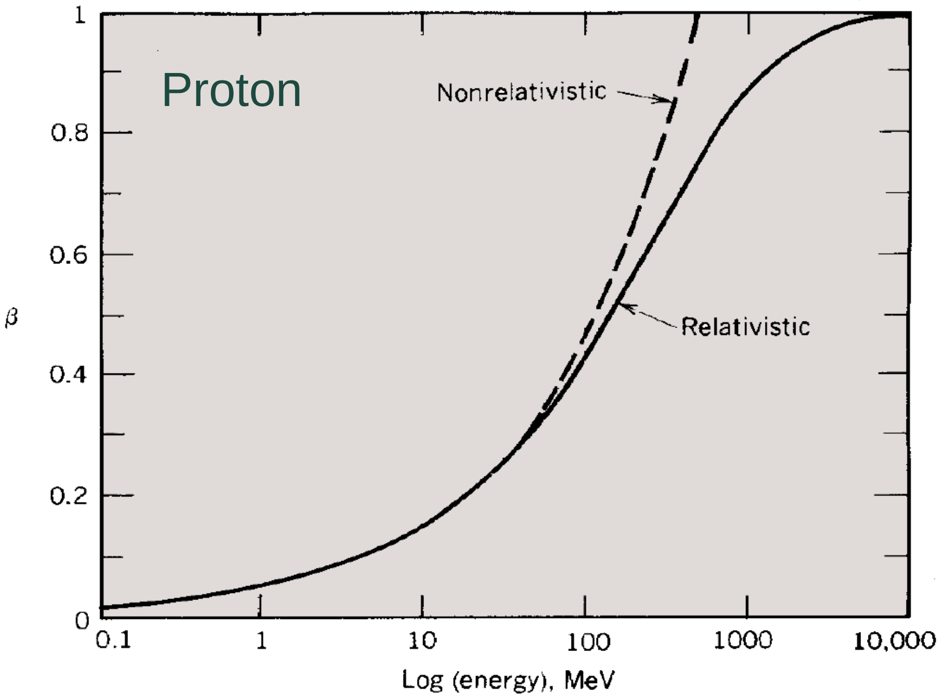
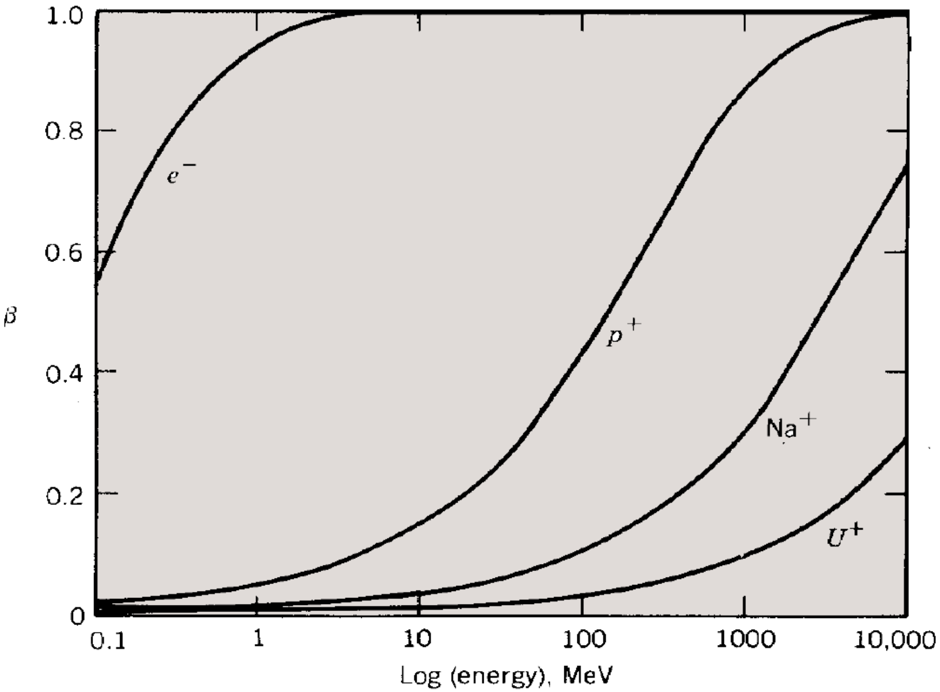
Charged particle properties

Particle	Charge (coulomb)	Mass (kg)	Rest Energy (MeV)	A	Z	Z^*
Electron (β particle)	-1.60×10^{-19}	9.11×10^{-31}	0.511	—	—	—
Proton	$+1.60 \times 10^{-19}$	1.67×10^{-27}	938	1	1	1
Deuteron	$+1.60 \times 10^{-19}$	3.34×10^{-27}	1875	2	1	1
Triton	$+1.60 \times 10^{-19}$	5.00×10^{-27}	2809	3	1	1
He^{+}	$+1.60 \times 10^{-19}$	6.64×10^{-27}	3728	4	2	1
He^{++} (α particle)	$+3.20 \times 10^{-19}$	6.64×10^{-27}	3728	4	2	2
C^{+}	$+1.6 \times 10^{-19}$	1.99×10^{-26}	1.12×10^{4}	12	6	1
U^{+}	$+1.6 \times 10^{-19}$	3.95×10^{-25}	2.22×10^{5}	238	92	1

1 eV = 1.6×10^{-19} J = 1240 nm = 241.8 THz

β for particles as a function of kinetic energy





Example

(a) What is the kinetic energy of an electron that travels at 99% of the velocity of light?

Solution

$$E_{\mathrm{k}} = m_0 c^2 \left[\frac{1}{\left(1-\beta^2\right)^{1/2}} - 1 \right]$$

$$= 9.11 \times 10^{-31}\ \mathrm{kg} \left(3 \times 10^8\ \frac{\mathrm{m}}{\mathrm{s}}\right)^2 \left\{ \frac{1}{\left[1-(0.99)^2\right]^{1/2}} - 1 \right\} = 4.99 \times 10^{-13}\ \mathrm{J}.$$

(b) How much additional energy is required to increase the velocity of this electron to 99.9% of the velocity of light, an increase in velocity of only 0.9%?

Solution

The kinetic energy of an electron whose velocity is 99.9% of the speed of light is

$$E_{\mathrm{k}} = 9.11 \times 10^{-31}\ \mathrm{kg} \left(3 \times 10^8\ \frac{\mathrm{m}}{\mathrm{s}}\right)^2 \left\{ \frac{1}{\left[1-(0.999)^2\right]^{1/2}} - 1 \right\} = 17.52 \times 10^{-13}\ \mathrm{J}.$$

The additional work necessary to increase the kinetic energy of the electron from 99% to 99.9% of the velocity of light is

$$\Delta W = (17.52 - 4.99) \times 10^{-13}\ \mathrm{J}$$
$$= 12.53 \times 10^{-13}\ \mathrm{J}.$$

Electric force

- Coulomb's law

$$F_e = k\frac{q_1 q_2}{r^2}, \qquad k_0 = \frac{1}{4\pi\epsilon_0} = 9.00\times10^9\,\frac{\mathrm{N\cdot m^2}}{\mathrm{C^2}}$$

- Dielectric constant or relative permittivity $K_e = \dfrac{\epsilon}{\epsilon_0}$

Compare the electrical and gravitational forces of attraction between an electron and a proton separated by 5×10^{-11} m.

Solution

The electrical force is given by Eq. (2.23):

$$f = k_0\frac{q_1 q_2}{r^2} = 9.00\times10^9\,\frac{\mathrm{N\cdot m^2}}{\mathrm{C^2}}\cdot\frac{1.6\times10^{-19}\,\mathrm{C}\cdot1.6\times10^{-19}\,\mathrm{C}}{\left(5\times10^{-11}\ \mathrm{m}\right)^2}$$

$$= 9.2\times10^{-8}\ \mathrm{N}.$$

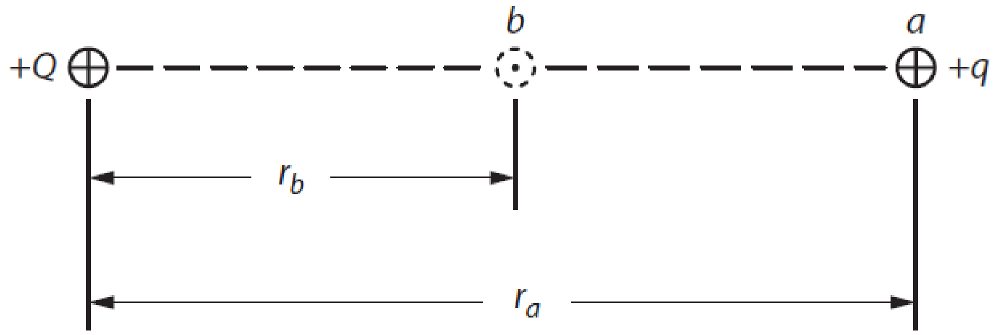
The gravitational force between the electron and the proton is

$$F = \frac{6.67\times10^{-11}\,\dfrac{\mathrm{N\cdot m^2}}{\mathrm{kg^2}}\cdot9.11\times10^{-31}\,\mathrm{kg}\cdot1.67\times10^{-27}\,\mathrm{kg}}{\left(5\times10^{-11}\,\mathrm{m}\right)^2}$$

$$= 4.1\times10^{-47}\ \mathrm{N}.$$

Electric potential

- An electric potential (also called the electric field potential, potential drop or the electrostatic potential) is the amount of work needed to move a unit of charge from a reference point to a specific point inside the field without producing an acceleration.



$$dW = -f\,dr = -k_0 \frac{Qq}{r^2} dr$$

$$W = -k_0\, Qq \int_{r_a}^{r_b} \frac{dr}{r^2} = k_0 Qq \left(\frac{1}{r_b} - \frac{1}{r_a} \right).$$

$$V_b = \frac{W}{q} = k_0 \frac{Q}{r_b}$$

Example

(a) What is the potential at a distance of 5×10^{-11} m from a proton?

