

ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
FAKULTA JADERNÁ A FYZIKÁLNĚ INŽENÝRSKÁ



Diplomová práce

**Dynamika pohybu antivodíku
v experimentu AEGIS**

Praha 2011

Michal Špaček

Prohlášení

Prohlašuji, že jsem svou diplomovou práci vypracoval samostatně a použil jsem pouze podklady (literaturu, projekty, SW atd.) uvedené v příloženém seznamu.

Nemám závažný důvod proti užití tohoto školního díla ve smyslu § 60 Zákona č. 121/2000 Sb., o právu autorském, o právech souvisejících s právem autorským a o změně některých zákonů (autorský zákon).

V Praze dne 5.1.2012

Abstrakt

Název práce:

Dynamika pohybu antivodíku v experimentu AEGIS

Autor: Bc. Michal Špaček

Obor: Jaderné inženýrství

Druh práce: Diplomová práce

Vedoucí práce: doc. RNDr. Vojtěch Petráček, CSc., Katedra fyziky, Fakulta jaderná a fyzikálně inženýrská, České vysoké učení technické v Praze

Abstrakt: Tato práce se zabývá pohybem atomů antivodíku v obecných elektrických a magnetických polích a v gravitačním poli Země. V úvodu autor objasňuje, které části experimentu AEGIS se práce dotýká a jaký význam pro experiment má rozřešení této problematiky. Podrobně jsou odvozeny kinematika nábojové výměny a kinematika deexcitace urychleného antivodíku – výsledky jsou ověřeny nezávislými postupy a demonstrovány na jednoduchých příkladech. V rámci kvaziklasického modelu, který je postupně budován a analyzován, je nalezena pohybová rovnice antivodíku ve vnějším poli a jsou rozebrána její omezení. Průběžně jsou zdůrazňovány důležité vlastnosti antivodíku.

Klíčová slova: AEGIS, antivodík, positronium, gravitace, rydbergovské atomy, nábojová výměna, deexcitace, neindukovaný elektrický dipól, indukovaný elektrický dipól, neindukovaný magnetický dipól, indukovaný magnetický dipól, pohybová rovnice dipólu, křížná pole, Starkův jev, Zeemanův jev, pohybová rovnice atomu.

Abstract

Title:

Dynamics of anti-hydrogen motion in the AEGIS experiment

Author: Bc. Michal Špaček

Branch of study: Nuclear engineering

Type of work: Master's thesis

Supervisor: doc. RNDr. Vojtěch Petráček, CSc., Department of Physics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague

Abstract: This thesis deals with the motion of antihydrogen atoms in general electric and magnetic fields and in the Earth's gravitational field. The author first clarifies which part of the AEGIS experiment is concerned and what is the importance of solving the problematics. Charge exchange kinematics and antihydrogen deexcitation kinematics are derived in detail – the outcomes are verified by independent derivation methods and illustrated with simple examples. Within a quasiclassical model which is being constructed and analysed progressively, the antihydrogen's equation of motion in an external field is found and its limits are analysed. The important qualities of the antihydrogen are stressed continuously.

Key words: AEGIS, antihydrogen, positronium, gravity, Rydberg atoms, charge exchange, deexcitation, not-induced electric dipole, induced electric dipole, not-induced magnetic dipole, induced magnetic dipole, dipole equation of motion, crossed fields, Stark effect, Zeeman effect, atomic equation of motion.

Obsah

1	Introduction	7
2	AEGIS design and thesis model	10
2.1	The theoretical model	13
3	Theoretical facts	14
3.1	Hydrogen atom in zero crossed fields	14
3.2	Lorentz force	15
3.3	Relativity	15
4	Experimental facts	18
4.1	Hydrogen and positronium	18
4.2	Differences between matter and antimatter	19
5	Charge exchange kinematics	20
6	Deexcitation	26
7	Elementar dipoles	32
7.1	Not-induced electric dipole – a water molecule	33
7.2	Induced electric dipole – a hydrogen atom in the ground state	35
7.3	Not-induced magnetic dipole – a neutron	36
7.4	Induced magnetic dipole – a parapositronium	39
7.5	Summary	40
8	Stark and Zeeman effect	41
8.1	Perturbation theory	42
8.2	Sommerfeld’s quantum conditions	43
8.3	Zeeman effect	44
8.4	Stark effect	46
8.5	Comments	48
9	Spectrum of a hydrogen atom in crossed fields	50
9.1	Hydrogen spectrum by Sommerfeld’s method	51
9.2	Electron spin influence	55
9.3	Strong fields effects	57
10	Special limit	58
11	Hydrogen dynamics in crossed fields	61
11.1	Angle dependence	62
11.2	Gradients	63
11.3	Stark and Zeeman limits	63
11.4	Antihydrogen	63
12	Summary	64
13	References	70

1 Introduction

This thesis examines the properties of hydrogen and antihydrogen atoms in electric and magnetic fields. The most appropriate qualities of both particles, concerning their presence in these fields within the chosen model, are the same in their absolute value and may differ in the sign. Chapters concerning the kinematics of reactions are written directly in the language of antimatter (antihydrogen). However, since it is easier to compare the intermediate and sideline results with the known laws, the following chapters (especially about external fields' dynamics) present the problematic from the point of view of normal matter (hydrogen). The conversion to the antimatter is discussed later.

The main theoretical aim of the text is to provide the AEGIS collaboration in CERN with the equation of motion of antihydrogen in combined (crossed) fields¹.

