Daniel Jirák František Vítek BASICS OF MEDICAL PHYSICS

KAROLINUM

Basics of Medical Physics

Daniel Jirák František Vítek

Reviewed by: Ing. Milan Hájek, DrSc., Institute for Clinical and Experimental Medicine, Prague doc. RNDr. Otakar Jelínek, CSc., Institute of Biophysics and Informatics, First Faculty of Medicine, Charles University, Prague

Published by Charles University Karolinum Press Prague 2017 Edited by Alena Jirsova Setting and layout by Studio Lacerta (www.sazba.cz) First English edition

© Charles University, 2017 © Daniel Jirák, František Vítek, 2017

ISBN 978-80-246-3810-2 ISBN 978-80-246-3884-3 (pdf)



Charles University Karolinum Press 2018

www.karolinum.cz ebooks@karolinum.cz

CONTENTS

1.	STR	RUCTURE OF MATTER	9		
	1.1	Particles and force interactions	9		
	1.2	Energy	11		
	1.3	Quantum effects.	13		
		1.3.1 Quantum numbers	15		
	1.4	Hydrogen atom			
		1.4.1 Spectrum of the hydrogen atom	20		
	1.5	Electron structure of heavy atoms	20		
	1.6	Excitation and ionisation of atoms			
		1.6.1 Binding energy of electrons in an atom.	23		
	1.7	Principle of mass spectroscopy			
	1.8	1.8 Atomic nuclei			
		1.8.1 Binding energy of a nucleus			
		1.8.2 Magnetic properties of nuclei			
	1.9	Forces acting between atoms.	29		
		1.9.1 Ionic bonds	29		
		1.9.2 Covalent bonds	30		
	1.10	0 Physical basis of nuclear magnetic resonance tomography	32		
2.	MO	DLECULAR BIOPHYSICS	41		
	2.1	Molecular Bonds and Forces	41		
	2.2	Phases of matter.	43		
		2.2.1 Gaseous phase	44		
		2.2.2 Liquid phase	49		
		2.2.3 Solids	49		
		2.2.4 Plasma	50		
	2.3	Change of phases	50		
		2.3.1 Phase diagram	50		
		2.3.2 Gibbs law of phases.	51		
	2.4	Classification of dispersion system	52		
		2.4.1 Analytical dispersions	53		
		2.4.2 Colloidal dispersions	54		
	2.5	Water	60		
	2.6	Transport phenomena	63		
		2.6.1 Basic laws of fluids	63		
		2.6.2 Law of Laplace	64		
		2.6.3 Viscosity	66		
		2.6.4 The Hagen-Poiseuille law	68		
		2.6.5 Stokes law	69		
		266 Diffusion	70		

	2.7	Colligative properties of solutions	71
		2.7.1 Raoult laws	72
		2.7.2 Osmotic pressure	73
	2.8	Phase border phenomena.	75
		2.8.1 Surface tension	75
		2.8.2 Adsorption	76
3.	THE	RMODYNAMICS	77
	3.1	Thermodynamic system	77
	3.2	Work and heat	79
	3.4	Heat transport	81
	3.5	Functions of state.	82
		3.5.1 Internal energy.	83
		3.5.2 Enthalpy	84
		3.5.3 Entropy	85
		3.5.4 Free energy	87
		3.5.5 Free enthalpy	87
	3.6	Chemical potential.	88
	3.7	Reaction heat	88
	3.8	Thermodynamics of biological system	89
	3.9	Transformation and accumulation of energy in biological system	91
	3.10	Measurement of temperature	92
		3.10.1 Liquid thermometers	92
		3.10.2 Medical thermometer	93
		3.10.3 Calorimetric thermometer	93
		3.10.4 Thermocouple	93
		3.10.5 Electrical resistance thermometer	93
		3.10.6 Thermistor	94
		3.10.7 Thermography	94
		3.10.8 A bimetallic strip.	94
	3.11	Calorimetry	94
	3.12	Thermal losses.	95
	3.13	The laws of thermodynamics	96
4.	BIO	PHYSICS OF ELECTRIC PHENOMENA	98
	4.1	Introduction	98
		4.1.1 Coulomb law and permittivity.	98
		4.1.2 Electric potential, potentials of phase boundary-lines.	100
		4.1.3 Donnan equilibrium.	103
	4.2	Electric phenomena in alive organism	103
		4.2.1 Resting membrane potential of nerve cell	104
		4.2.2 Action potential of nerve fibre	106
		4.2.3 Action potential in heart cell	110
		4.2.4 Electrocardiogram (ECG)	111
		4.2.5 Heart's electrical sequence and interpretation of electrocardiogram	113
		4.2.6 Electroencephalograph (EEG) and Electromyograph (EMG).	115
	4.3	Electric field, electric current and voltage.	115
		4.3.1 Conduction of electric current in organism	115
		4.3.2 Effect of electric current on organism	118
		4.3.3 Conductometry	120
	4.4	Oscilloscope	122
5.	ACC	DUSTICS AND PHYSICAL PRINCIPLES OF HEARING	123
	5.1	Introduction	123
		5.1.1 Basic quantities	124