Solution

$$V = k_0 \frac{Q}{r} = 9.00 \times 10^9 \frac{\mathrm{N \cdot m^2}}{\mathrm{C^2}} \cdot \frac{1.6 \times 10^{-19}\,\mathrm{C}}{5 \times 10^{-11}\,\mathrm{m}} = 28.8 \frac{\mathrm{N \cdot m}}{\mathrm{C}}$$

$$= 28.8 \frac{\mathrm{J}}{\mathrm{C}} = 28.8\ \mathrm{V}$$

(b) What is the potential energy of another proton at this point?

Solution

According to Eq. (2.31), the potential energy of the proton is equal to the product of its charge and the potential of its location. Therefore,

$$E_\mathrm{p} = qV = 1.6 \times 10^{-19}\ \mathrm{C} \cdot 28.8\ \mathrm{V} = 4.6 \times 10^{-18}\ \mathrm{J}.$$

Electric current

- A flow of electrically charged particles constitutes an electric current. The unit for the amount of current is the ampere (A), which is a measure of the time rate of flow of charge.
- 1 A (1 Coulombs per 1 second) means

$$\frac{1\,\mathrm{C/s}}{\mathrm{A}} \cdot \frac{1}{1.6\times 10^{-19}\,\dfrac{\mathrm{C}}{\mathrm{electron}}} = 6.25\times 10^{18}\,\frac{\mathrm{electrons/s}}{\mathrm{A}}.$$

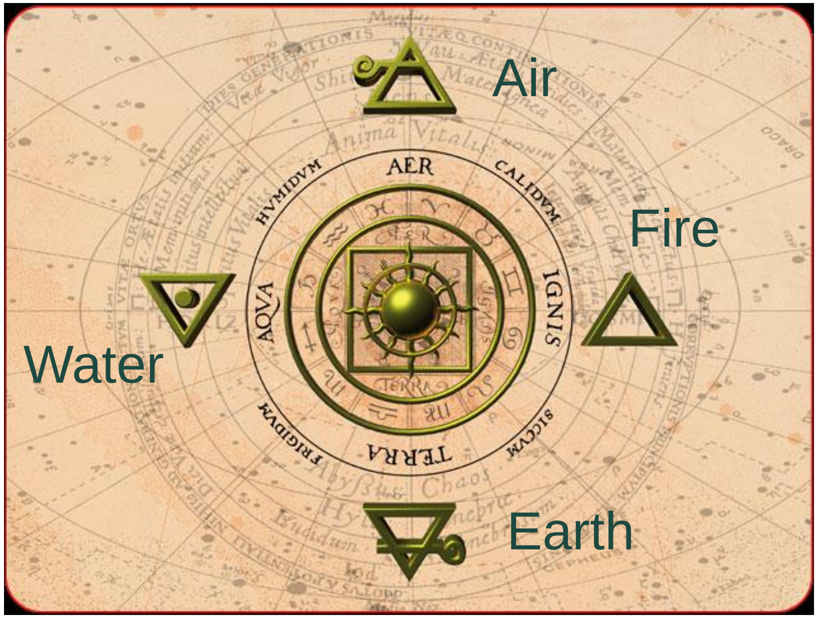
A 100-μA electron beam in an X-ray tube represents an electron flow rate of

$$100\times 10^{-6}\,\mathrm{A}\cdot 6.25\times 10^{18}\,\frac{\mathrm{electrons/s}}{\mathrm{A}} = 6.25\times 10^{14}\ \mathrm{electrons/s}.$$

Current is determined only by the flow rate of charge. For example, in the case of a beam of alpha particles, whose charge $= 2(1.6\times 10^{-19}\ \mathrm{C}) = 3.2\times 10^{-19}$ C, 1 A corresponds to 3.125×10^{18} alpha particles.

Atom: philosophical approach

- The four elements (Empedocles, 490 BC ~ 430 BC and Aristotle, 384 BC ~ 322 BC)



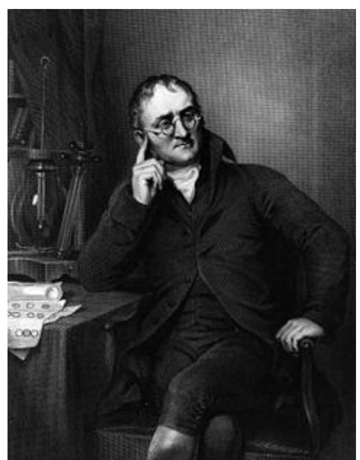
- Atomic hypothesis (“Atomos” = “unsplittable”, Democritus, 460 BC ~ 370 BC)

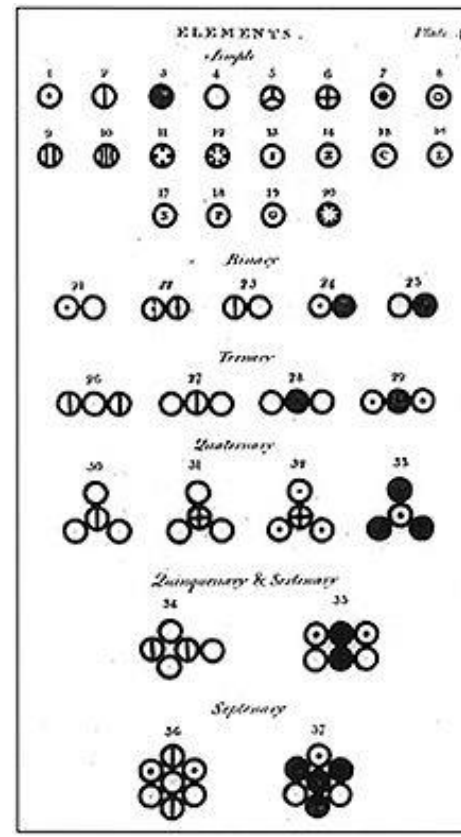
  Everything is composed of "atoms", which are physically, but not geometrically, indivisible; that between atoms, there lies empty space; that atoms are indestructible, and have always been and always will be in motion; that there is an infinite number of atoms and of kinds of atoms, which differ in shape and size.

Atomic nature of matter

- Dalton's atomic theory (John Dalton, 1808)

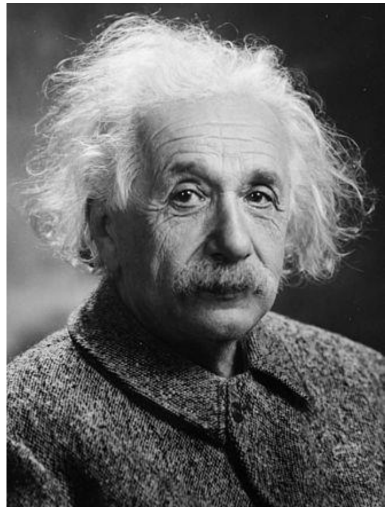
  1. Elements are made of extremely small particles called atoms.
  2. Atoms of a given element are identical in size, mass, and other properties; atoms of different elements differ in size, mass, and other properties.
  3. Atoms cannot be subdivided, created, or destroyed.
  4. Atoms of different elements combine in simple whole-number ratios to form chemical compounds.
  5. In chemical reactions, atoms are combined, separated, or rearranged.

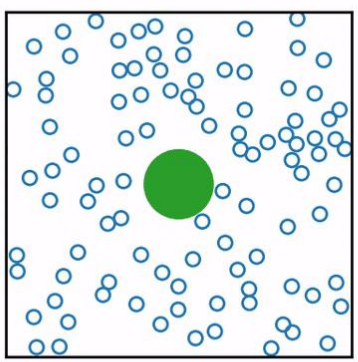




Evidence that atoms and molecules exist

- Brownian motion (Robert Brown, 1827)





열 분자운동 이론이 필요한, 정지 상태의 액체 속에 떠 있는 작은 부유입자들의 운동에 관하여 (아인슈타인, 1905)

Annalen der Physik 322, 549 (1905)

5. *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen;*
von A. Einstein.

In dieser Arbeit soll gezeigt werden, daß nach der molekularkinetischen Theorie der Wärme in Flüssigkeiten suspendierte Körper von mikroskopisch sichtbarer Größe infolge der Molekularbewegung der Wärme Bewegungen von solcher Größe ausführen müssen, daß diese Bewegungen leicht mit dem Mikroskop nachgewiesen werden können. Es ist möglich, daß die hier zu behandelnden Bewegungen mit der sogenannten „Brownschen Molekularbewegung" identisch sind; die mir erreichbaren Angaben über letztere sind jedoch so ungenau, daß ich mir hierüber kein Urteil bilden konnte.