Definition: *Throughout the following text, the term "crossed fields" refers to a pair of electric and magnetic fields described by the vectors as follows:*

$$\left(\vec{E}(\vec{R}), \vec{B}(\vec{R}) \right) \quad (1.1)$$

The first scientific goal of the AEGIS experiment (Antimatter Experiment: Gravity, Interferometry, Spectroscopy) is to directly measure the gravitational acceleration of antimatter in Earth's gravitational field. For this purpose, a device has been designed for antihydrogen production and experimental use [1]. If successful, this would be the first known measurement of this kind in history. The experiment is situated in CERN, Geneva, on the Antiproton Decelerator (AD).

There are many difficulties when considering the study of antimatter: The antimatter itself, whether natural or artificially produced, is extremely rare; a significant measure of antimatter is charged particles (positrons, antiprotons, ...) and much of antimatter propagates at the speeds close to the speed of light (antineutrinos). If the gravitational and electrostatic forces are compared, the ratio gives 10^{-36} approximately².

Gravity is the weakest of all fundamental interactions and for the enormous ratio, it dominates only under certain conditions: Gravity can prevail if the distances are immense and if the two interacting bodies are huge – huge bodies (separated by long distances) naturally possess neutral charges. On the other hand, many microscopic particles have no chance of neutralizing and are thus governed by the Lorentz force. However, in AEGIS, any long distance measurements cannot be afforded – even when one of the interacting bodies (the Earth) is huge enough, the second (an antimatter particle) is always microscopic.

Fortunately, there is no need for the gravity to prevail in this sense – as the interaction's other characteristic is that it cannot be "cancelled"³. If an area is prepared with both electric and magnetic fields screened out ("cancelled"), the gravity would remain weak but also the only effective interaction. This is the general methodology for gravity measurement on antimatter at AEGIS.

There are three major theories of gravity interaction on antimatter [2]. The first theory predicts for antimatter the exact same behaviour as is known for classical matter; the second theory proposes an analogy to Coulomb force in which antimatter particle would fall up in the Earth's gravitational field; and the third theory suggests existence of two more exotic potentials, hence antimatter would fall down but a bit faster than a classical matter.

¹The term crossed field is considered more accurate and is used mainly in this text.

²The value is obtained after evaluating magnitudes of gravitational and electrostatic forces between two protons at Bohr radius.

³According to one of the theories of antimatter's gravitational interaction, the gravity could be "cancelled" in the same way as the electric interaction of the Earth in space is – the both charge types are of the same number and space distribution. However, the antimatter amount is easily overwhelmed by the mass of the Earth. Therefore, the statement regarding gravity's uncancellation remains valid.

No matter which of these theories is valid, due to the small dimensions of the AEGIS experiment device, it is clearly reasonable to treat the gravitational acceleration (positive or negative) as constant in the device's volume – the gravitational field would be uniform.

A particle in a uniform gravitational field – g is the acceleration due to the gravity – follows a parabola set forth by the initial conditions. Variables X_1 , X_2 and X_3 (the latter oriented in the \vec{g} direction) simply mean the Cartesian coordinates as time functions and the dot-signs introduce their derivatives:

$$X_1 = X_1(0) + \dot{X}_1(0)t \quad (1.2a)$$

$$X_2 = X_2(0) + \dot{X}_2(0)t \quad (1.2b)$$

$$X_3 = X_3(0) + \dot{X}_3(0)t + \frac{1}{2}gt^2 \quad (1.2c)$$

Variables with "(0)" stand for initial conditions. The time variable t may be eliminated and the three equations reduce to one formula⁴:

$$X_3 = X_3(0) + \dot{X}_3(0)t + \frac{1}{2}g \frac{(X_1 - X_1(0))^2 + (X_2 - X_2(0))^2}{\dot{X}_1^2(0) + \dot{X}_2^2(0)} \quad (1.3)$$

Direct gravitational measurement in a uniform gravitational field means that the parabola is necessary to fit. If gravity is the only effective interaction, one has to measure the positions and time-of-flight very precisely⁵. Therefore the velocities should not be too high – if so, the parabola would then become a line indistinguishable from a parabola and any fitting would fail.

In the case of a charged particle and because of gravity's relative weakness, parabola fitting would also fail if both electric and magnetic fields were not screened off with an extremely high precision. This seems to be impossible, thus the only promising method is to experimentally test electrically neutral antimatter particles.

For AEGIS, antihydrogen was found to be the only possible particle for gravitational studies and measurements. It is (when not ionised) electrically neutral⁶. There are known ways to account for its production and it can be handled at velocities small enough to make gravity measurements feasible.

An antihydrogen atom is a compound state of one antiproton (negative elementary charge) and one positron (positive elementary charge) in a general quantum state $\psi_{n,l,m,s}$ – with the state and the quantum numbers n , l , m and s referring to the positron. Its mass is equal to a hydrogen atom in the same state. Antihydrogen is not likely to exist in nature close to the Earth, thus one has to produce it artificially through a so called charge exchange reaction. In charge exchange, a positronium (a compound state of one positron and one electron) hits an antiproton which displaces the electron in the positronium. One antihydrogen and one electron are obtained as products.

Note that the quantum state of the gained antihydrogen depends on the quantum state of the positronium. These quantum states are called Rydberg states if the particles are on higher internal energy levels.

Due to the nature of antimatter, the contact of any antihydrogen atom with a particle of matter leads to a complete annihilation of both of them. To account for that, one has to keep antimatter in a space with a very high vacuum and slow the antiparticles down so that they remain in their preparation volume until the experimental device is ready for measurements.