		5.1.2 The Doppler effect.	127
		5.1.3 Weber-Fechner's law.	129
		5.1.4 Complex tones.	131
	5.2	The principles of hearing	133
	5.3	Ultrasound .	135
		5.3.1 Piezoelectric effect	135
		5.3.2 Ultrasound imaging.	136
		5.3.3 Effect of ultrasound on tissue	141
	5.4	Shock waves	141
6.	OP	TICS	143
	6.1	Propagation of light	143
	6.2	Ray optics	145
	6.3	Dispersion of light	149
	6.4	Light scattering	149
	0	6.4.1 Rayleigh scattering	150
		642 Raman scattering	150
	65	Absorption of light	151
	6.6	Polarisation of light	152
	0.0	6.6.1 Polarimetry	154
	67	Ouentum enties	154
	6.9	Wava antias	155
	0.8	(0.1 Just - frame - flight	155
		6.8.1 Interference of light.	155
	()	6.8.2 Diffraction of light	15/
	6.9		158
	< 10	6.9.1 Compound microscope	160
	6.10	Laser	162
	6.11	Optics of the human eye	164
		6.11.1 Eye defects	166
		6.11.2 Biophysics of vision	167
-	VD		
7.	X-R		169
	7.1	General features of X-rays	169
		7.1.1 Production of braking radiation (bremsstrahlung)	170
		7.1.2 Production of characteristic X-rays.	172
		7.1.3 The attenuation of X-radiation	172
		7.1.4 X-ray contrast	174
	7.2	Use of X-rays for diagnostic purposes	177
		7.2.1 X-ray imaging methods	179
		7.2.2 Computed tomography	180
		7.2.3 Risks of X-ray radiation	184
	7.3	Therapeutic application of X-rays.	185
8.	RAI	DIOACTIVITY AND IONISING RADIATION	187
	8.1	Natural and artificial radioactivity.	187
		8.1.1 Basic law of radioactive decay	188
		8.1.2 Radioactive equilibrium	190
		8.1.3 Radioactive series	192
		8.1.4 Types of radioactive decay	193
	8.2	Ionising radiation and its sources	196
	-	8.2.1 Positively charged particles.	196
		8.2.2 Linear accelerators	196
		823 Circular accelerators	197
		8.2.4 Negatively charged particles – electrons	198
		8.2.5 Neutrons	199
			- / /

	8.2.6	Radionuclide sources of neutrons	. 199
	8.2.7	γ-radiation	. 199
	8.2.8	Cosmic rays	. 200
8.3	Interac	ction of radiation with matter	. 200
	8.3.1	Interaction of α-particles	. 201
	8.3.2	Interaction of β-radiation.	. 201
	8.3.3	Interaction of γ-radiation	. 203
	8.3.4	Neutron interactions	. 207
8.4	Detect	ion of ionising radiation	. 208
	8.4.1	Ionisation chambers	. 209
	8.4.2	Geiger-Müller counter	. 210
	8.4.3	Scintillation counter	. 212
	8.4.4	Semiconductor-based detector	. 213
	8.4.5	Integral and selective detection of γ-radiation	. 214
8.5	Basic	quantities in radiation dosimetry	. 215
	8.5.1	Personal dosimeters	. 216
8.6	Use of	f nuclear medicine in therapy	. 217
8.7	Use of	f nuclear medicine in diagnostics	. 217
	8.7.1	Radionuclides	. 218
	8.7.2	Scintigraphy (planar gamma radiography)	. 218
	8.7.3	Single photon emission computerised tomography	. 220
	8.7.4	Positron emission tomography	. 221

STRUCTURE OF MATTER

1.1 PARTICLES AND FORCE INTERACTIONS

There are two forms of matter: particles and fields. Under physical conditions, particle forms of matter exist in four states: solid, liquid, gas and plasma. Force interactions are characteristic of individual field types, of which there are four: gravitational and electromagnetic fields (existing as part of the environment) and strong and weak nuclear fields (existing at the atomic level).

Individual forms of matter can mutually transform, e.g. the formation of an electromagnetic wave due to the annihilation of particles and antiparticles. The creation of an electron-positron pair during the absorption of γ -radiation is an example of the opposite transformation of a field into particles.