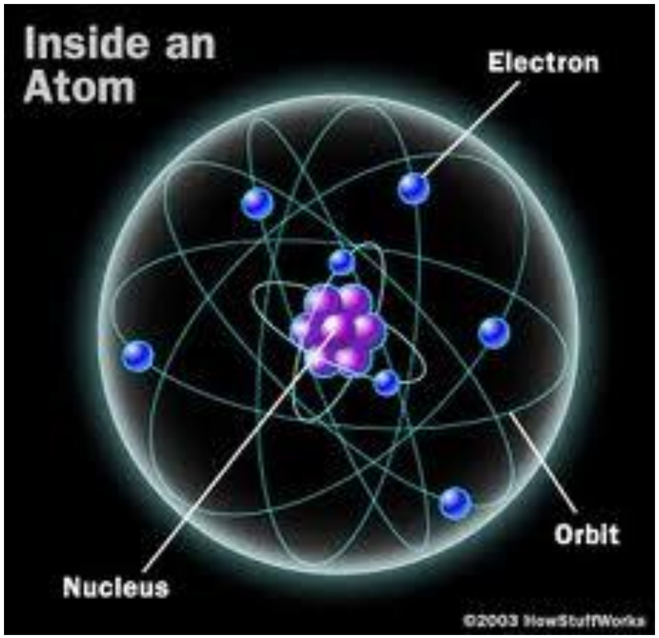
Wenn sich die hier zu behandelnde Bewegung samt den für sie zu erwartenden Gesetzmäßigkeiten wirklich beobachten läßt, so ist die klassische Thermodynamik schon für mikroskopisch unterscheidbare Räume nicht mehr als genau gültig anzusehen und es ist dann eine exakte Bestimmung der wahren Atomgröße möglich. Erwiese sich umgekehrt die Voraussage dieser Bewegung als unzutreffend, so wäre damit ein schwerwiegendes Argument gegen die molekularkinetische Auffassung der Wärme gegeben.

§ 1. Über den suspendierten Teilchen zuzuschreibenden osmotischen Druck.

Im Teilvolumen V^* einer Flüssigkeit vom Gesamtvolumen V seien z-Gramm-Moleküle eines Nichtelektrolyten gelöst. Ist das Volumen V^* durch eine für das Lösungsmittel, nicht aber für die gelöste Substanz durchlässige Wand vom reinen Lösungs-

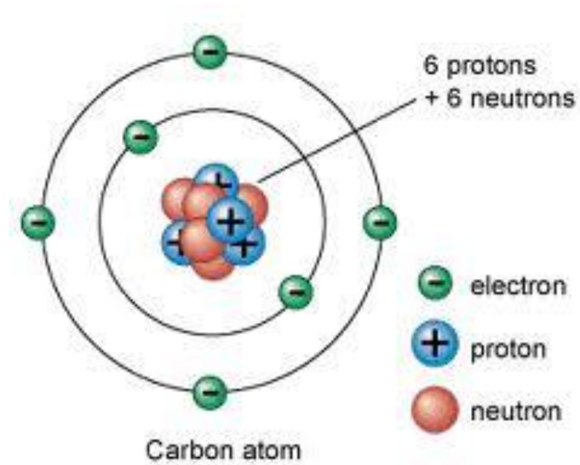
The structure of atom

- Every atom is composed of a nucleus and one or more electrons bound to the nucleus. The nucleus is made of one or more protons and typically a similar number of neutrons. Protons and neutrons are called nucleons.
- More than 99.94% of an atom's mass is in the nucleus.



$$\frac{m_p}{m_e} \approx 1837 \qquad \left|\frac{q_p}{q_e}\right| = 1$$

- Proton (p, H^+)
  - mass (m_p) = 1.67×10^{-27} kg
  - charge (q_p) = $+1.6 \times 10^{-19}$ C (+e)
- Electron (e)
  - mass (m_e) = 9.11×10^{-31} kg
  - charge (q_e) = -1.6×10^{-19} C (-e)



$${}^{12}_{6}\mathrm{C}$$

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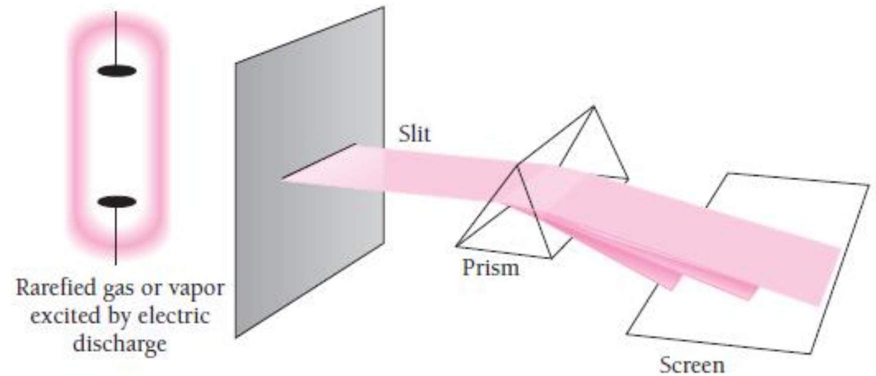
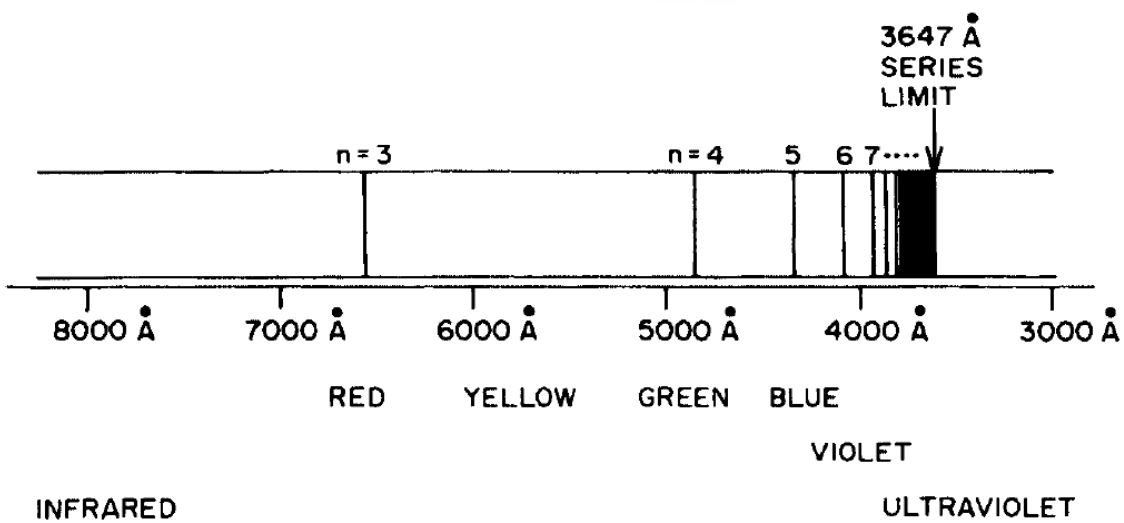
Line spectrum

- In 1885, Balmer published an empirical formula that gives the observed wavelengths, λ, in the hydrogen spectrum.

$$\frac{1}{\lambda} = R_\infty \left(\frac{1}{2^2} - \frac{1}{n^2} \right)$$





- The Balmer formula was derived theoretically by Bohr in 1913.

Discovery of electron: J. J. Thomson (1897)

THE

LONDON, EDINBURGH, AND DUBLIN

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[FIFTH SERIES.]

OCTOBER 1897.

XL. *Cathode Rays.* *By* J. J. THOMSON, *M.A., F.R.S., Cavendish Professor of Experimental Physics, Cambridge**.

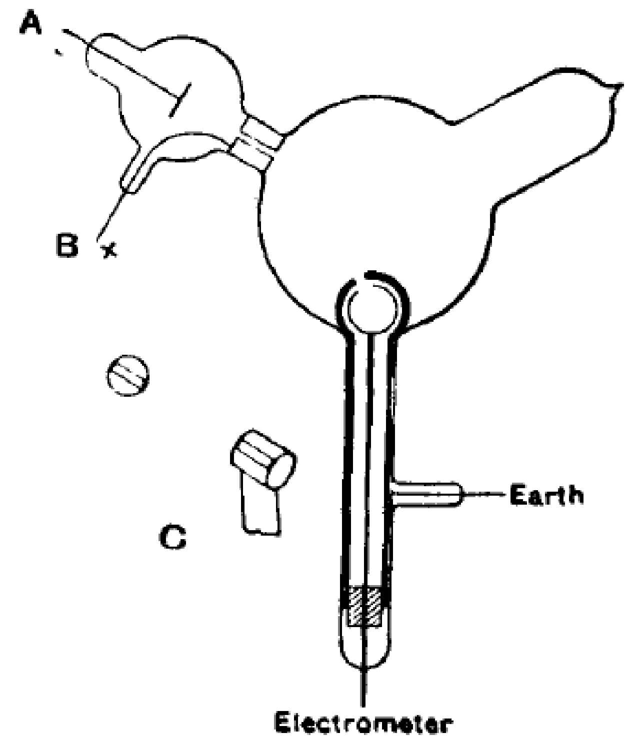
THE experiments† discussed in this paper were undertaken in the hope of gaining some information as to the nature of the Cathode Rays. The most diverse opinions are held as to these rays; according to the almost unanimous opinion of German physicists they are due to some process in the æther to which—inasmuch as in a uniform magnetic field their course is circular and not rectilinear—no phenomenon hitherto observed is analogous: another view of these rays is that, so far from being wholly ætherial, they are in fact wholly material, and that they mark the paths of particles of matter charged with negative electricity. It would seem at first sight that it ought not to be difficult to discriminate between views so different, yet experience shows that this is not the case, as amongst the physicists who have most deeply studied the subject can be found supporters of either theory.