⁴In case of $\dot{X}_1(0) = 0$ along with $\dot{X}_2(0) = 0$, the gravitational fall is simply given by (1.2c).

⁵In the second formula, the time is eliminated. However, precise time-of-flight measurements are still necessary to determine the initial velocity conditions.

⁶Even though a particle is electrically neutral as a whole, it can still exhibit electrical qualities and its behaviour in electric and magnetic fields may not be trivial, especially if it possesses a non-uniform space charge distribution. In these instances, the crossed fields play roles and may affect the gravitational measurements. However, this fields' screening-off requirement does not have to be as extremely precise as a charge particle would demand.

In AEGIS, it is impossible to keep antihydrogen in the vacuum volume at small velocities for a long time and the experimental device cannot work continuously. However, one is able to successfully handle its element – antiproton – with a system of electrodes (Malmberg-Penning trap) inside a strong magnetic field where it follows a closed curve. The experiment is designed so that clusters of antiprotons and positroniums meet every few minutes. Thus, all the antihydrogen atoms of a pulse exist for a time short enough to handle the antiatoms but long enough to carry out the necessary gravitational measurements.

As a result of this design, the antihydrogen atoms undergo a complicated motion in crossed fields before the expected parabola behaviour.

All the antihydrogen atoms rise in an area with a strong magnetic field and a time-dependent electric field. However, for direct gravitational measurements they have to reach a zone where gravity dominates. By using an accelerator, the antiatoms are forced to pass gradients of electric and magnetic fields, where their motion is quite non-trivial. At the end, there is a position sensitive detector for reading the vertical coordinate in (1.3). For every pulse, the interval between the antihydrogen production (which almost completely coincides with the start of the acceleration) and reaching of the detector is called total time-of-flight.

As mentioned above, one needs to know the initial conditions with precision but unfortunately this does not seem to be measurable. In AEGIS it is possible to control the conditions of the just produced antihydrogen. However, these are not the values which are present in the gravitational parabola fitting formula (1.3) because they account for particles present in crossed fields, not in a pure gravitational field like in (1.3). One has to know how the set of these variables for particles in the crossed fields are transformed into another set of true initial conditions in a pure gravitational field (at any place of the trajectory where gravity dominates).

The questions are thus: how much of the total time-of-flight is spent in the final (gravity-only) area and whether the antihydrogen keeps flying horizontally or is elevated or dropped or side-tilted a bit by the electric and magnetic fields.

Based on the obtained data, only an appropriate understanding of antihydrogen dynamics can help to quantify the gravitational acceleration. This text's aim is to provide a deeper analysis of how to deal with the antihydrogen atoms kinematics and dynamics in the AEGIS experiment at CERN. Note that the focus is not on the individual antiatoms but on their clusters.

The whole physics is strictly in SI units. Einstein summation convention is not applied anywhere. Upper case letters ($\vec{R} = (X_1, X_2, X_3)$, $\vec{P} = (P_1, P_2, P_3)$, M) are often primarily used to refer to compound particles (hydrogen, antihydrogen, positronium) whereas the lower case letters ($\vec{r} = (x_1, x_2, x_3)$, $\vec{p} = (p_1, p_2, p_3)$, m) are linked to the particles' constituents (electrons, positrons, protons, antiprotons); only \vec{L} always means the angular momentum of a constituent. Alternative notations of total and partial derivatives are $\dot{A} = \frac{d}{dt}A$ or $A^{.i} = \frac{\partial}{\partial X_i}A$ respectively.

2 AEGIS design and thesis model

This chapter will provide some brief facts about the AEGIS technical and about the model of fields and particles used in the further theoretical analysis.

The AEGIS experiment's status early in 2012 is "in construction". When completed, more phases of measurements are planned and the goal of the first one is the direct measurement of gravitational acceleration of antimatter in the Earth's gravitational field with intention of 1 % accuracy.

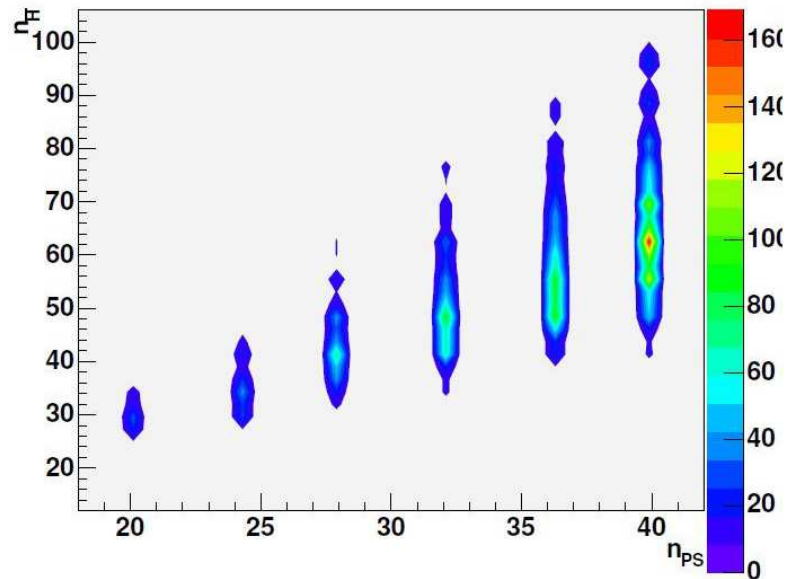
The AEGIS experiment is situated in CERN, Geneva, which is important to know for the prediction of the acceleration if it equals that of classical matter and for taking the natural magnetic field of the Earth into account.

