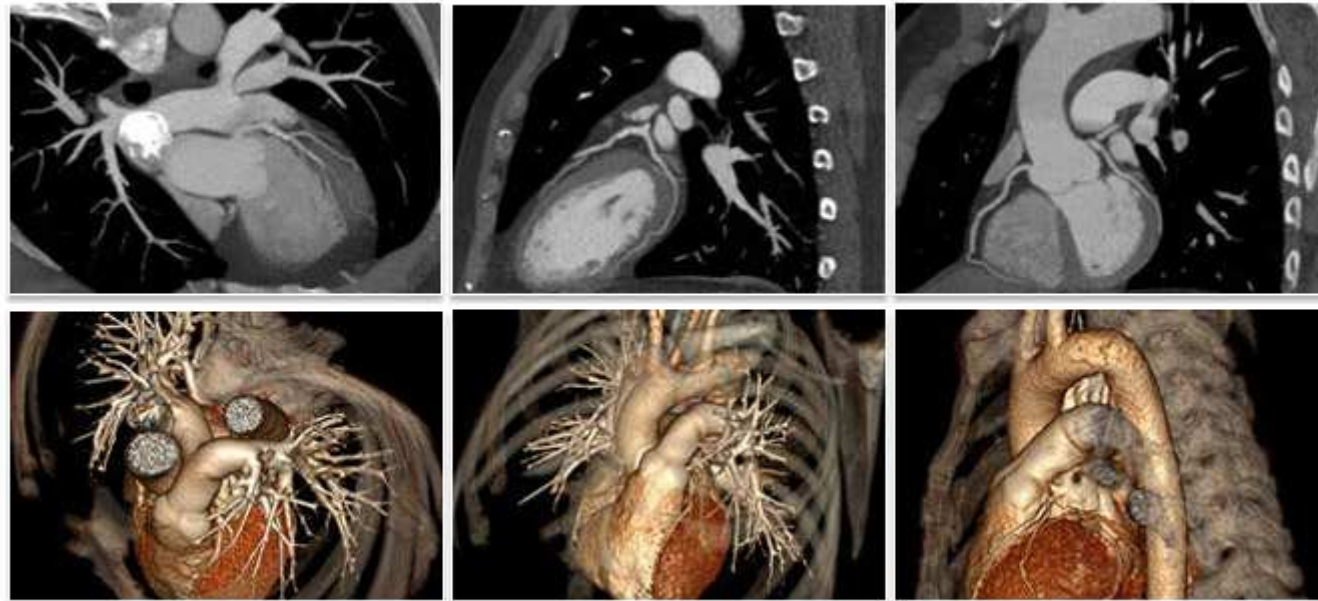

Quantum, atomic and nuclear physics

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Introduction

- The principles and applications of modern physics, which encompasses a lot of quantum, atomic and nuclear physics, are extremely important for biomedical sciences.
- Almost all imaging methods used in medicine are based on this part of physics.



Basics

- Before we start to describe the processes occurring on the atomic and subatomic level of matter, it is necessary to define a “new” unit of energy, which is very often used when speaking about individual particles and their small assemblies – molecules. The main SI unit of energy – the joule – is too big for that purpose. Therefore, the small amounts of energy carried by individual elementary particles, atoms, chemical bonds etc. are measured in units called electron volts:

$$1 \text{ electron volt [eV]} = 1.602 \times 10^{-19} \text{ J.}$$

- 1 electron volt is the energy obtained by one electron when accelerated in an electrostatic field by 1 V potential difference. The potential energy of charged particle $E=W=eU$ changes into its kinetic energy during the acceleration.
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Basics

- 1 mole is such an amount of substance which contains such number of particles as present in a sample of the nuclide carbon-12 which mass is equal to 0.012 kg.
 - Avogadro's constant: $N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$
 - Is the number of particles in 1 mole of any substance.
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Basics

- Atomic mass constant is 1/12 of the mass of carbon-12 nuclide atom: $m_u = 1.66 \times 10^{-27}$ kg.
- Molar mass (M_m) is the mass of 1 mole of a substance. It is equal to the sum of atomic masses of the atoms forming one molecule expressed in grams.
- Molar volume (V_m) is the volume of 1 mole of a substance:

$$V_m = M_m / \rho$$

where ρ is density of the substance.