The corpuscular form of matter consists of two groups of fundamental particles: *leptons* and *quarks*. Leptons do not interact with strong nuclear forces. Both groups consist of three generations. The first generation of leptons contains an electron and an electron neutrino, the second contains a muon and a muon neutrino and the third contains particle τ and its neutrino (See Table 1.1).

Lon	tons	Quarks		
Сер	tons	Flavour	Charge	
electron	electron neutrino	u (up)	+2/3	
e	v _e	d (down)	-1/3	
muon	muon neutrino	c (charm)	+2/3	
μ	v _m	s (strange)	-1/3	
tau	tau neutrino	t (top)	+2/3	
τ	ν_t	b (bottom)	-1/3	

Table 1.1 Fundamental particle	Table	Fundamental partic	les
---------------------------------------	-------	--------------------	-----

The three generations of quarks differ according to a property called *flavour*. Each generation has two flavour quarks: u quarks (up) and d quarks (down) in the first, c quarks (charm) and s quarks (strange) in the second and t quarks (top) and b quarks (bottom) in the third. As

well as flavour, each quark is characterised by a non-integer electric charge that equals $\pm 2/3$ of the elementary charge for the first quark of each pair and -1/3 for the second quark of the corresponding generation (Table 1.1). Quarks also differ according to another property known as *colour*. Each quark possesses a red, green or blue colour. All fundamental particles, leptons and quarks are also distinguished by a spin quantum number equalling $\pm 1/2$. Each particle has its own antiparticle. When charged, the antiparticle possesses an opposite electric charge. In the case of flavour and colour, these properties are denoted by the prefix anti-, i.e. the flavours (quarks) anti*u* and anti*d* and the colours antired, antigreen and antiblue. Although the antiparticle has the same mass as the particle and the same value of spin (integer or half-value), it has opposite rotation (clockwise or counter-clockwise) and opposite magnetic moment (see Table 1.2). If a particle and antiparticle are in the appropriate quantum states, then they can annihilate each other and produce other particles.

Table	1.2	Selected	basic	characteristics	of	antiparticles
-------	-----	----------	-------	-----------------	----	---------------

Same mass
Identical value of spin (integer, non-integer) but opposite rotation (clockwise, counter-clockwise)
Opposite magnetic moment (positive, negative) – if half-value
Opposite charge – if not without charge
Opposite colour (anticolour)

Quarks also form composite particles called *hadrons*. Hadrons must possess an integer electric charge and have a colour combination that is colourless or white. These conditions are achieved in two different ways. Hadrons of the first group are composed of two quarks called *mesons* (a quark and an antiquark). Mesons have an integer value of spin. A typical example is the pion particle, π . It is formed by a *u* quark and an anti*u* in the case of meson π^0 , by a *u* quark and an anti*d* in the case of meson π^- .

Baryons are another group of hadrons. Baryons are composed of three quarks of different colours (red, green and blue). Baryons have half-value spin. For example, a proton consists of two u quarks and one d quark, while a neutron consists of two d quarks and one u quark.

Elementary particles (fundamental hadrons and quanta of fields) consist of two large groups according to spin value. The first are *fermions*, which are characterised by a half-value spin quantum number. Their behaviour can be explained using Fermi-Dirac statistics. They also function in accordance with Pauli's exclusion principle, i.e. no two fermions of identical energies can exist in one system. The particles of the second group are called *bosons*, which possess an integer spin quantum number value. Their behaviour can be explained using Einstein-Bose statistics. In the case of bosons, the number of particles at the same energy level is not limited.

Table 1.3 H	adrons
-------------	--------

Particles composed of quarks	s – have an integer value of ele	ectric charge
	- are white (colourless)	
Mesons	-2 quarks: quark + antiquark	k (integer spin)
Baryons	– 3 quarks:	(half-value spin)

As previously mentioned, there are four types of force interactions: strong, electromagnetic, weak and gravitational. The force interactions of all field types contain non-contact and exchange characters, i.e. they occur due to the exchange of the quanta of these fields. Basic Bose particles represent the excitations of these fields. Thus, the *photon* corresponds to the electromagnetic field, gluons (of three different colours) to strong nuclear force, the particles W^{\pm} and Z^{0} to weak interaction and the hypothetical graviton to gravitational interaction. The ranges of the gravitational field (source is mass) and electromagnetic field (source is electric charge) are not limited, whereas the range of the strong interaction (source is colour) is approximately 10^{-15} m and the range of the weak interaction (enabling the change of flavour) is approximately 10⁻¹⁸ m. These last two are called saturated fields. At distances corresponding to the sizes of the respective atomic nuclei, i.e. approximately 10^{-15} m, the relative ratios of the strong, electromagnetic, weak and gravitational interactions are $1:10^{-3}:10^{-15}:10^{-40}$. These ratios indicate that gravitation is negligible in particle physics but very important for macroscopic objects. Gravitational interaction occurs only in particles with mass; it cannot be absorbed, transformed or shielded against and it always attracts and never repels. The electromagnetic force acts between electrically charged particles and can be cancelled out; it can also attract and repel. The weak interaction is responsible for changing one quark to another. The strong interaction binds protons and neutrons together to form the nucleus of an atom.