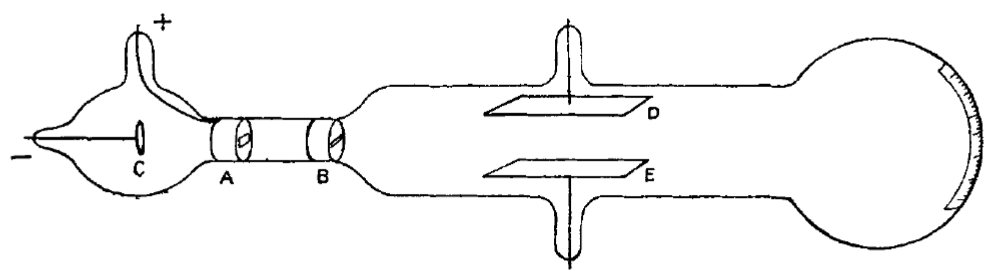
The electrified-particle theory has for purposes of research a great advantage over the ætherial theory, since it is definite and its consequences can be predicted; with the ætherial theory it is impossible to predict what will happen under any given circumstances, as on this theory we are dealing with hitherto

* Communicated by the Author.

† Some of these experiments have already been described in a paper read before the Cambridge Philosophical Society (Proceedings, vol. ix. 1897), and in a Friday Evening Discourse at the Royal Institution ('Electrician,' May 21, 1897).

Phil. Mag. S. 5. Vol. 44. No. 269. *Oct.* 1897. Y





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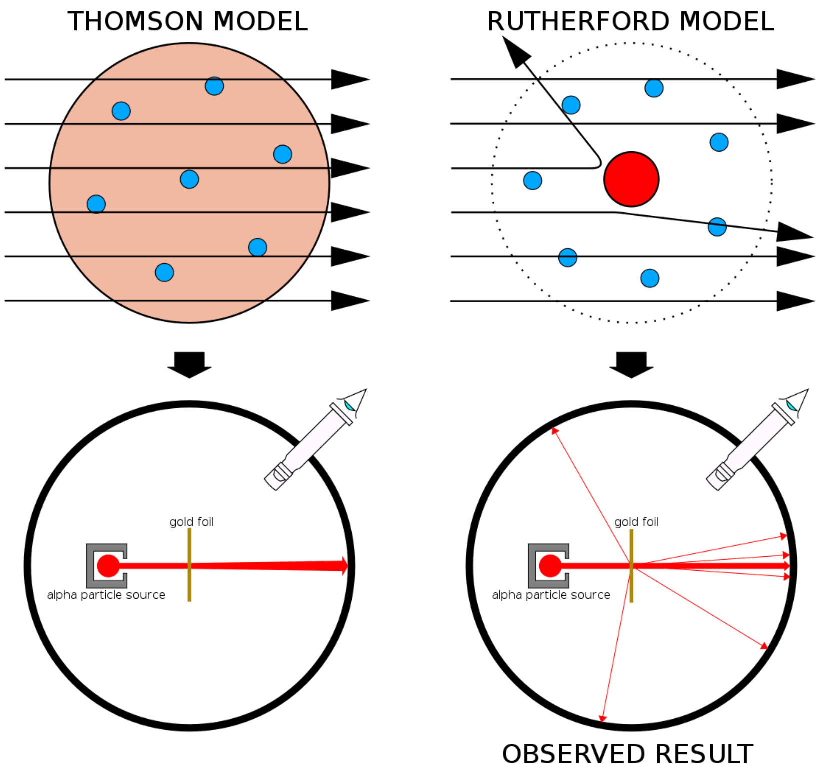
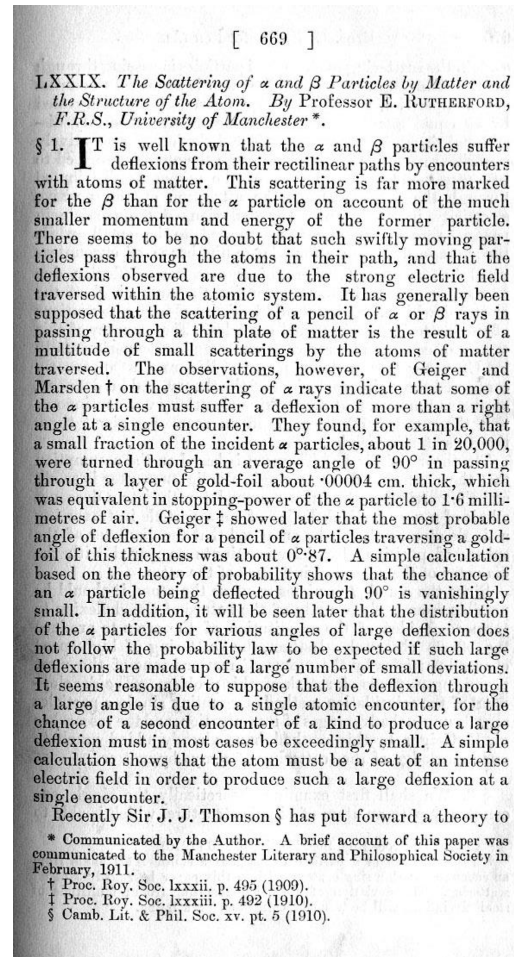
Gold foil experiment: Rutherford model (1911)

- Rutherford directed the famous Geiger–Marsden experiment in 1909 which suggested, upon Rutherford's 1911 analysis, that J. J. Thomson's plum pudding model of the atom was incorrect.

Philosophical Magazine 21, 669 (1911)



$$s = \frac{Xnt \csc^4\left(\frac{\phi}{2}\right)}{16r^2} \cdot \left(\frac{2Q_n Q_\alpha}{mv^2}\right)^2$$



[669]

LXXIX. *The Scattering of α and β Particles by Matter and the Structure of the Atom.* By Professor E. RUTHERFORD, *F.R.S., University of Manchester* *.

§ 1. IT is well known that the α and β particles suffer deflexions from their rectilinear paths by encounters with atoms of matter. This scattering is far more marked for the β than for the α particle on account of the much smaller momentum and energy of the former particle. There seems to be no doubt that such swiftly moving particles pass through the atoms in their path, and that the deflexions observed are due to the strong electric field traversed within the atomic system. It has generally been supposed that the scattering of a pencil of α or β rays in passing through a thin plate of matter is the result of a multitude of small scatterings by the atoms of matter traversed. The observations, however, of Geiger and Marsden † on the scattering of α rays indicate that some of the α particles must suffer a deflexion of more than a right angle at a single encounter. They found, for example, that a small fraction of the incident α particles, about 1 in 20,000, were turned through an average angle of 90° in passing through a layer of gold-foil about ·00004 cm. thick, which was equivalent in stopping-power of the α particle to 1·6 millimetres of air. Geiger ‡ showed later that the most probable angle of deflexion for a pencil of α particles traversing a gold-foil of this thickness was about 0°·87. A simple calculation based on the theory of probability shows that the chance of an α particle being deflected through 90° is vanishingly small. In addition, it will be seen later that the distribution of the α particles for various angles of large deflexion does not follow the probability law to be expected if such large deflexions are made up of a large number of small deviations. It seems reasonable to suppose that the deflexion through a large angle is due to a single atomic encounter, for the chance of a second encounter of a kind to produce a large deflexion must in most cases be exceedingly small. A simple calculation shows that the atom must be a seat of an intense electric field in order to produce such a large deflexion at a single encounter.

Recently Sir J. J. Thomson § has put forward a theory to

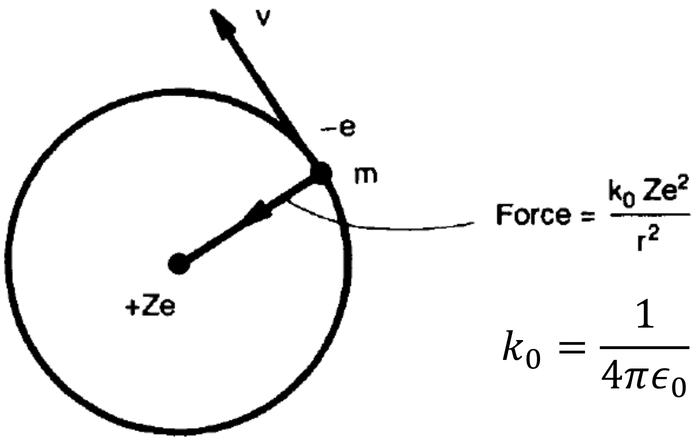
* Communicated by the Author. A brief account of this paper was communicated to the Manchester Literary and Philosophical Society in February, 1911.
† Proc. Roy. Soc. lxxxii. p. 495 (1909).
‡ Proc. Roy. Soc. lxxxiii. p. 492 (1910).
§ Camb. Lit. & Phil. Soc. xv. pt. 5 (1910).