Basics

- Subatomic particles (e.g. electrons, protons, neutrons) are not only small rigid balls, but also possess some wave properties. Their wave motion (oscillation) manifest itself as de Broglie waves, with wavelength given by formula:

$$\lambda = h/p = h/mv,$$

where λ is the wavelenghts of the de Broglie waves [m], h is the Planck's constant and p is the momentum of the particle [kg.m.s⁻¹].

- Evidences for the wave properties of the particles are the diffraction and interference phenomena.
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Basics

- Each atom consist of a nucleus and electron shells.
 - The internal energy of atoms is **quantized**. It means that only discrete values of energy are possible or achievable.
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Basics - Electron shells

Schrödinger's Equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r}, t) \psi(\mathbf{r}, t)$$

i is the imaginary number, $\sqrt{-1}$.

\hbar is Planck's constant divided by 2π : 1.05459×10^{-34} joule-second.

$\psi(\mathbf{r}, t)$ is the wave function, defined over space and time.

m is the mass of the particle.

∇^2 is the Laplacian operator, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.

$V(\mathbf{r}, t)$ is the potential energy influencing the particle.

- The wave function is a complex mathematical function. Is a solution of the Schrödinger equation and determining the possible states of electrons located in electromagnetic field.
- Important is to know that the absolute squared value of wave function expresses the probability that a particle exists in a certain part of space (in the close vicinity of the atomic nucleus) called „**orbital**“ (electron cloud theory...)

Electron shells

- Quantum mechanics model of the hydrogen atom:
- Quantum numbers:
 - 1. **Principal quantum number** $n = 1, 2, 3, \dots$
 - It determines mainly energy of electrons.
 - The respective electron shells are marked by capital letters K ($n=1$), L ($n=2$), M ($n=3$), ...
 - For the simplest atom hydrogen we can write:





$$E_n = -\frac{E_1}{n^2}$$

where E_1 is the energy of the ground state of the electron ($n = 1$).

Note that the value of energy is negative because some work must be done to liberate the electron from the shell.

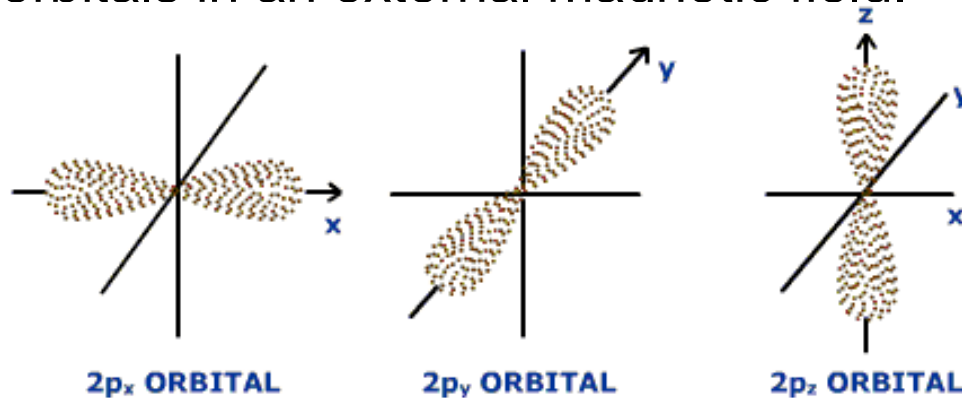
Electron shells

- Quantum mechanics model of the hydrogen atom:
 - Quantum numbers:
 - **2. Orbital momentum quantum number.**
 - It can take value 0, 1, 2, 3 ... $n - 1$ for each principal quantum number n .
 - The respective orbitals, i.e. the defined parts of space in which the electrons can be found with highest probability, are marked by letters s ($l = 0$), p ($l = 1$), d ($l = 2$), f ($l = 3$)...
 - These numbers determine the angular momentum of the electron, i.e. the shape of the orbital.
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Angular Momentum Quantum Number, ℓ	Name of Subshell	Shape	
0	s	Sphere	
1	p	Dumbbell	
2	d	Complex/double dumbbell	
3	f	More complex/multiple lobes	