Of the particles with a mass other than zero, only electrons and protons are stable; other particles are unstable. For example, a free neutron decays after approximately 10^3 s due to β -decay into a proton, electron and electron antineutrino, $n \rightarrow pe^-v'_e$. This decay corresponds to the transmutation of a *d* quark into a *u* quark.

Of the particles with non-zero mass, muon μ^- possesses the longest life span (2.10⁻⁶ s). Most hadrons decay immediately after formation since they exist no longer than 10⁻¹² s.

1.2 ENERGY

Energy is a scalar physical quantity and represents the ability to work. The law of conservation of energy states that the total amount of energy in an isolated system remains constant over time. This means that energy cannot be created or destroyed and that it is capable of being transformed from one form to another or transferred from one place to another. For example, the result of the annihilation of an electron and a positron (with a weight equal to the energy equivalent of 0.51 MeV) is two light quanta (photons) of the same energy. Total energy E of a particle (or system of particles) in a force field is given by the sum of its resting energy E_{0} , kinetic energy E_{k} and potential energy E_{n}

$$E = E_0 + E_k + E_p \tag{1.1}$$

where E_0 is the energy related to the particle mass according to Einstein's relationship

$$E_0 = m_0 c^2, (1.2)$$

where m_0 is the mass at rest and *c* is the velocity of light in a vacuum (the highest velocity of propagation of energy). A photon, which possesses zero mass and a rest energy of zero, does not exist at rest and moves throughout a system of coordinates at velocity *c*.

The mass m of a particle moving with relativistic velocity v (almost at the velocity of light in a vacuum) increases according to the relation

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}},$$
(1.3)

where *v* is the velocity related to the observer.

Particles with non-zero mass $m_0 > 0$, energy *E*, velocity of movement *v* and momentum p = mv are related by the equation

$$E^2 = m_0^2 c^4 + p^2 c^2 \tag{1.4}$$

Kinetic energy E_k is defined by the following equation

$$E_k = \frac{mv^2}{2} = \frac{p^2}{2m}$$
(1.5)

Kinetic energy is energy due to motion. It is also independent of direction and can only possess positive or zero values, $E_k \ge 0$. Generally, potential energy may be positive or negative according to the zero level chosen. In central fields of Newton-type forces where the force of interaction is inversely proportional to the squared distance, (e.g. Coulomb's law, Newton's law of gravitation), the zero level is set where there is no interaction, i.e. at "infinity"; therefore, potential energy E_p is negative ($E_p < 0$). It must be negative because positive force is required to remove the particle (body, electric charge), which is attracted to the distance. Here, the force of interaction is negligible and energy equals zero. In the mechanics of a mass point, the equation for potential energy is as follows: $E_p = mgh$, where *m* is mass, *g* is gravity acceleration and *h* is height. In this case, if the zero energy level is defined at the surface of the earth and h > 0, then the potential energy will be positive and will equal the product, *mgh*.

Energy is expressed in joules. However, in atomic physics and radiation physics, this unit is not suitable. In these cases, energy is mostly expressed in *electronvolts* (eV). 1 eV is the energy obtained by an electron accelerated by the potential difference of 1 *volt*. Since 1 J = 1 C.1 V and charge 1 C equals a total charge of approximately 6×10^{18} electrons, 1 eV = 1.6×10^{-19} J. The relation of 1 eV to 1 J is the same as that for the charge of 1 electron to 1 C. In the physics of elementary particles, the unit eV is also applied as a unit of mass according to equation (1.2). Based on this relationship, the rest mass of electron $m_e = 0.51 \text{ MeV/c}^2$. The c² unit is usually omitted. Thus, similarly, the mass of proton $m_p = 938.28$ MeV and the mass of neutron $m_n = 939.57$ MeV.

1.3 QUANTUM EFFECTS

The laws of classical physics are not sufficient to describe the physical processes that occur at the atomic level. Within the region of very small distances, there are processes that exist separate to the macro-level and that have other physical quantities. One of them is an effect related to *Planck's constant h* or *Dirac's constant*, $\hbar = 1.05 \times 10^{-34}$ J.s. These constants are related by $\hbar = h/2\pi$. Planck's constant in circular motion with radius *r* represents the smallest amount of radiated energy.