The experiment is considered to be quite small, in the number of participants, in the budget and in the space area, too. AEGIS is not independent – for antiproton production, which is a very complex process, it shares the so called Antiproton Decelerator (AD) with other experiments.

As already mentioned, the experiment is designed to produce antihydrogen atoms for the gravitational measurements through the so called charge exchange reaction:



In the charge exchange reaction, an antiproton replaces an electron in a positronium and an antihydrogen atom is formed; both positronium and antihydrogen are on general energy levels. The reaction takes place in the so called antihydrogen production chamber. For the most probable principal (energy) quantum number of an antihydrogen atom $\langle n \rangle$, it holds that $\langle n \rangle = \sqrt{2}n_{\text{Ps}}$ [1]. For a monoenergetic sample of positroniums, the energy spectrum of antihydrogen atoms leaving the charge exchange satisfies that the higher n_{Ps} is, the wider the spectrum $\{n_{\text{min}}, \dots, \langle n \rangle, \dots, n_{\text{max}}\}$ becomes – the simulations are in the Figure 2.1:



Obrázek 2.1: Distributions of antihydrogen's principal numbers n for chosen n_{Ps} 's. Taken from [1].

To catch the delivered antiprotons, a strong time-independent magnetic field (~ 3 T) has to be present. This is a complication for the gravity measurement but also the main aim of this thesis to cope

up with on the theoretical level.

Whereas antiprotons will be obtained from the AD, AEGIS has its own positron source, namely a sample of ^{22}Na isotope; its half-life is $8.214 \cdot 10^7$ s [3] and the whole sample in the apparatus is expected to provide $1.5 \cdot 10^{10}$ Bq intensity¹. Both positrons and antiprotons are stored in separate traps for a while and undergo various types of cooling.

The positrons are transferred from their origin further through a special silicon aerogel whose purpose is to transform the positrons into positroniums. In the aerogel, there are very complicated systems of microchambers and microtunnels ("emental-like" structure) where the positrons meet electrons and form positronium particles. The positroniums head then for the charge exchange. Before the charge exchange, both reactants' clouds are focused to improve their geometric overlap.

There are two possible positronium configurations – orthopositronium $o\text{-Ps}$ and parapositronium $p\text{-Ps}$ (see the chapter Experimental facts). They differ in their half-life – they both undergo internal annihilation in a very short time. However, parapositronium does not even survive passing through the aerogel.

Only every thirtieth positron is transformed in a positronium capable of reaching the antihydrogen production chamber. The loss processes are: some of the positrons do not produce positroniums at all; half of the positroniums are short living parapositroniums; some of the orthopositroniums are too sensitive to the magnetic field; some of the orthopositroniums do not succeed in escaping from the aerogel; and some of the orthopositroniums escape into wrong directions. The positroniums are being cooled as they travel in the systems of tunnels and hit the internal surfaces².

Only a few of the orthopositroniums which travel in the right direction to the antihydrogen production chamber would live long enough to undergo the charge exchange. Therefore short after escaping the aerogel, laser pulses are applied to the orthopositroniums which excite them and extend their half-lives. As a side effect, as it should be called, there is a very important advantage of having the positroniums on a higher energy level n_{Ps} – the cross section of the charge exchange reaction is proportional to n_{Ps}^4 [1]. The higher n_{Ps} is reached, the more positroniums approach the antihydrogen production chamber and the more antihydrogen atoms are produced.

On the other hand, too high n_{Ps} cannot be afforded. As shown above, for very high positronium energy levels, the spectrum of antihydrogen energy levels would be very wide and many antiatoms would be lost due to the fact that their motions in crossed fields are very different from the average, for which the particular AEGIS crossed fields are designed. Moreover, a very high $\langle n \rangle$ would make the antihydrogen too sensitive to the magnetic field. The optimal value is thought to be $\langle n \rangle = 25$.

There are electrodes inside the antihydrogen production chamber which will serve as a Stark accelerator only few nanoseconds after the charge exchanges occur.

For better performance, it was decided to handle with both antiprotons and positrons (positroniums) in pulses – the preparation of them is continuous but the charge exchange itself is strobe-like. The particles are first accumulated in traps and after a certain time, when their numbers are high, they are sent simultaneously to the antihydrogen production chamber. When the two particles' clouds mix and an antihydrogen cloud rises, a sudden electric field of the Stark accelerator forces the Rydberg antiatoms to exit the chamber horizontally towards the gravitational acceleration measurement zone. Before, they have to pass crossed fields' gradients. Finally, they hit the detector at the very end of the apparatus and their vertical position is measured.

The typical velocities in the measurements are expected to be between 100 m/s and 1000 m/s.

The main direct advantage of the pulse mode is that for all antihydrogen atoms hitting the final detector, the time-of-flight is almost the same and can be easily measured (much easier than for every antiatom separately).

There are more detectors intended to control the measurement process: the main in the antihydrogen production chamber which will read the velocities of those antihydrogens which would not leave the

¹The real frequency of positrons after their cooling with a neon gas will be $8 \cdot 10^6$ s⁻¹.

²About 17000 hits are necessary to effectively cool the keV ($\sim 10^{-16}$ J) positroniums down to 1 eV ($\sim 10^{-19}$ J).