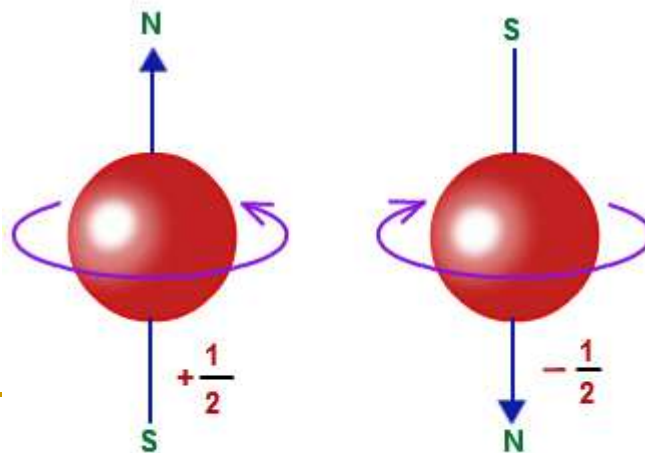
Electron shells

- Quantum mechanics model of the hydrogen atom:
- Quantum numbers:
 - 3. **Magnetic quantum number m .**
 - This can take values $0, \pm 1, \pm 2, \text{ and } \pm 3 \dots \pm l$ for each orbital quantum number l .
 - These numbers determine the allowed spatial orientations of electron orbitals in an external magnetic field.



Electron shells

- Quantum mechanics model of the hydrogen atom:
- Quantum numbers:
 - 4. **Spin quantum number s .**
 - It can take only two values: $\pm\frac{1}{2}$.
 - This number quantizes the intrinsic angular momentum of an electron, which can be imagined as being the rotation of an electron (say, clockwise and anti-clockwise).



Electron shells

- **Pauli's exclusion principle** states:

No two electrons in an atom can exist with the same set of four quantum number values.

- In atoms with a higher number of electrons, the energy of the electron depends also partly on the quantum numbers l , m , and s .
 - **Excitation** is a process in which an atom absorbs energy.
 - **Deexcitation** is a process in which an atom emits energy in the form of a photon.
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Spectral analysis

- Various physical bodies can absorb or emit ultraviolet, visible or infrared light.
 - This phenomenon can be explained on the basis of excitation and deexcitation processes.
 - Light is emitted mainly from hot bodies in which the atoms (or molecules) become repeatedly excited and then returning to the ground energetic state by deexcitation. Light absorption can be considered an important excitation process.
 - The dependence of intensity of emitted or absorbed light on light wavelength is called a **spectral curve**.
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Spectral analysis

- To obtain such a curve, it is necessary to disperse (separate) polychromatic light into its components which differ in their wavelength.
 - It can be done e.g. by prisms because the index of refraction depends on wavelength so that light of different wavelength is refracted through various angles. Another possibility is the use of diffraction gratings.
 - The instruments used to study absorbed and emitted light are called spectrographs (these serve only for visualization of absorption or emission spectra on a screen) or **spectrophotometers** (these serve for objective measurement of light absorption or emission).
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Spectral analysis

- The **emission spectrum** is obtained after passage of the light beam emitted from the substance under study through the prism or grating.
 - The **absorption spectrum** can be seen and measured after passage of polychromatic light through a solution of the substance under study followed by spectral analysis of the transmitted light.
 - In gases formed by atoms or very simple molecules, only light of certain (discrete) values of wavelength is absorbed or emitted. In such a case, we can see only bright lines on a black background (in emission spectra) or dark lines on a background of spectral colours (in absorption spectra) – we speak about **line spectra** in both cases.
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Spectral analysis

- Many molecules are so sensitive to high temperatures that they cannot emit light due to heating. Complex molecules dissolved in solution absorb light in a relatively wide interval of wavelength values. Thus, we can speak about **band spectra**. The **continuous spectra** of emitted light are found in hot solid bodies.
 - The existence of line spectra can be simply explained taking into account the discrete values of electron energies in atomic electron shells (they are given by the principal quantum numbers, $n = 1, 2, 3 \dots$).
 - Therefore, the changes of electron energy and energy values of emitted photons can also have only discrete values.
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Luminiscence



- **Chemiluminescence**, the emission of light as a result of a chemical reaction
 - **Mechanoluminescence**, a result of a mechanical action on a solid
 - **Photoluminescence**, a result of absorption of photons
 - Fluorescence, lifetime: nanoseconds
 - Phosphorescence, lifetime: milliseconds to hours
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Photoelectric effect

- We can observe this with electromagnetic radiation the energy of which is high enough to liberate electrons from matter.
- We already know that electromagnetic radiation propagates in the form of small quanta of energy, which are called photons. The energy of one photon is given by Planck's formula:

$$E = hf,$$

where h is the Planck's constant and f is the frequency.

