Structure of matter, matter wave

Tamás Bozó

Nanobiotechnology and Molecular Biophysics Workgroup
Department of Biophysics and Radiation Biology

03 October 2018

Overview

Topics:

- atomic structure
- atomic modells
- dual nature of electron
- propagation of free and bound electron
- quantum states

Related exam questions:

6. Proofs of particle-wave duality in case of electron. Matter waves in bound and free cases.

***Textbook chapters:* I/1.1 -1.4**

Related practices: *Light emission, Light absorption*

Matter

elements | **compounds**

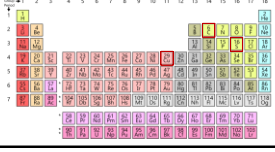
e.g.:

carbon sulphur copper

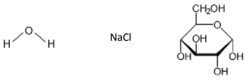
e.g.:

water salt glucose

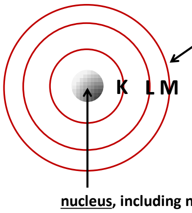
building blocks: atoms
(chemically undividable)



building blocks: molecules



Atomic structure



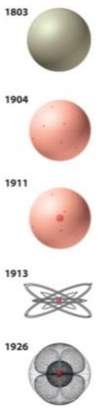
energy levels (shells) with
K: max. 2 e^-
L: max. 8 e^-
M: max. 18 e^-
N: max. 32 e^-
O: max. 50 e^-
P: max. 64 e^-
Q: max. 98 e^-

nucleus, including nucleons:
protons (p^+)
neutrons (n^0)

chemical properties!

***Z*: atomic number = number of protons (= number of electrons)**
***N*: neutron number**
***A*: mass number = Z+N**
(Nuclear structure will be detailed in Lecture 11.)

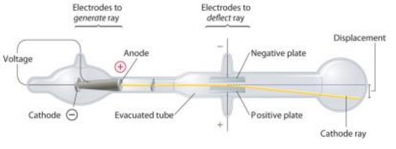
History of the atom



~ 400 B.C.	**Demokritus:** atoms (ἄτομος) are miniscule quantities of matter.
1803	**J. Dalton:** stoichiometric law, every elements consists of identical constituens, billiard ball model
1900	**M. Plack:** Radiation law, quantum physics
1897-1904	**J.J. Thomson:** cathode ray: discovery of electron, mass of electron „plum pudding" model
1910	**R.A. Millikan:** charge of electron
1909-11	**E. Rutherford:** discovery of nucleus, planetary model
1913	**N. Bohr:** discrete energy states, Bohr-model
1914	**J. Franck, G.L. Hertz:** evidence of energy quanta
1923	**L.V. de Broglie:** electron wave
1926	**E. Schrödinger:** wave function, quantummechanical atomic model
1927	**W. Heisenberg:** uncertainty relation
1927-28	**C.J. Davisson, L.H. Germer, G.P. Thomson:** evidence of electron waves
1932	**J. Chadwick:** discovery of neutron

Discovery of electron (1897)

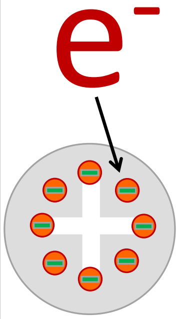
Sir Joseph John Thomson
1856-1940



Thomson's cathode ray tube

Observations	Conclusions
Ray deflects in electric and magnetic field toward positively charged electrode	CR consist of negatively charged particles („corpuscules") .
Very low *m/q* ratio.	These particles are either very light or highly charged.
The *m/q* ratio is independent of the nature of cathode (or filling gas).	These particles are fundamental components of all atoms.

Thomson's plum-pudding model (1904)

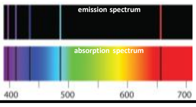


- Particles of small mass and negative charge (electrons)
- distributed symmetrically around the center of a
- homogeneous,
- positively charged,
- liquid-like substance that
- gives the vast majority of mass of the atom.

$m_{electron} = 9.109 \cdot 10^{-31} kg$

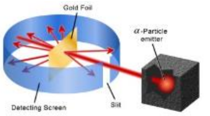
$q_{electron} = -e = 1.602 \cdot 10^{-19} C$

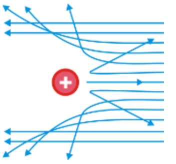
Problems with the model:
- e.g.: Could not explain the line spectrum of H_2 gas.