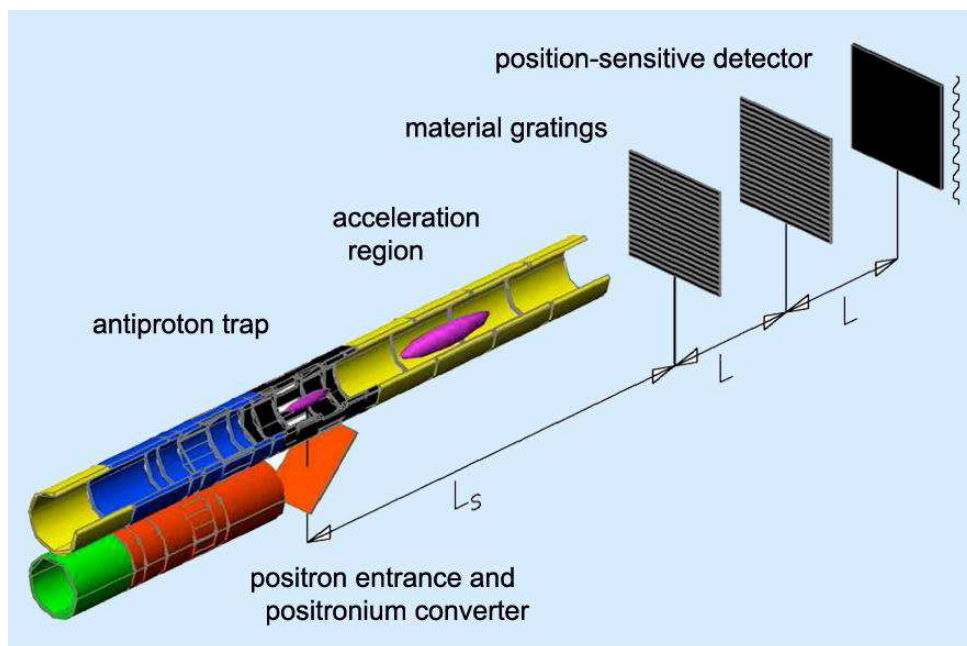
chamber in the proper horizontal direction. The detector will prove that the antiatoms are really produced as well. All in all, only 10^5 antiatoms are expected to travel in the right direction in one pulse in the best maximum.

As common in most particle experiments, ultra-cold temperatures are necessary. A cryostat ensures temperatures under 4 K in almost all the experiment volume and as low as 100 mK is reached in the antihydrogen production chamber. The antiatoms of this temperature may be cooled even more by a Doppler laser method³.

An interesting geometrical trick is about to use in the experiment: Two parallel gratings (with the period $A = 80 \mu\text{m}$) will be equidistantly placed before the detector. This would mean another big loss of the already low number of 10^5 antihydrogen atoms but, on the other hand, the signal from the position sensitive detector will be summed in modulo A and will give more accurate information to compute the gravitational acceleration. The distances between the gratings or the latter grating and the detector will be 40 cm. The whole system of the two gratings and the detector is called Moire deflectometer.

The strip width in the position-sensitive detector will be $25 \mu\text{m}$ which is twice the ideal. However, when an antiatom hits the detector, the signal is from about 5 strips – their relative responses help to improve the position accuracy down to $13 \mu\text{m}$ or better.

A basic scheme of the experiment is in the Figure 2.2:



Obrázek 2.2: A scheme of the AEGIS experiment: the antihydrogen production chamber is in black; the traps for positrons and antiprotons are in orange and blue; the orange plate is the aerogel where positroniums are produced; on the right-hand side, the three vertical squares constitute the Moire deflectometer. The crossed fields are strong in the left half whereas the right half (where the gravitational measurements take place) is screened from them – any particle going from the left to the right has to pass the crossed fields' gradients. Taken from [1].

³In numerical simulations of antihydrogen trajectories, this effect can be implemented as a sudden change in their transversal linear momentum.

2.1 The theoretical model

A hydrogen atom and an antihydrogen atom themselves are very complex systems. Furthermore, they become even more difficult to comprehend when placed in crossed fields.

The goal of this thesis is to find a force on such particles in crossed fields for tracing their trajectories – the Lorentz force on a charged particle is the very motivation. First of all, a model is necessary to establish which would respect all the qualities significant for the dynamics and neglect anything which does not play a role in the macroscopic behaviour.

The maximal achievable magnitude of the magnetic field in AEGIS is 3 T and the limit of the electric field's absolute value is 100 kV/m [1]. For these values, the principal quantum number n of each antiatom is well-defined and the ionisation is avoided⁴.

The main principle is that the atomic spectrum is adiabatic invariant in these particular crossed fields of AEGIS. This means that when the antiatoms move, the crossed fields' change in space and in time is small enough to preserve the instantaneous eigenstates.

In this sense, it is reasonable to regard any crossed fields available for AEGIS as locally uniform on atomic space scales and time-independent on a time scale of numerical iterations. The local uniformity and temporary time-independence help quite a lot to find the spectrum of the atoms.

It is exactly the particular quantum state of a hydrogen or an antihydrogen atom what determines the response of the atom to the external crossed fields. The problem is therefore retroactive – the instant external crossed fields form the instant internal properties of the atoms and these properties are responsible for the particles' dynamics in those fields. Therefore, to determine the force on an antihydrogen atom, its internal energy has to be found first.