Photoelectric effect

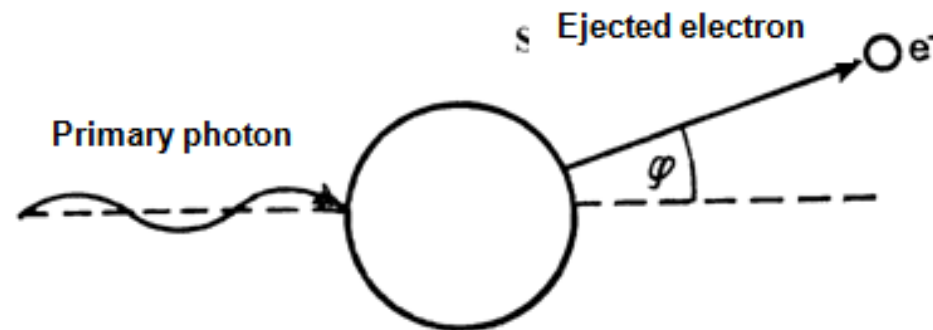
- The photoelectric effect is an energy transformation which is described by Einstein formula:

$$h.f = W_b + \frac{1}{2} mv^2$$

where hf is the energy of the incident photon, W_b is the binding energy of the electron (this energy must be delivered to eject an electron from an atom), m is the electron mass, v is its velocity, and the term $\frac{1}{2}mv^2$ is the kinetic energy of the ejected electron. When the ejected electron has no or only very small kinetic energy, i.e. $hf_0 = W_b$, f_0 is called the threshold (or limit) frequency. When $f > f_0$ the electrons are liberated from atoms.

Photoelectric effect

- Consequence:
- The energy carried by the ejected electrons does not depend on the intensity of the incident radiation (light) but on the energy (i.e. on the frequency and/or wavelength) of individual incident photons.



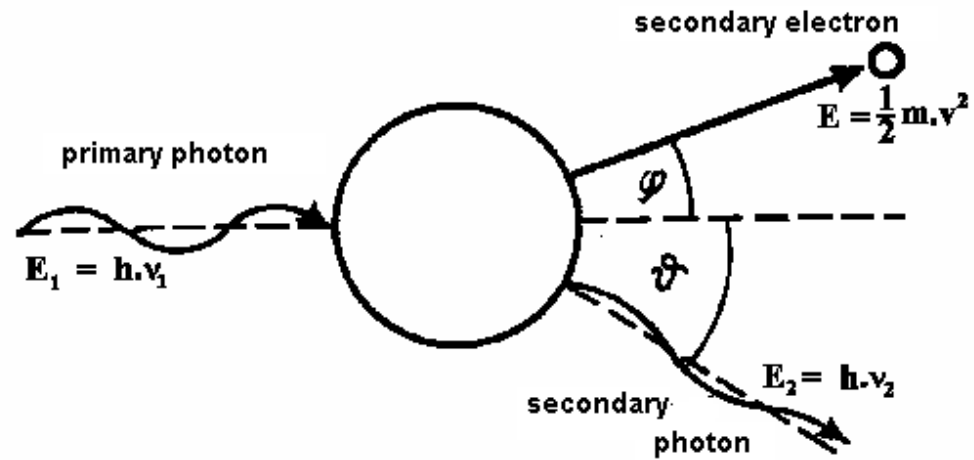
Compton scatter (effect)

- This is a phenomenon related to the photoelectric effect, occurring at higher energies of incident photons. The photon energy is not fully transformed into the kinetic energy of ejected electron and the energy necessary for ejection of the electron (binding energy W_b) so that a secondary photon of lower energy appears. Moreover, this binding energy is (in comparison with the energy of the secondary photon and the kinetic energy of electron) is so small that it can be neglected. The secondary photon does not travel in the same direction as the primary photon – it is scattered. So we can write:

$$hf = (W_b) + 1/2mv^2 + hf'$$

where hf' is the energy of the secondary photon ($f' < f$).

Compton scatter



Momentum of a photon

- A photon is a discrete amount of energy connected with oscillations of an electromagnetic field. Photons behave sometimes as particles with zero rest mass. They have even their own momentum which is given by the following equations:

$$p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda} \quad \left(\lambda = \frac{c}{f} \right)$$

- This photon momentum manifests clearly photons obey the Law of momentum conservation.
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