Discovery of atomic nucleus (1909)

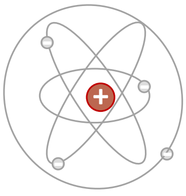

Sir Ernest Rutherford
1871-1937





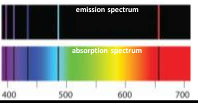
Observations	Conclusions
99.995% of all α particles suffered only slight deflection.	Density of the atom is inhomogeneous. bulk mass is concentrated in a small volume inside. This volume in 10^5 times smaller than that of the atom.
0.005% of all α particles bounced back through 180°.	This core has to be positively charged.

Rutherford's modell



- „Tiny solar system"
- Electrons (light, negatively charged particles) orbiting around the nucleus (heavy, positively charged particle).
- Coulomb interactions keep electrons orbiting.

Problems with the model:
- Such an atom cannot be stable (orbiting electrons accelerates→ accelerated charges radiate → they lose energy and fall into nucleus)
- Could not explain the line spectrum of H_2 gas.



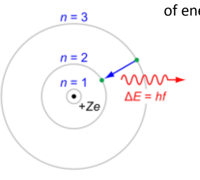
Niels Bohr's atomic model (1913)


Niels Henrik David Bohr
1885-1962

Postulate I: Electrons can occupy only certain distinct orbits (numbered as n=1, 2, 3, ...). Being on these orbits they do not radiate, but have constant energy (E_1, E_2, E_3,...).

$$\underbrace{m_e \cdot v \cdot r}_{\substack{\text{angular momentum} \\ L\ [kg \cdot m^2 \cdot s^{-1}]}} = n \cdot \frac{h}{2\pi} = n \cdot \hbar$$

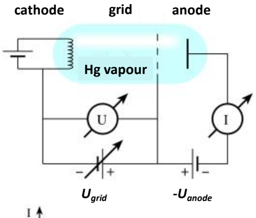
Postulate II: Emission (radiation) take place when an electron jumps to a lower energy orbit. Upon absorption of energy electron can jump to a higher energy orbit.

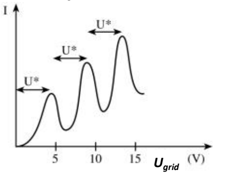


$$\Delta E = E_m - E_i = h \cdot f$$

- Explained well the line spectrum of H_2.
- BUT failed to explain the spectra of larger atoms, relative intensities of spectral lines, and a few further phenomena.

Franck-Hertz experiment (1914)






James Franck
1882-1964

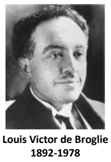

Gustav Ludwig Hertz
1887-1975

Conclusion
Energy cannot change continously but only by certain discrete values: quanta. *(Direct evidence of energy quanta!)*

The wave nature of the electron (1923)

Einstein: mass-energy equivalence	**Planck:** radiation law	**Maxwell:** speed of light
$E = mc^2$	$E = h \cdot f$	$c = \lambda \cdot f$

de Broglie: If light is a particle, can electron be a wave?


Louis Victor de Broglie
1892-1978

$$\left.\begin{matrix} m \cdot c^2 = h \cdot \dfrac{c}{\lambda} \\ \\ p = m \cdot v \end{matrix}\right\} \quad \begin{matrix} \lambda = \dfrac{h}{m \cdot v} = \dfrac{h}{p} \\ \\ p = \dfrac{h}{\lambda} \end{matrix}$$

Wave-particle duality: Electron is at once a subatomic particle, with well defined mass and charge AND a wave.

Generalization: Matter waves (particles of matter have wave-like properties.)

Interference experiments (1927-28)

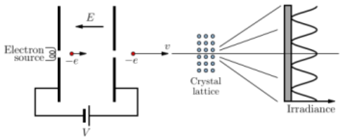
J.Davisson and L.H.Germer

G. P. Thomson

Experimental proof of wave nature: Interference of electron beams on crystals and metal foils.

Davisson, *Germer* and *Thomson* used electron beams to induce diffraction on a thin metal foils or crystals.

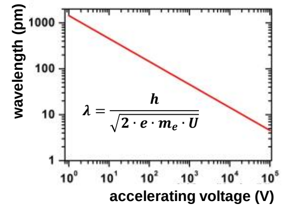
Interference pattern appeared, which is a clear evidence of wave-like properties.