Bohr model (1913)

- Bohr model included several non-classical constraints (quantum nature).
  - An atomic electron moves without radiating only in certain discrete orbits about the nucleus.
  - The transition of the electron from one orbit to another must be accompanied by the emission or absorption of a photon of light, the photon energy being equal to the orbital energy lost or gained by the electron.

- Orbit radius

$$\frac{m_e v^2}{r} = \frac{Ze^2}{4\pi\epsilon_0 r^2} \qquad L = m_e v r = n\frac{h}{2\pi} = n\hbar$$



$$k_0 = \frac{1}{4\pi\epsilon_0}$$

⇩

$$r_n = \frac{n^2 h^2 \epsilon_0}{\pi m_e Z e^2}$$

$$r_n = \frac{n^2(1.05457\times10^{-34})^2}{(8.98755\times10^9 Z)(1.60218\times10^{-19})^2(9.10939\times10^{-31})}$$

$$= 5.29\times10^{-11}\frac{n^2}{Z}\ \text{m}.$$

Bohr radius (a_0) = 0.529 Å

Bohr model (1913)

- Orbital velocity

$$v_n = \frac{Ze^2}{2nh\epsilon_0}$$

$$v_n = \frac{k_0 Ze^2}{n\hbar} = 2.19 \times 10^6 \frac{Z}{n}\ \mathrm{m\,s^{-1}}.$$

- Fine structure constant: determines the relativistic corrections to the Bohr energy levels, which give rise to a fine structure in the spectrum of hydrogen.

$$\alpha = \frac{v_1}{c} \approx \frac{1}{137}$$

- Total energy of the electron in the nth orbit:

$$\mathrm{KE}_n = \frac{1}{2} m v_n^2 = \frac{k_0^2 Z^2 e^4 m}{2n^2\hbar^2}$$

$$\mathrm{PE}_n = -\frac{k_0 Ze^2}{r_n} = -\frac{k_0^2 Z^2 e^4 m}{n^2\hbar^2}$$

⇨

$$E_n = \mathrm{KE}_n + \mathrm{PE}_n = -\frac{k_0^2 Z^2 e^4 m}{2n^2\hbar^2} = -\frac{13.6 Z^2}{n^2}\ \mathrm{eV}.$$

Q. What is E_K for W (Z=74)?

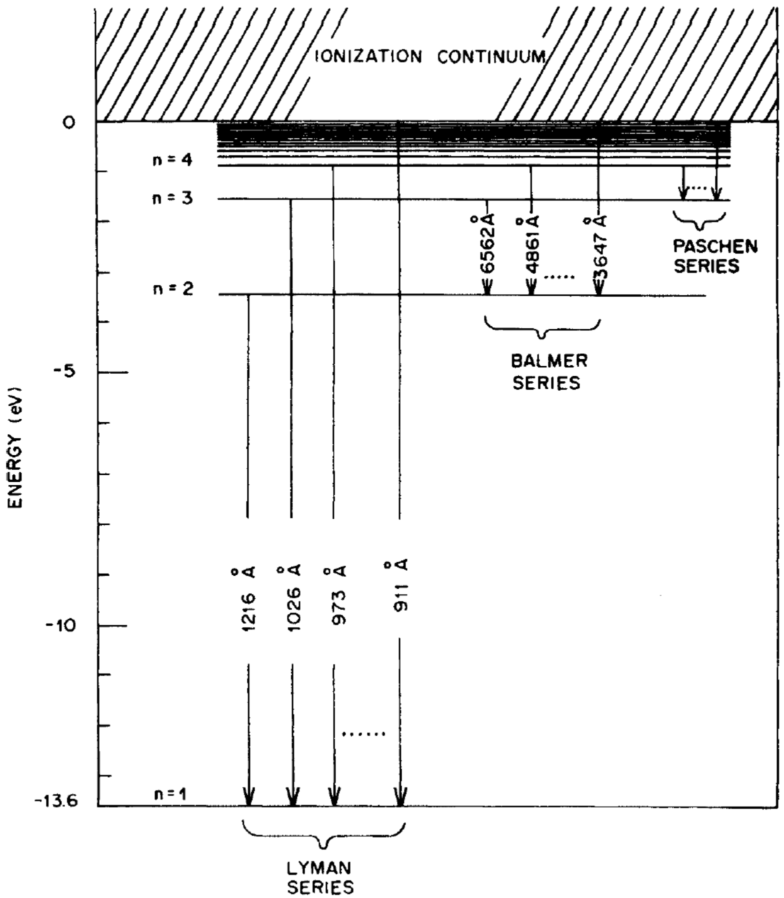
Bohr model (1913)

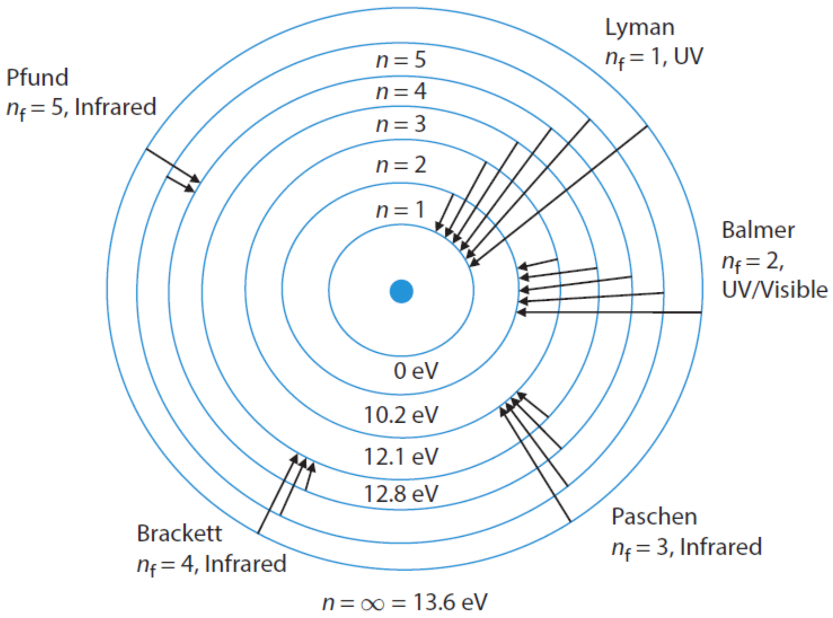
- Bohr model explains the line emissions well.

$$h\nu = \frac{hc}{\lambda} = \frac{k_0^2 Z^2 e^4 m}{2\hbar^2}\left(-\frac{1}{n_i^2} + \frac{1}{n_f^2}\right)$$

$$\frac{1}{\lambda} = \underline{1.09737 \times 10^7} Z^2 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \text{m}^{-1}$$

Rydberg constant





Example

Example

Calculate the wavelength of the third line in the Balmer series in Fig. 2.1. What is the photon energy in eV?

Solution

$$\frac{1}{\lambda} = 1.09737 \times 10^7 \left(\frac{1}{4} - \frac{1}{25}\right) = 2.30448 \times 10^6 \text{ m}^{-1} \qquad = 434 \text{ nm}$$

$$E = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{4.34 \times 10^{-7}} = 4.58 \times 10^{-19} \text{ J} \qquad = 2.86 \text{ eV}$$

Example

Calculate the angular velocity of the electron in the ground state of He^+.

Solution

With quantum number n, the angular velocity ω_n in radians s^{-1} is equal to $2\pi f_n$, where f_n is the frequency, or number of orbital revolutions of the electron about the nucleus per second. In general, $f_n = v_n/(2\pi r_n)$; and so $\omega_n = v_n/r_n$. With $n = 1$ and $Z = 2$, Eqs. (2.8) and (2.9) give $\omega_1 = v_1/r_1 = 1.66 \times 10^{17}$ s^{-1}, where the dimensionless angular unit, radian, is understood.

de Broglie wave (1924)

- The wavelength of a photon is specified by its momentum according to the relation

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

- de Broglie suggested that this is a completely general one that applies to material particles as well as to photons. The momentum of a particle of mass m and velocity v is $p = \gamma m v$, and its de Broglie wavelength is accordingly

$$\lambda = \frac{h}{\gamma m v}$$

Example

Calculate the de Broglie wavelength of a 10-MeV electron.