One of the effects of quantum properties is the discrete value of angular momentum. Angular momentum L is defined as a vector product (cross-product) of position vector r and the vector of momentum, p = mv.

$$\boldsymbol{L} = [\boldsymbol{r} \times \boldsymbol{p}] \tag{1.6}$$

In general, the cross-product of two vectors is the vector perpendicular to the plane determined by the vectors multiplied. Its magnitude equals the product of their magnitudes multiplied by the sine of their angle. In the case of regular circular motion, the directions of momentum of vector p and position vector r change at every moment, whereas the magnitude and direction of the cross-product remain constant (see Fig. 1.1). The two vectors r and v are perpendicular to each other. Therefore, angular momentum L = rmv, since $\sin(\pi/2) = 1$.



Figure 1.1: Orbital angular momentum L of a particle with momentum p at circular motion with the radius r.

According to quantum mechanics, the angular momentum of the orbital motion of a particle can possess only certain discrete values, which are multiples of Dirac's constant. Similarly, the projections of angular momentum of an atom in the direction of the coordinate axes can only possess well-defined values (see later).

As well as orbital angular momentum, elementary particles possess their own angular momentum, *spin* and *magnetic moment* due to rotation. Particles with half-value spin are called *Fermi particles (fermions)* and those with integer-value spin are called *Bose particles (bosons)*. For example, the spin of an electron or of a nucleon equals $\frac{1}{2}$ and the spin of a photon equals 1 (in multiples of \hbar). The spin value determines the behaviour of the particle. Thus, Fermi particles with identical spin cannot exist at the same energy level. This explains why all of the electrons in heavy atoms occupy the higher energy levels more distanced from the nucleus instead of the lowest energy levels. On the other hand, Bose particles tend to occupy the same energy state.

Elementary particles and their system (atom, molecule) possess both corpuscular and wave properties – a finding originally resulting from experimentation into the properties of light. Interference or diffraction of light demonstrates that light is represented by waves, while the photoelectric effect demonstrates that light is a flux of quanta of energy in the form of photons. Energy *E* of a photon (J) is related to frequency $f(s^{-1})$ of the wave and to its wavelength λ (m) by the equation

$$E = hf = hc/\lambda, \tag{1.7}$$

where *c* is the velocity of light in a vacuum and $h = 6.63 \times 10^{-34}$ J.s = 4.13×10^{-15} eV.s is Planck's constant. Therefore, Planck's constant reflects the sizes of energy quanta in quantum mechanics.

The motion of each particle with mass *m*, momentum *p* and energy *E* is related to wavelengths λ of the de Broglie wave given by the equation

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \tag{1.8}$$

and to frequency f given by the equation

$$f = \frac{E}{h} \tag{1.9}$$

Equation (1.8) reveals that the wavelengths of elementary particles are very short. In the case of a wavelength of an electron in an electron microscope accelerated by a voltage of l kV, its energy (expressed in eV) will be $1 \text{ keV} = 10^3 \text{eV} \times 1.6 \times 10^{-19} \text{ J/eV} = 1.6 \times 10^{-16} \text{ J}.$

Using equation (1.8) we get

$$\lambda = \frac{6.63 \times 10^{-34} \,\text{J.s}}{\sqrt{(2 \times 9.11 \times 10^{-31} \,\text{kg}).(1.6 \times 10^{-16}) \,\text{J}}} = 3.88 \times 10^{-11} \,\text{m} = 0.039 \,\text{nm}$$

Therefore, the wavelength of this electron is four orders shorter than that of visible light. That is why the resolving power of an electron microscope is more accurate than that of an optical microscope (see later in Chapter 6).

The corpuscular-wave dualism of a subatomic particle has consequences. For example, it is not possible to *simultaneously* estimate position vector \mathbf{r} of a particle (or its coordinates) or its momentum p with an arbitrary accuracy. *Heisenberg's uncertainty principle* holds for the uncertainty of position vector Δr and momentum Δp

$$\Delta r.\Delta p \ge \hbar \tag{1.10}$$

Thus, the smaller region of motion results in a higher uncertainty of momentum. A similar relation also holds for the simultaneous determination of an energy level and its duration. If the uncertainty of an energy level is ΔE and the time interval in which the measurement is performed is Δt , then

$$\Delta E . \Delta t \ge \hbar \tag{1.11}$$

Therefore, if the given energy state lasts for a long time, its energy may be established with a high degree of certainty. For example, the mean time between atom excitation and photon emission during de-excitation is approximately 10^{-8} s. With respect to the above equation, the uncertainty of estimating the energy level is

$$\Delta E = \frac{\hbar}{\Delta t} = \frac{1.05 \times 10^{-34} \,\mathrm{Js}}{10^{-8} \,\mathrm{s}} \cong 1.1 \times 10^{-26} \,\mathrm{J} \cong 7 \times 10^{-6} \,\mathrm{eV}$$

Quantum effects can be quantitatively described by quantum mechanics.