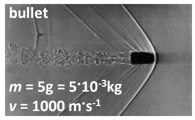
Wavelength of electron (e.g.: in a cathode ray tube)

$$\left.\begin{array}{l}\lambda = \dfrac{h}{p}\\ p = m_e \cdot v\end{array}\right\} \lambda = \frac{h}{m_e \cdot v}$$

$$\left.\begin{array}{l}E_{pot} = e \cdot U\\ E_{kin} = \dfrac{1}{2} \cdot m_e \cdot v^2\\ E_{kin} = E_{pot}\end{array}\right\} v = \sqrt{\frac{2 \cdot e \cdot U}{m_e}}$$



Why don't we observe the wave properties of macroscopic objects?

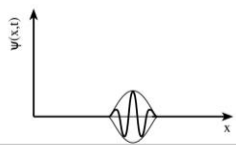


$$\lambda = \frac{h}{m \cdot v} = \frac{6.626 \cdot 10^{-34}\ m^2 \cdot kg \cdot s^{-1}}{5 \cdot 10^{-3}\ kg \cdot 1000\ m \cdot s^{-1}} = \mathbf{1.325 \cdot 10^{-34} m}$$

The wave nature of the electron

Ervin Schrödinger
1887-1961

A wave function (or state function) ***Ψ(x,t)*** is used to describe the amplitude of the electron wave as a function of position ***(x)*** and time ***(t)***.
Electron is pictured as a continous charged cloud of finite size with a charge density proportional to ***Ψ²*** at any point in space.



visualization: wave package

location: where *Ψ(x,t)* ≠ 0
momentum (*p*): given by the shape

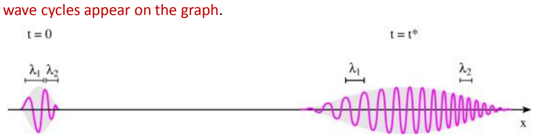
Propagation law of free electrons (1926) (e.g. vacuum tube electron)

1. Ψ(x,t) ≠ 0 holds for more than one point → position cannot be determined with a simple numeric value.

2. The function is nonperiodic → cannot be characterised by a single wavelength → Any λ between an approximate largest λ_1 and smallest λ_2 wavelength can characterize the wave package.

Since $p = \dfrac{h}{\lambda}$, $v = \dfrac{p}{m_e}$ and $s = v \cdot t$

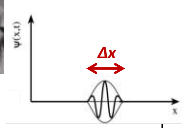
Neither momentum (p), nor speed (v) nor displacement (s) can be described by a well determined single value → they can be characterised by any value between p_1 and p_2, v_1 and v_2, s_1 and s_2 → Ψ(x,t) will disperse while propagating and new wave cycles appear on the graph.



Heisenberg uncertainty relation (1927):

Werner Karl Heisenber
1901-1976

A wave function(or state function) ***Ψ(x,t)*** is completely determined, although some pieces of the information it carries (e.g. position, momentum, velocity of the electron) are uncertain.



$$\Delta x \cdot \Delta p \geq h$$

Δx: uncertainty of position
Δp: uncertainty of momentum
h: Planck's constant

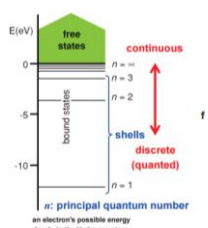
Conclusion: *The more determined the positon (x) of an electron, the less determined the momentum (p), and vice versa.*

It can be extended to other pairs of physical properties (complementary variables) of a particle, eg. energy and time:

$$\Delta E \cdot \Delta t \geq h$$

What about electrons bound in an atom?

1. External force field is present due to the positively charged nucleus.
2. The field will move (distort) the state function of the electron to its own direction.
3. Electrons do not have enough energy to leave the proximity of the nucleus, they are in bound state.
4. Electrons disperse due to the uncertainty of their momentum.



As a result:
A dynamic equilibrium evolves between the attractive effect of nucleus and the dispersing nature of the state function.
Stationary , symmetric state functions emerge to form discrete, strictly differentiated, well defined atomic electron states.