Solution

$$10 = 0.511(\gamma - 1) \qquad \gamma = 20.6$$

$$\lambda = \frac{h}{\gamma m c} = \frac{6.63 \times 10^{-34}}{20.6 \times 9.11 \times 10^{-31} \times 3 \times 10^{8}} = 1.18 \times 10^{-13} \text{ m.}$$

Schrodinger equation (1926)

- In quantum mechanics, the wave function Ψ is not itself a measurable quantity and may therefore be complex.

$$\Psi = Ae^{-i\omega(t-x/v)} \quad \Rightarrow \quad \Psi = Ae^{-2\pi i(\nu t - x/\lambda)}$$

- In terms of the total energy E and momentum p of the particle

$$\Psi = Ae^{-(i/\hbar)(Et-px)} \quad \Leftarrow \quad E = h\nu = 2\pi\hbar\nu \quad \text{and} \quad \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$$

- Differentiating it, and using energy-momentum relation

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi$$

$$p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2}$$

$+$

$$\frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi$$

$$E\Psi = -\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}$$

$+$

$$E\Psi = \frac{p^2\Psi}{2m} + U\Psi$$

Time-dependent Schrödinger equation in one dimension

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

Schrodinger equation (1926)

- Separation of variables

$$\Psi = Ae^{-(i/\hbar)(Et-px)} = Ae^{-(iE/\hbar)t}e^{+(ip/\hbar)x} = \psi e^{-(iE/\hbar)t}$$

$$E\psi e^{-(iE/\hbar)t} = -\frac{\hbar^2}{2m} e^{-(iE/\hbar)t}\frac{\partial^2\psi}{\partial x^2} + U\psi e^{-(iE/\hbar)t}$$

Steady-state Schrödinger equation in one dimension

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U$$

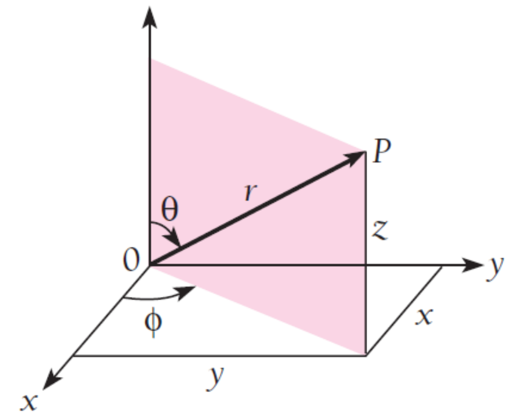
Schrödinger's equation

$$\hat{H}\psi_{\mathrm{n}} = E_n\psi_n$$

Schrodinger equation for hydrogen atom

- In spherical polar coordinates, Schrödinger's equation is written

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}(E-U)\psi=0$$



$x = r\sin\theta\cos\phi$
$y = r\sin\theta\sin\phi$
$z = r\cos\theta$

Electric potential energy

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

Hydrogen atom

$$\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r}+E\right)\psi=0$$

Schrodinger equation for hydrogen atom

- Separation of variables

Hydrogen-atom wave function

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Equation for Φ

$$\frac{d^2\Phi}{d\phi^2} + m_l^2\Phi = 0$$

Equation for Θ

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left[l(l+1) - \frac{m_l^2}{\sin^2\theta}\right]\Theta = 0$$

Equation for R

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[\frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r} + E\right) - \frac{l(l+1)}{r^2}\right]R = 0$$

Principal quantum number $n = 1, 2, 3, \ldots$

Orbital quantum number $l = 0, 1, 2, \ldots, (n-1)$

Magnetic quantum number $m_l = 0, \pm 1, \pm 2, \ldots, \pm l$

Schrodinger equation for hydrogen atom

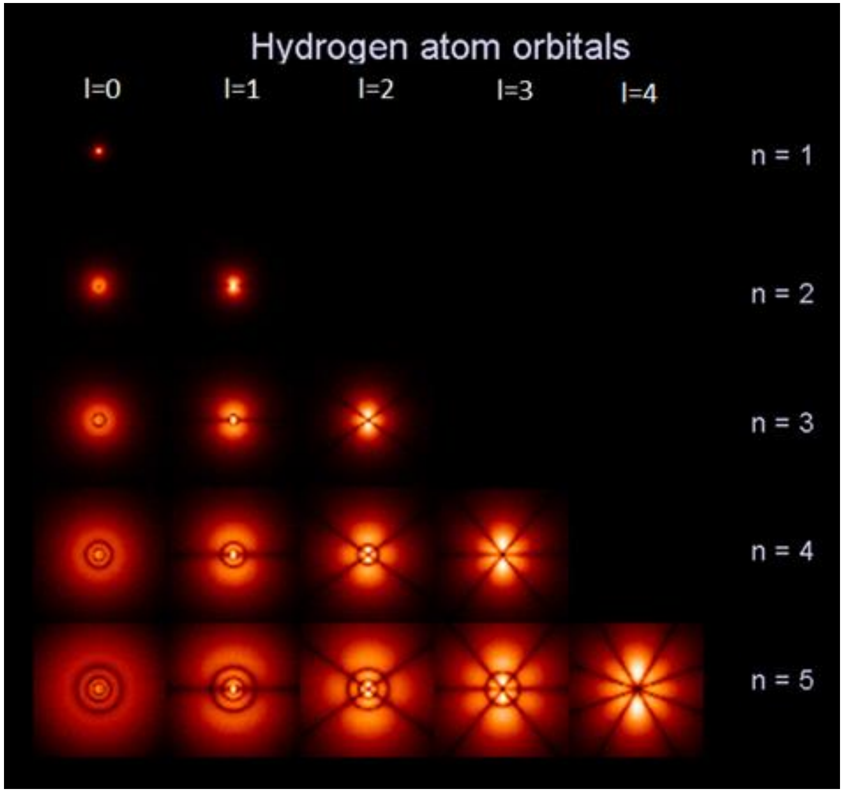
- The electron wave functions of the hydrogen atom

$$\psi = R_{nl}\Theta_{lm_l}\Phi_{m_l}$$

Table 6.1 Normalized Wave Functions of the Hydrogen Atom for $n = 1, 2,$ and 3*

n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r, \theta, \phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\,a_0^{3/2}}e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\,a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\,a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$
2	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\,a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\,a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\cos\theta$
3	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}(3\cos^2\theta-1)$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}(3\cos^2\theta-1)$
3	2	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	$\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin^2\theta\, e^{\pm 2i\phi}$

*The quantity $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 5.292 \times 10^{-11}$ m is equal to the radius of the innermost Bohr orbit.



Fine structure: quantum numbers

- To describe an atom completely, it is necessary to utilize four quantum numbers: principal, azimuthal, magnetic, and spin.

Spin angular momentum

$$S = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

Table 7.1 Quantum Numbers of an Atomic Electron

Name	Symbol	Possible Values	Quantity Determined
Principal	n	$1, 2, 3, \ldots$	Electron energy
Orbital	l	$0, 1, 2, \ldots, n-1$	Orbital angular-momentum magnitude
Magnetic	m_l	$-l, \ldots, 0, \ldots, +l$	Orbital angular-momentum direction
Spin magnetic	m_s	$-\frac{1}{2}, +\frac{1}{2}$	Electron spin direction

Table 7.3 Subshell Capacities in the M ($n = 3$) Shell of an Atom

	$m_l = 0$	$m_l = -1$	$m_l = +1$	$m_l = -2$	$m_l = +2$	
$l = 0$:	↓↑					↑$m_s = +\frac{1}{2}$
$l = 1$:	↓↑	↓↑	↓↑			↓$m_s = -\frac{1}{2}$
$l = 2$:	↓↑	↓↑	↓↑	↓↑	↓↑	

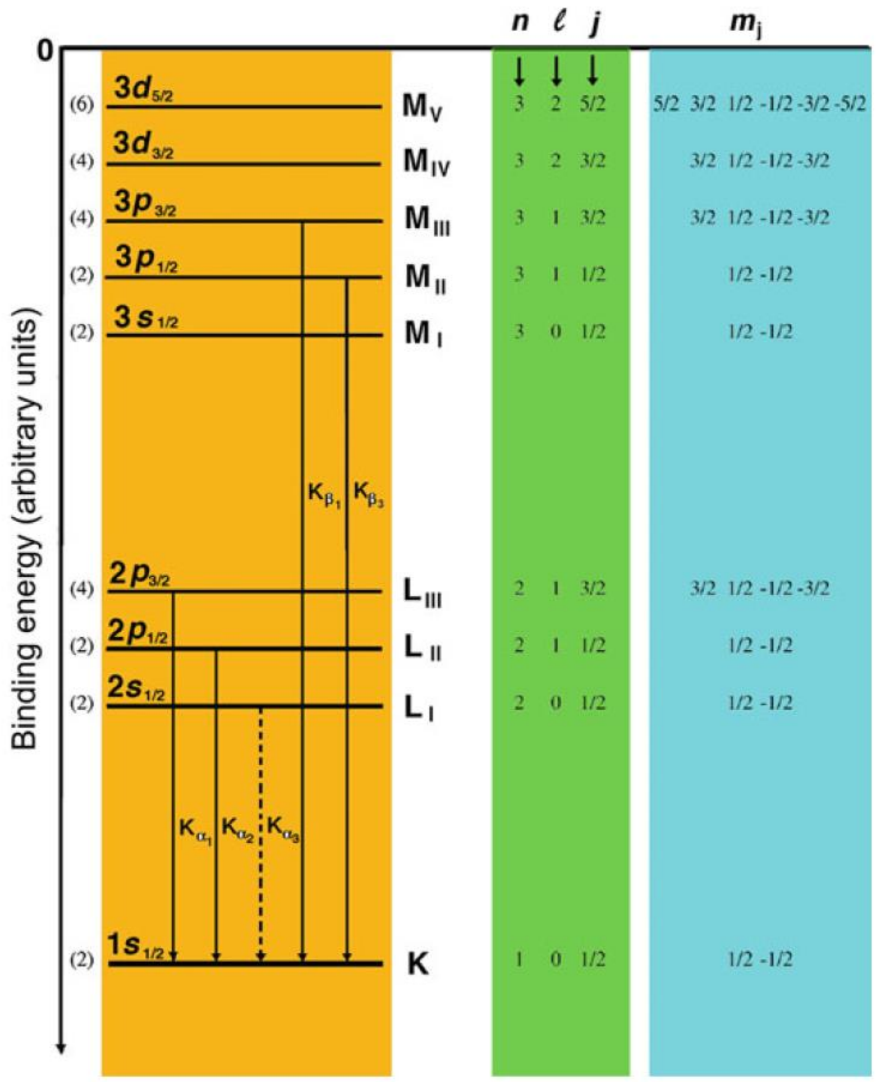
Selection rule

- Total angular momentum

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$J = \sqrt{j(j+1)}\hbar \qquad j = l + s = l \pm \tfrac{1}{2}$$