It will be showed⁵ further that the total force on an antihydrogen atom in crossed fields is proportional only to the fields' first derivatives ("gradients"). Therefore the only required information provided by the crossed fields $(\vec{E}(\vec{R}), \vec{B}(\vec{R}))$ are $|\vec{E}(\vec{R}, t)|$, $|\vec{B}(\vec{R}, t)|$, $\frac{\partial E_j(\vec{R}, t)}{\partial X_i}$ and $\frac{\partial B_j(\vec{R}, t)}{\partial X_i}$, the first pair to compute the spectrum and the second pair to find the external force.

In effect, the crossed fields are allowed to be time-dependant and to have gradients but around a current position of a particle, the gradients and time-variability of the crossed fields are neglected anytime when the spectrum is necessary to calculate (that is in each iteration step).

In such a step, the crossed fields are regarded as uniform and time-independent in the volume of an antiatom (their average values in that volume are chosen, for example). In these local uniform crossed fields, the internal energies of the antiatoms are found and consequently, when the gradients are taken back into account, the force on them can be determined. The force together with the initial conditions and the time step Δt determine the displacement $\Delta \vec{R}$ of the antiatom and the same process is applied for new crossed fields $(\vec{E}(\vec{R} + \Delta \vec{R}, t + \Delta t), \vec{B}(\vec{R} + \Delta \vec{R}, t + \Delta t))$: local crossed fields' uniformity is temporally re-established and so on.

To sum up, the model used in this thesis considers the crossed fields as locally uniform on the atomic scales which makes it easier to determine the internal energies of (anti)atoms. However, an (anti)atom as a whole responses to the crossed fields' gradients outside its volume but the response is determined by the internal energy following from the locally uniform crossed fields.

⁴This hold for $\langle n \rangle = 25$.

⁵This is a result of the analysis and an experimental fact, too.

3 Theoretical facts

In this chapter, some theoretical results are presented for their application in next chapters.

3.1 Hydrogen atom in zero crossed fields

When a hydrogen atom is placed in zero crossed fields $(\vec{E}(\vec{R}, t), \vec{B}(\vec{R}, t)) = (0, 0)$, its spectrum is called unperturbed. The energies, which are possible to label with the principal quantum number n , are

$$W_0 = -\frac{R}{n^2}, \quad (3.1)$$

where $R = 2.179872 \cdot 10^{-18}$ J is the Rydberg constant of a hydrogen atom [3]. The formula (3.1) is the solution of the Schrödinger equation

$$\hat{H}_0\psi = W_0\psi, \quad (3.2)$$

where \hat{H}_0 denotes the unperturbed Hamiltonian of a hydrogen atom:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} \quad (3.3)$$

In (3.3), \hat{p} is the electron's linear momentum operator, \hat{r} stands for the electron's position operator, $m_e = 9.109383 \cdot 10^{-31}$ kg denotes the rest mass of the electron, $e = 1.602177 \cdot 10^{-19}$ C means the elementary charge of the electron and $\epsilon_0 = 8.854187 \frac{C^2}{Nm^2}$ refers to the vacuum permittivity [3].

For a given n , there are n^2 different eigenfunctions (when the electron spin is ignored). There is a further discussion in the chapter Stark and Zeeman effect. In general nonzero locally uniform crossed fields (\vec{E}, \vec{B}) , one needs to solve the Schrödinger equation (3.2) for a general crossed fields Hamiltonian (instead of \hat{H}_0) [4] which is

$$\begin{aligned} \hat{H} = & \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} - \frac{\hat{p}^4}{8m_e^3c^2} + \frac{e^2\hbar^2}{4\pi\epsilon_0m_e^2c^2r^3}\hat{L} \cdot \hat{S} + \frac{e^2\hbar^2}{8\epsilon_0m_e^2c^2}\delta(\vec{r}) + \\ & + \frac{e\hbar}{2m_e}B \left(\hat{L}_3 + 2\hat{S}_3 \right) + \frac{e^2B^2}{8m_e}\hat{r}^2 \sin^2 \theta - eE (\hat{x} \sin \gamma + \hat{z} \cos \gamma), \end{aligned} \quad (3.4)$$

if the local crossed fields are $(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = ((E \sin \gamma, 0, E \cos \gamma), (0, 0, B))^1$ where γ denotes the angle between the crossed fields constituents ($\gamma = \arccos \frac{\vec{E} \cdot \vec{B}}{|\vec{E}| \cdot |\vec{B}|}$). The spin is fully taken into account in (3.4).

When the spin is ignored and one keeps only the most significant terms, the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} + \frac{e\hbar}{2m_e}B\hat{L}_3 - eE (\hat{x} \sin \gamma + \hat{z} \cos \gamma) \quad (3.5)$$

or for general local crossed fields (\vec{E}, \vec{B}) simply

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} + \frac{e\hbar}{2m_e}\vec{B}\hat{L} - e\vec{E}\hat{r}. \quad (3.6)$$

¹For any crossed fields configuration, such a Cartesian coordinate system can be found.

3.2 Lorentz force

The force on a particle with a charge Q is given as

$$\vec{F} = Q \left(\vec{E}(\vec{R}) + \dot{\vec{R}} \times \vec{B}(\vec{R}) \right) \quad (3.7a)$$

or by the Cartesian coordinates with the Levi-Civita symbol $\epsilon_{ijk} = \frac{1}{2} (i - j) (j - k) (k - i)$ it is

$$F_i = Q \left(E_i(\vec{R}) + \sum_{j,k=1}^3 \epsilon_{ijk} \dot{X}_j B_k(\vec{R}) \right). \quad (3.7b)$$

These two expressions valid for a charged particle are the motivation of this thesis to find their analogy for the motion of a dipole-like particle.