1.3.1 Quantum numbers

From a quantum-mechanical perspective, the motion of an electron in the force field of the atomic nucleus is not represented by a certain trajectory but by a "cloud". Its form and distance from the nucleus is determined by other parameters such as orbital angular momentum, magnetic moment and spin. The region of space in which the electron moves is called the *orbital*. The electron state is described by the wave function, which involves a number of dimensionless parameters that equal the number of degrees of freedom. With regard to the rotation of the electron, the number of degrees of freedom is 4. Therefore, the state of the electron can be completely expressed by four *quantum numbers*. These numbers are natural integers (with the exception of spin) that determine the geometry and symmetry of the electron cloud. No two electrons in the same atom can have the same four quantum numbers.

Principal quantum number n determines the total electron energy. In accordance with the quantum theory of the hydrogen atom, an electron may exist at various energy levels E_n given by the equation

$$E_0 = -\frac{me^4}{8\varepsilon_0^2 h^2} \cdot (\frac{1}{n^2}), \tag{1.12}$$

where $m = 9.11 \times 10^{-31}$ kg is the rest mass of the electron, $\varepsilon_0 = 8.854 \times 10^{-12}$ F.m⁻¹ is the permittivity of the vacuum and $e = 1.6 \times 10^{-19}$ C is the electron charge. The principal quantum number is a natural number, which can possess values of n = 1, 2, 3 and so on. Moreover, its value estimates the shell in which the electron appears. The shells K, L, M, N, O, P and Q correspond to the values n = 1, 2, 3, 4, 5, 6 and 7, respectively. As *n* increases, the orbital becomes larger and the electron spends more time farther from the nucleus. The electron also moves at a higher potential energy and is, therefore, less tightly bound to the nucleus. *n* also expresses the maximal number of electrons in the shells according to the relation $2n^2$ (for more detail, see paragraph 1.5).

Orbital quantum number ℓ of an electron in a shell expressed by *n* may possess the values $\ell = 0, 1, 2, ..., (n-1)$ and determines the form and symmetry of the electron cloud, which is in turn determined by angular momentum *L*. The magnitude of *L* is given by equation

$$L = \hbar \sqrt{\ell(\ell+1)} \tag{1.13}$$

The orbital quantum number is used for notating states in spectroscopy. Values of ℓ are denoted by letters so that the values of $\ell = 0, 1, 2, 3, 4$ and 5 correspond to the letters *s*, *p*, *d*, *f*, *g* and *h*, respectively. According to equation (1.13), the value of orbital angular momentum corresponding to state *s* equals zero and the value corresponding to state *p* is $\sqrt{2}\hbar$, etc. The notation of states is a combination of the principal quantum number and letter. Thus, a state with n = 2 and $\ell = 0$ is 2*s*, a state with n = 4 and $\ell = 2$ is 4*d*, etc.

If an arbitrary direction (axis z) is chosen in the space, then the values of projection of the angular momentum in this direction, L_z , are discrete values given by the product $m_i\hbar$ where m_i is the magnetic quantum number.

Magnetic quantum number m_l can possess the values $m_l = \pm 0, \pm 1, \pm 2, ..., \pm \ell$ for a given ℓ , which determines the spatial position of the orbital. The magnitudes of the orbital angular momentum can only have discrete values given by equation (1.13). Moreover, the direction of angular momentum is not arbitrary and is limited with respect to the orientation of the external magnetic field. The magnetic quantum number estimates the direction of vector L by determining its component in the direction of the external magnetic field.

Orbital magnetic moment $\vec{\mu}_{orb}$ is related to angular momentum \vec{L} (see Fig. 1.1) and given by the equation

$$\vec{\mu}_{orb} = -(\frac{e}{2m_e})\vec{L},\tag{1.14}$$

where m_e is the mass of the electron.

The unit used to express the orbital magnetic moment of the electron is the *Bohr magneton*, $u_B = e\hbar/2m_e = 9.28 \times 10^{-24} \text{ A.m}^2$ (or J.T⁻¹, since J/T = J/(Wb.m⁻²) = J.m²/Wb = J.m²/(V.s) = C.V.m²/(V.s) = A.m²). For a given ℓ , the number of possible orientations of the orbital angular momentum in the external magnetic field equals $2\ell+1$ since the values of *m* may vary within a range from $-\ell$ through 0 to $+\ell$. Thus, the magnetic quantum number estimates the magnitude of the projection of mechanical angular momentum \vec{L} and of magnetic moment $\vec{\alpha}$ in a certain direction. For the z-component of orbital magnetic moment $\vec{\mu}_{orb,z}$, it holds that $\mu_{orb,z} = m_l \cdot \mu_B$. Orbital magnetic dipole moments are multiples of u_B .