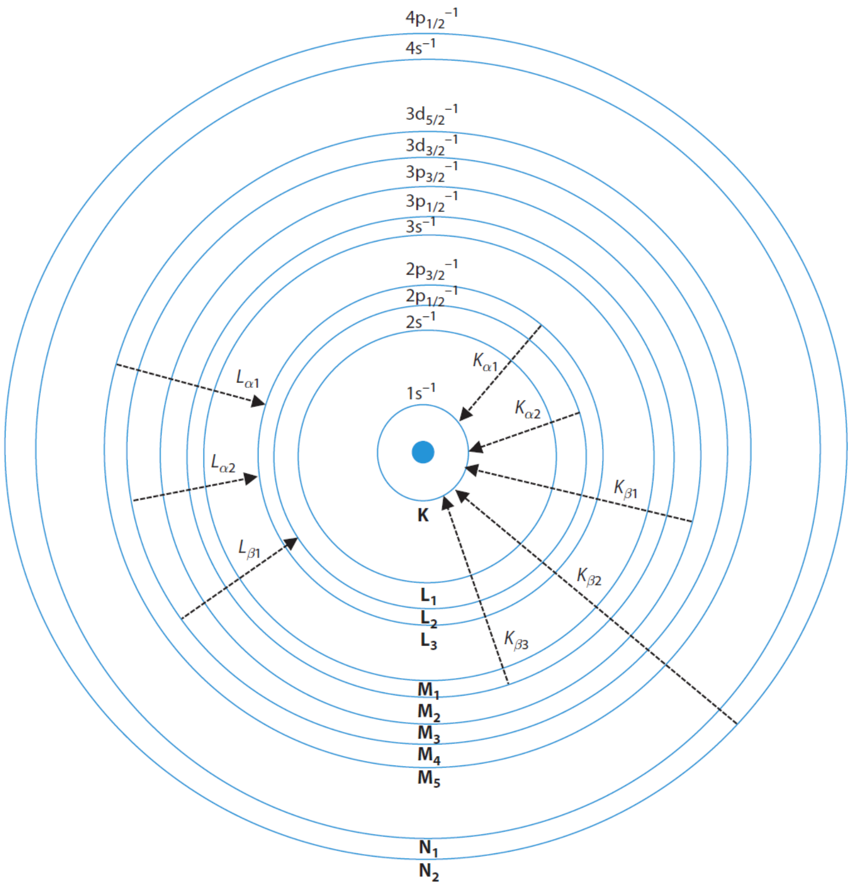
$$J_z = m_j\hbar \qquad m_j = -j, -j+1, \ldots, j-1, j$$

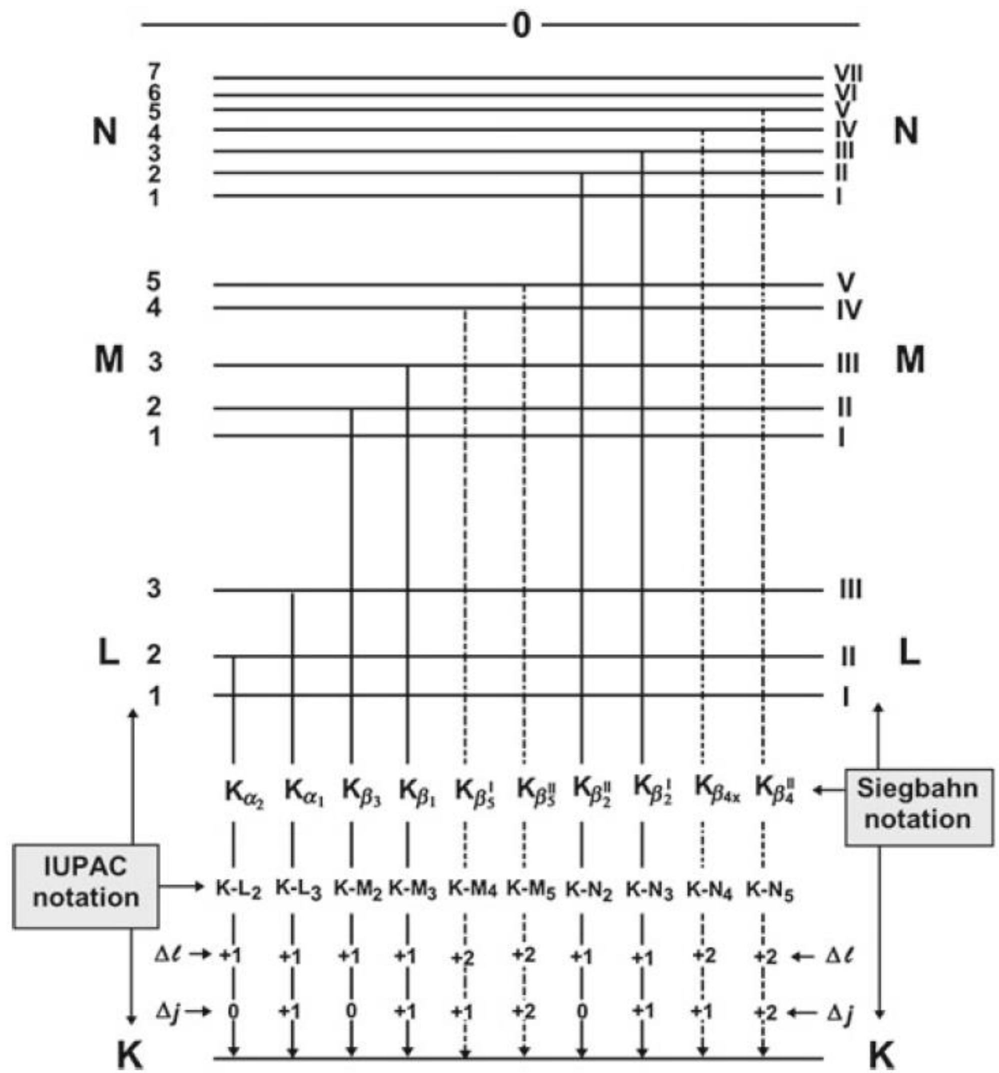


- Allowed transitions

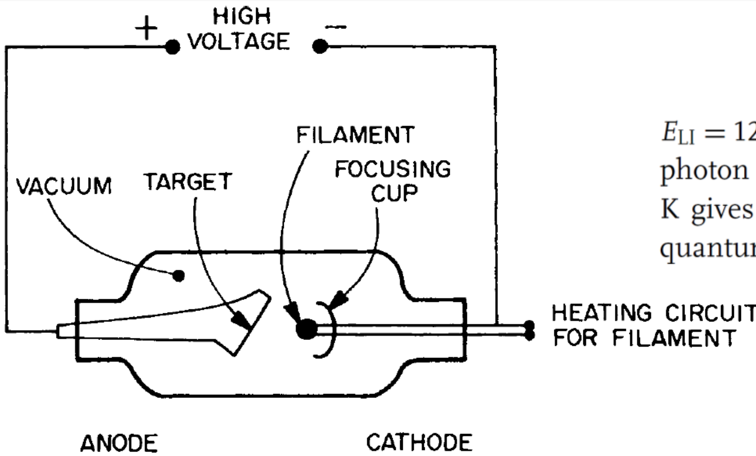
$$\Delta\ell = \pm 1 \quad \text{and} \quad \Delta j = 0 \quad \text{or} \quad \pm 1.$$