Note the differences between (3.7) and known properties of a hydrogen (or antihydrogen) atom. First, the Lorentz force does not depend on quantum numbers. Given a sample of identical charged particles with the same initial conditions and in the same crossed fields, they all follow the same curve. On the contrary, a sample of hydrogen or antihydrogen atoms splits into groups which is the result of the explicit dependence of the force on atoms' internal states.

Next, the charged particles accelerate ($\ddot{\vec{R}} \neq 0$) in uniform crossed fields, whereas there is no force on (anti)hydrogen atoms in gradientless crossed fields.

And finally, there seem to be no corrections to (3.7) in extremely strong fields. For (anti)hydrogen atoms, one has to treat the fields' magnitudes first to decide on the form of the force on them since the weak and strong fields effects differ.

3.3 Relativity

The force (3.7) satisfies the general covariance principle, that is its form is the same in any reference frame, although the particular values of \vec{E} , \vec{B} , $\dot{\vec{R}}$ or \vec{F} may vary. Anyway, this holds for the right-hand side of an equation of motion; on the left-hand side, there is the total time derivative of the particle's linear momentum. The momentum in special relativity is

$$\vec{P} = \frac{M \dot{\vec{R}}}{\sqrt{1 - \frac{\dot{\vec{R}}^2}{c^2}}}, \quad (3.8a)$$

whereas in classical mechanics it equals

$$\vec{P} = M \dot{\vec{R}}, \quad (3.8b)$$

hence the difference is given by the factor $1/\sqrt{1 - \frac{\dot{\vec{R}}^2}{c^2}}$. The maximum values of antihydrogen velocities in AEGIS are expected not to exceed 1000 m/s, therefore the factor of difference between classical and relativistic approach is

$$\frac{1}{\sqrt{1 - \frac{1000^2}{299792458^2}}} \approx 1 + 5,6 \cdot 10^{-12} \quad (3.9)$$

and the classical Newtonian left-hand side (3.8b) of the equation of motion can be used.

In the general theory of relativity, the dynamics of a particle in a pure gravitational field is given by the Einstein field equation. If one is interested in a passive problem where the test particle has no effect on the given arbitrary spacetime, the equation of motion of such a particle is the geodesic equation

$$\frac{d^2 x^\rho}{d\tau^2} = - \sum_{\mu, \nu=0}^3 \Gamma_{\mu\nu}^\rho \frac{dx^\mu}{d\tau} \frac{dx^\nu}{d\tau}, \quad (3.10)$$

where $\Gamma_{\mu\nu}^\rho = \frac{1}{2} \sum_{\sigma=0}^3 g^{\rho\sigma} (g_{\sigma\mu, \nu} + g_{\nu\sigma, \mu} - g_{\mu\nu, \sigma})$ stands for the Christoffel symbols of the second kind, $g^{\mu\nu}$ denotes the metric tensor of the given spacetime, x^ρ are the global coordinates of the curve in the spacetime along which the particle moves and τ means the particle's proper time parametrising the curve.

Consider a weak gravitational field. The spacetime geometry is almost Minkowski-like and there are coordinates where it holds that $g^{\mu\nu} = \eta^{\mu\nu} - h^{\mu\nu}$ and $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ with "h" small with respect to 1 (including its derivatives). Then:

$$\sum_{\sigma=0}^3 g^{\sigma\nu} g_{\mu\sigma} = \sum_{\sigma=0}^3 (\eta^{\sigma\nu} - h^{\sigma\nu}) (\eta_{\mu\sigma} + h_{\mu\sigma}) = \delta_\mu^\nu + h_\mu^\nu - h_\mu^\nu + O(h^2) = \delta_\mu^\nu. \quad (3.11)$$

If the test particle moves very slowly, that is if $|\frac{dx^i}{d\tau}| \ll c$ for $i = 1, 2, 3$, the geodesic equation (3.10) reduces to

$$\begin{aligned} \frac{d^2 x^\rho}{d\tau^2} &= -\Gamma_{00}^\rho \left(\frac{dt}{d\tau} \right)^2 = -\frac{1}{2} \sum_{\sigma=0}^3 g^{\rho\sigma} (g_{\sigma 0, 0} + g_{0\sigma, 0} - g_{00, \sigma}) \left(\frac{dt}{d\tau} \right)^2 = \\ &= -\frac{1}{2} \sum_{\sigma=0}^3 g^{\rho\sigma} (-g_{00, \sigma}) \left(\frac{dt}{d\tau} \right)^2 = \frac{1}{2} \sum_{\sigma=0}^3 g^{\rho\sigma} g_{00, \sigma} \left(\frac{dt}{d\tau} \right)^2, \end{aligned} \quad (3.12)$$

which with (3.11) gives

$$\frac{d^2 x^\rho}{d\tau^2} = \frac{1}{2} \sum_{\sigma=0}^3 \eta^{\rho\sigma} h_{00, \sigma} \left(\frac{dt}{d\tau} \right)^2 = \frac{1}{2} h_{00, \rho} \left(\frac{dt}{d\tau} \right)^2 = \frac{1}{2} \cdot \frac{\partial h_{00}}{\partial x_\rho} \left(\frac{dt}{d\tau} \right)^2. \quad (3.13)$$

To make this limit match with Newton's law of gravity $\ddot{X} = -\frac{\partial\phi}{\partial X}$, where $\phi \left[\frac{m^2}{s^2} \right]$ denotes the scalar gravitational potential (per unit mass), one sets simply $h_{00} = -2\phi$.