Spin quantum number s is a value that describes the angular momentum of an electron. An electron possesses its own, internal angular momentum, which does not depend on its orbital angular momentum. However, it also possesses its own magnetic moment, which is related to its internal angular momentum. The magnitude of angular momentum S due to the

spin of the electron is given for any electron, bound or free, by $S = \hbar \sqrt{s(s+1)}$ where $s = \frac{1}{2}$ is

the spin quantum number of the electron. In an external magnetic field, the vector of the spin angular momentum can have two orientations. Component S_z of the spin angular momentum of an electron along the external magnetic field in direction z is determined by spin magnetic quantum number $m_{s'}$ which has two values, $\pm \frac{1}{2}$, and thus the value of this component is $\pm \frac{1}{2}\hbar$. Similar to orbital angular momentum, spin dipole magnetic momentum μ_s is also related to spin angular momentum S by $\mu_s = -\frac{e}{m}S$, where e is the charge and m is the mass of the electron. Spin dipole moments of electrons (and of other elementary particles) are multiples of u_B .

Thus, the state of an electron in an atom is completely determined by a set of 4 quantum numbers: n, ℓ , m and s. Electron configurations of atoms with more electrons are governed by the *Pauli exclusion principle*, which states that any two electrons in an atom cannot exist in an identical quantum state. There is a different set of quantum numbers for each electron in a given atom.

An electron can transit from one state to another due to the absorption or emission of energy. Transitions between quantised states occur as a result of two photon processes: emission and excitation. Absorption of energy is connected with the transition of electrons from lower to higher energy levels. A downward transition involves the emission of energy (photons). All of these processes require that the photon energy given by the Planck relationship defined in equation 1.7 is equal to the energy separation of the participating pair of quantum energy states (see Fig. 1.2.).



Figure 1.2: Energy separation between energy states.

During electron transitions from one state to another due to the absorption or emission of energy, only these transitions occur. By means of this process, the principal quantum number can vary arbitrarily, whereas the orbital quantum number varies only by ± 1 . These transitions are called *allowed* while other transitions are called *forbidden*. Thus, of the $3 \times 2 = 6$ possible transitions from shell M (n = 3, $\ell = 0$, 1, 2) to shell L (n = 2, $\ell = 0$, 1), only those from 3d to 2p, from 3p to 2s and from 3s to 2p are allowed (see Fig. 1.3).



Figure 1.3: Transitions from orbital n = 3 to orbital n = 2.

1.4 HYDROGEN ATOM

The simplest system composed of nucleons and electrons is the hydrogen atom. In this system, one electron moves in the central electric field of one proton. The distance from the nucleus, at which the electron appears with the highest probability, can be estimated from the relationship of uncertainty (see equation 1.10).

If the electron moves at distance r from the nucleus then the uncertainty only equals r. From equation (1.10), the uncertainty of momentum p is

$$\Delta p = \frac{\hbar}{r} \tag{1.15}$$

The total energy of the electron in the field of the atom is given by the sum of its kinetic and potential energies. According to equation (1.5) via equation (1.15), *kinetic energy* E_k is

$$E_k = \frac{p^2}{2m_e} = \frac{\hbar^2}{2m_e r^2},$$
(1.16)

where m_e is the mass of the electron. *Potential energy* E_p of an electron with charge -e in the force field of a proton with charge +e at distance r is given by

$$E_p = -\frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r}$$
(1.17)

where ε_0 is the permittivity of the vacuum. The potential energy of an electron in the field of the nucleus is negative. It reaches the highest (zero) value at "infinite" distance from the nucleus, where the force action of charges of the electron and nucleus is negligible. Thus, total energy *E* of an electron in the field of one proton is

$$E = E_k + E_p = \frac{\hbar^2}{2m_e r^2} - \frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r}$$
(1.18)

Values of total electron energy can be calculated and plotted as a function of distance r from the nucleus (see Fig. 1.4). This curve of total energy manifests in a minimum value for a certain distance, r_0 . It holds generally in physics that each system is stable at the minimum value of its energy. Therefore, the highest probability of the appearance of an electron is only at this distance. An electron in its stable state does not emit energy.