$\psi(x)$

Properties of quantized atomic electron states

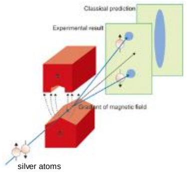
Bound electrons – quantized energy levels. Their state of the electron can be described by **quantum numbers**:

quantum number	possible values	characterizes	describes
principal	n=1,2,3...7	electron shell	energy level
azimuthal	l=0,1,2,...(n-1) or: s, p, d, f	subshell	magnitude of orbital angular momentum
magnetic	m_l=-l,....0,....+l	specific orbital within subshell	direction of orbital angular momentum
spin	m_s=±1/2	intrinsic angular momentum (spin*) of an electron	direction of the spin (magnitude is constant)

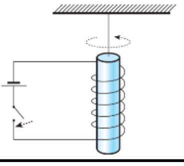
All the four quantum numbers are required to characterize a bound-state electron.

*Intrinsic angular momentum (spin) of the electron

Stern-Gerlach experiment

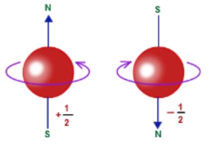


Einstein-de Haas experiment



Conclusions:

- Electrons possess an intrinsic magnetic moment.
- Electrons possess an intrinsic angular momentum.
- Spin takes a quantized value and direction



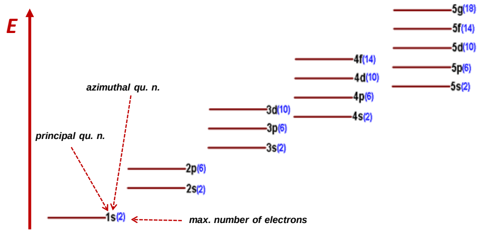
Spin quantum number: m_s or s= ±1/2

How will electrons occupy their quantum states?

Pauli exclusion principle: Within an atom there cannot be two electrons with all four quantum numbers being identical.

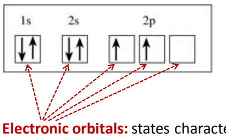
Principle of minimum energy: The total energy of the system should be minimized.

Hund principle: For a given electron configuration, the state with maximum total spin has the lowest energy.



How will electrons occupy their quantum states?

An example: **carbon** , Z=6

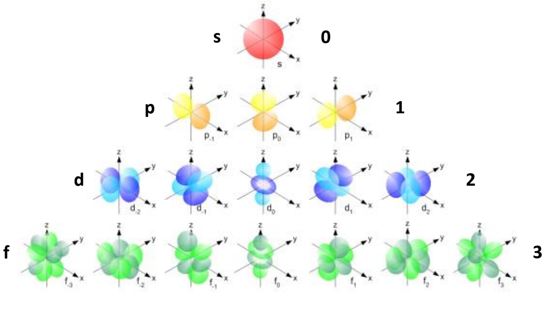


diamond graphite

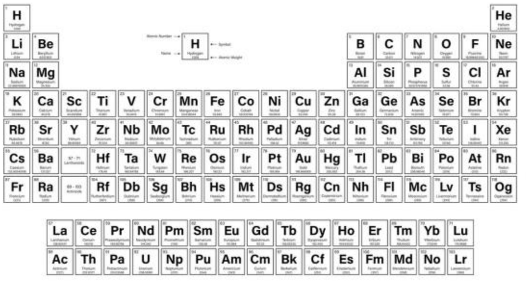
Electronic orbitals: states characterized by n, l and m_l quantum numbers, which may be occupied by at most 2 electrons of oposite spins.

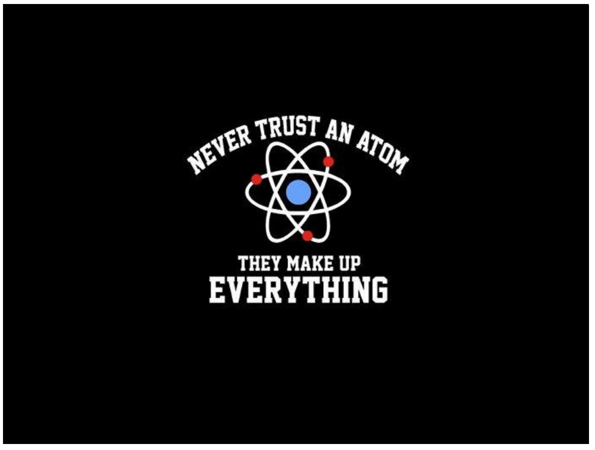
Configuration: Gives the (partially or fully) occupied subshells and the number of equivalent (same subshell)electrons.

Visualization of subshell structure



Periodic Table of the Elements




NEVER TRUST AN ATOM
THEY MAKE UP
EVERYTHING