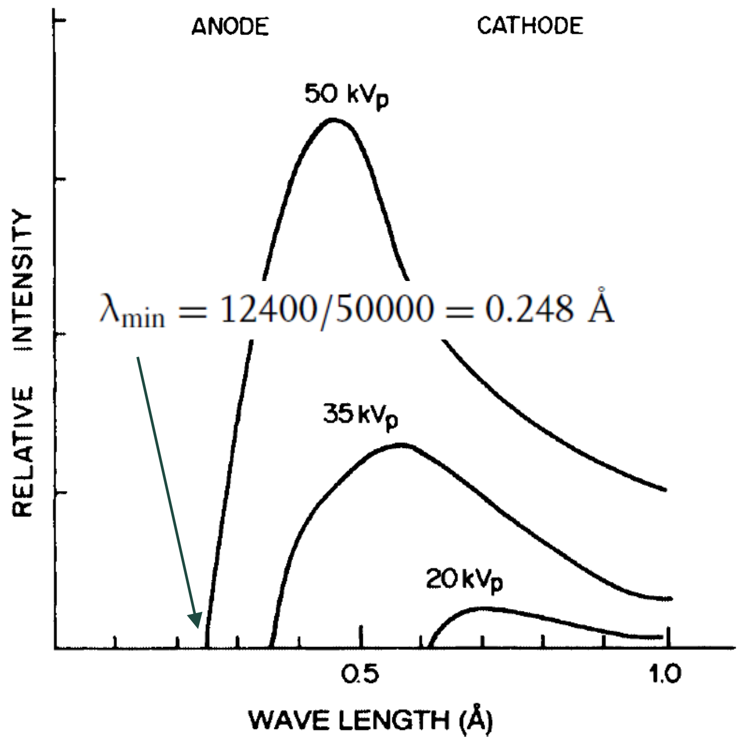
Characteristic X-ray





Continuous and characteristic X-rays

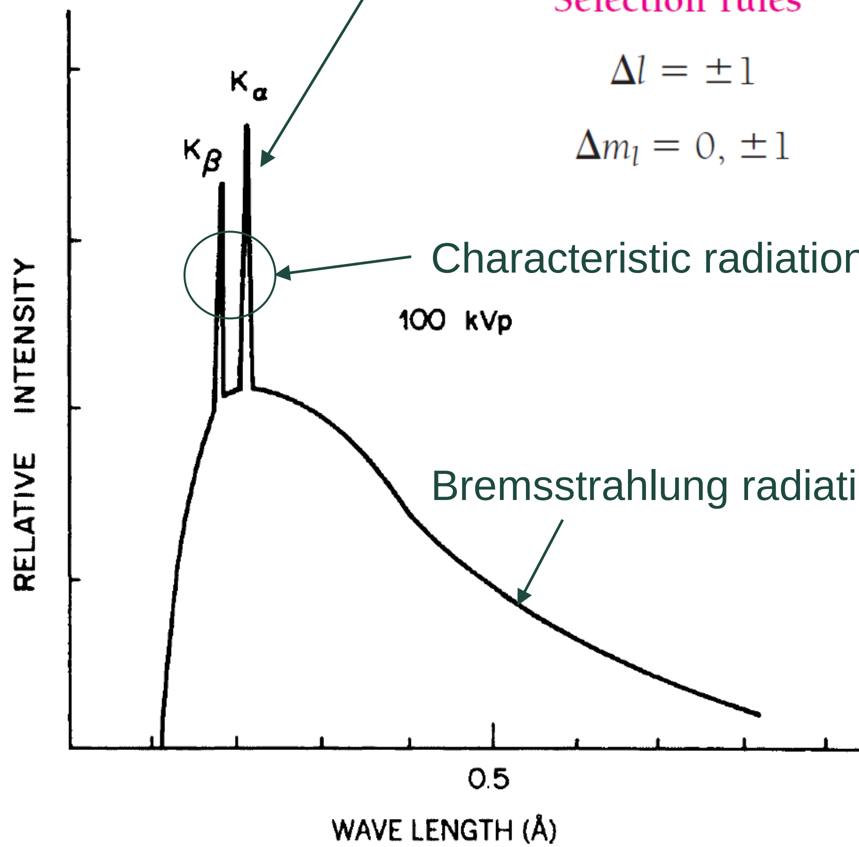




$\lambda_{\min} = 12400/50000 = 0.248$ Å

K-shell binding energy E_K = 69.525 keV for W

$E_{\mathrm{LI}} = 12.098$, $E_{\mathrm{LII}} = 11.541$, and $E_{\mathrm{LIII}} = 10.204$. The transition LIII → K gives a $K_{\alpha 1}$ photon with energy $E_{\mathrm{K}} - E_{\mathrm{LIII}} = 69.525 - 10.204 = 59.321$ keV; the transition LII → K gives a $K_{\alpha 2}$ photon with energy 57.984 keV. The optical transition LI → K is quantum mechanically forbidden and does not occur.



Selection rules

$$\Delta l = \pm 1$$

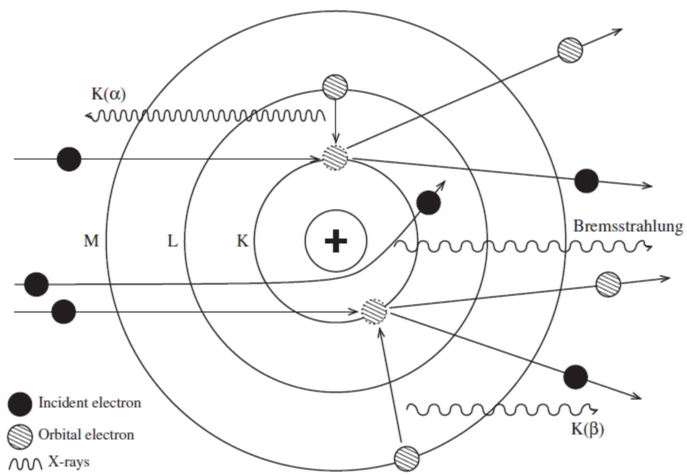
$$\Delta m_l = 0, \pm 1$$

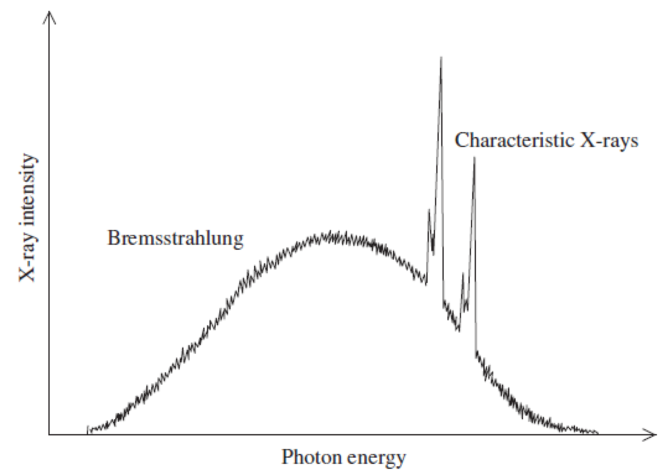
Characteristic radiation

Bremsstrahlung radiation

Bremsstrahlung and characteristic X-rays

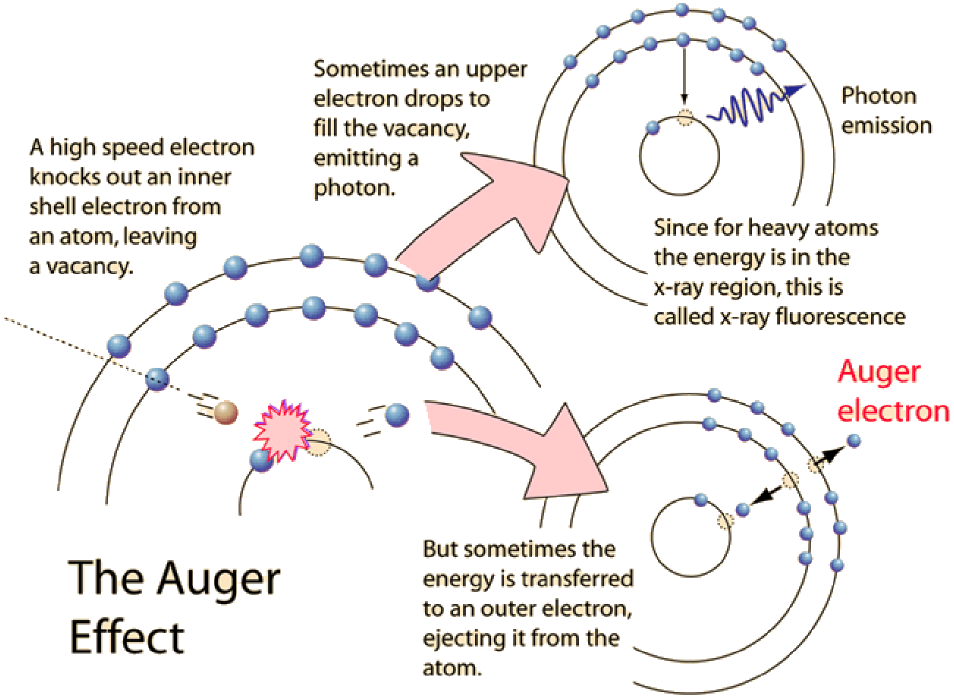
- Bremsstrahlung (braking radiation) refers to the radiation emitted by charged particles when they decelerate in a medium. In the case of X-rays, the high-energy electrons decelerate quickly in the target material and hence emit Bremsstrahlung. The emitted X-ray photons have a continuous energy spectrum since there are no quantized energy transitions involved in this process.
- The electrons incident on a target may also attain sufficient energies to knock off electrons from the internal atomic shells of target atoms, leaving them in unstable states. To regain atomic stability, the electrons from higher energy levels quickly fill these gaps. During this, so-called characteristic X-ray photons have energies equal to the difference between the two energy levels are emitted. The energy of emitted photons does not depend on the energy or intensity of the incident electron.





Auger effect

- The Auger effect is a physical phenomenon in which the filling of an inner-shell vacancy of an atom is accompanied by the emission of an electron from the same atom. When a core electron is removed, leaving a vacancy, an electron from a higher energy level may fall into the vacancy, resulting in a release of energy. Although most often this energy is released in the form of an emitted photon, the energy can also be transferred to another electron, which is ejected from the atom; this second ejected electron is called an Auger electron.



Homework

- J. Turner, Atoms, Radiation, and Radiation Detection, Wiley (2007), chapter 2

  Problems: 14, 19, 35, 53