Distance r_0 calculated from equation (1.18) using dE/dr = 0 (the extreme of the function can be calculated on the condition that its first derivative equals zero) is given by

$$r_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2} \tag{1.19}$$

If numerical values are substituted for electron mass $m_e = 9.1 \times 10^{-31}$ kg, permittivity of vacuum $\varepsilon_0 = 8.8 \times 10^{-12}$ F.m⁻¹, electron charge $e = 1.6 \times 10^{-19}$ C and $\hbar = 1.05 \times 10^{-34}$ Js, then $r_0 = 5.29 \times 10^{-11}$ m. This distance is called the *Bohr radius*. After substituting r_0 back into



Figure 1.4: Total electron energy E as a function of its distance r_0 from the nucleus.

equation (1.18) for the total electron energy, the energy of the hydrogen atom in its basic state is given by the equation

$$E = -\frac{1}{32\pi^2 \varepsilon_0^2} \cdot \frac{m_e e^4}{\hbar^2}$$
(1.20)

Equation (1.20) corresponds to the solution provided by Schrödinger's equation for an electron in the field of a proton where n = 1. A state n = 1 is the basic state, while states n = 2, 3, ... are excited states to which an electron may transit after the absorption of energy. If numerical values are substituted for the quantities in equation (1.12), subsequently n = 1, 2, 3, ... up to infinity according to the following energy values: $E_1 = -13.6 \text{ eV}, E_2 = -3.38 \text{ eV}, E_3 = -1.5 \text{ eV}$, etc. up to $E_{\circ} = 0$, respectively.

It can be demonstrated that for each energy level, value E_n corresponds to the most probable distance r_n from the nucleus, given by the following equation

$$r_n = n^2 r_0 \tag{1.21}$$

The most probable distance from the nucleus increases with n^2 .

Based on the wave theory of matter, the wavelength of an electron depends on its momentum as defined by equation (1.8). It can be shown that it equals the value of path $2\pi r_0 = 3.3 \times 10^{-10}$ m. In simplistic terms, an electron can move around the nucleus for an infinitely long period without emitting energy if its path is an integer multiple of the de Broglie wavelength, i.e. if

$$n\lambda = 2\pi r_n,\tag{1.22}$$

where n is the principal quantum number. During transitions from higher to lower energy levels, the hydrogen atom emits photons that possess a discrete (line) spectrum.

1.4.1 Spectrum of the hydrogen atom

An electron at a higher energy level than its ground state is not stable. A fast transition to either a lower or ground state occurs with the simultaneous emission of a photon. If the state changes from energy E_k to energy E_n , k > n, then according to equation (1.12) a quantum of radiation is emitted with the following energy

$$E = E_k - E_n = \frac{m_e e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \left(\frac{1}{n^2} - \frac{1}{k^2}\right)$$
(1.23)

The frequency or wavelength of this radiation is given by equation (1.7) when the energy value is substituted into the above equation. Since there are discrete values of electron energies, only certain energies (frequencies, wavelengths) may be emitted by the atom. Therefore, a *line spectrum* of radiation is observed.

The set of spectral lines observed during transitions from all higher levels to a certain energy level (corresponding to a given *n*) is called a *series* (see Fig. 1.5). The spectral emission lines of the hydrogen atom correspond to a transition to the basic energy level (with n = 1). They can be observed in the ultraviolet region of light, forming the *Lyman series*. The *Balmer series* corresponds to a transition to a level of n = 2 and only this series can be observed within the region of visible light. The series corresponding to n = 3 (*Paschen series*) and to higher values of *n* are within the region of infrared light. Thus, the highest energy emitted due to a transition from *n* equal to infinity to a basic state of n = 1 will correspond to equation (1.23)

$$E = \frac{m_e e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} = \frac{0.91 \times 10^{-30} \times (1.6 \times 10^{-19})^4}{32 \times (3.14)^2 \times (8.86 \times 10^{-12})^2 \times (1.05 \times 10^{-34})^2} = 2.16 \times 10^{-18} \text{ J} = 13.6 \text{ eV}$$

It corresponds to the wavelength

$$\lambda = \frac{hc}{E} = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{2.16 \times 10^{-18}} = 9.2 \times 10^{-8} \text{ m} = 92 \text{ nm}$$

Analogously, the highest energy in the Balmer series (n = 2) is

$$E_{n=2} = \frac{m_e e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{1}{2^2} = 0.54 \times 10^{-18} \text{ J} = 3.38 \text{ eV}$$

Its wavelength is 368 nm, which reaches the region of visible light.

1.5 ELECTRON STRUCTURE OF HEAVY ATOMS

The electron structure of atoms with multiple electrons is mainly determined by two rules:

- 1. The system of particles is stable at a minimum total energy.
- 2. Only one electron exists in each individual quantum state of the atom.