Anyway, (3.13) holds for a matter particle in a field "generated" by massive objects. The question is how the theory treats the problem of an antimatter particle in the same field. Matter and antimatter are connected with the Charge-Position-Time (CPT) symmetry. If the CPT-operation (or PT, since the charge is missing in the last equation) is applied on (3.13), the four-vector transforms as

$$dx^\rho \rightarrow -dx^\rho, \quad (3.14)$$

since it is linked to the just introduced antimatter particle, whereas the gravitational potential gradient $\frac{\partial h_{00}}{\partial x_\rho}$ stays invariant. The equation (3.13) transforms as

$$\frac{d^2(-x^\rho)}{d\tau^2} = \frac{1}{2} \cdot \frac{\partial h_{00}}{\partial x_\rho} \left(\frac{d(-t)}{d\tau} \right)^2, \quad (3.15)$$

which gives

$$\frac{d^2 x^\rho}{d\tau^2} = -\frac{1}{2} \cdot \frac{\partial h_{00}}{\partial x_\rho} \left(\frac{dt}{d\tau} \right)^2. \quad (3.16)$$

In effect, there is one extra minus-sign when compared to (3.13), the meaning of which can be the gravitational repulsion. Therefore the general relativity together with CPT-symmetry may predict

opposite gravitational acceleration of antimatter in the Earth's gravitational field. Hence the gravitational accelerations g and $-g$ of antimatter in the field of matter are acceptable in the general relativity theory [2].

The Kaluza-Klein theory expands the 4-dimensional tensor $g^{\mu\nu}$ in order to connect the gravity and electromagnetism. As a result, there are two more gravitational potentials aside ϕ . If valid, these two may modify the gravitational acceleration to $\pm g + \Delta g$.

Anyway, in the small volume of the AEGIS experiment, it is reasonable to treat the gravitational acceleration as constant, positive or negative, as discussed in the Introduction. The trajectory of antimatter particles is expected to be parabolic.

4 Experimental facts

In this chapter, the most important non-trivial phenomenological facts about the hydrogen and anti-hydrogen physics will be presented.

4.1 Hydrogen and positronium

There are no forces on (anti)hydrogen atoms of any quantum state in zero crossed fields (excluding gravity). If the crossed fields are nonzero but gradientless as well, there is also no force on the atoms.

The spectrum of (anti)hydrogen atoms depends on the angle between the crossed field vectors.

In very strong crossed fields, new effects are dominant. Especially, the spectrum is proportional to the second power of the fields' magnitudes.

Both a hydrogen (an antihydrogen) and a positronium have a well-defined ground states which are the lowest of all their possible energy levels. The ground state can be labelled with the principal number $n = 1$ while for higher states it is $n > 1$. The states with very high n are called Rydberg states and the particle decomposes to its constituents for $n \rightarrow +\infty$.

The Rydberg constant of a two-component particle is proportional to its reduced mass μ as

$$R = \frac{e^4}{32\pi^2\hbar^2\epsilon_0^2}\mu = \frac{e^4}{32\pi^2\hbar^2\epsilon_0^2}\frac{m_1m_2}{m_1 + m_2} \quad (4.1)$$

and the relation between R_H , $R_{\bar{H}}$ and R_{Ps} is

$$\frac{R_{\bar{H}}}{R_{Ps}} = \frac{R_H}{R_{Ps}} = \frac{\mu_H}{\mu_{Ps}} = \frac{\frac{m_p m_e}{m_p + m_e}}{\frac{m_e^2}{2m_e}} = \frac{2m_p m_e^2}{(m_p + m_e) m_e^2} \approx \frac{2m_p m_e^2}{m_p m_e^2} = 2 \quad (4.2)$$

and therefore

$$2R_{Ps} = R_{\bar{H}} = R_H = R = 2.179872 \cdot 10^{-18} \text{ J}. \quad (4.3)$$

For the energy levels of the positronium it holds that

$$W(n_{Ps}) = -\frac{R_{Ps}}{n_{Ps}^2} = -\frac{R}{2n_{Ps}^2}. \quad (4.4)$$

For any higher energy level of a hydrogen, an antihydrogen or a positronium, the half-life of the deexcitation to the particle's ground state can be defined. The magnetic field is able to delay the process. The problem is studied in the paper [5]. Based on the paper's findings, it takes around 5 ms for a monochromatic $n = 25$ hydrogen atoms' distribution to populate the ground state by 90 % in a 3 T magnetic field. This is comparable with the AEGIS typical time-of-flight of the antihydrogen atoms and therefore the evolution of the distribution should be taken into account¹.

¹In the chapter Deexcitation, it will be proved that the linear momentum changes can be neglected but the change of the energy level itself cannot since the dynamics in the crossed fields depends on the particular state.

Unlike a hydrogen or an antihydrogen, there are two possible configurations of positronium's ground state distinguished by the orientations of the spins of an electron and a positron. The antiparallel configuration is called parapositronium (p -Ps) and the parallel one is orthopositronium (o -Ps). The latter is a triplet of three possible projections s_{Ps} of the total spin S_{Ps} with three different properties in external crossed fields; parapositronium is a singlet. The second important difference is in their lifetimes τ . Their forming and decay branching ratios are also mentioned:

Quantity	Parapositronium	Orthopositronium
Formation	$e^- + e^+ \rightarrow p\text{-Ps}$ [50%]	$e^- + e^+ \rightarrow o\text{-Ps}$ [50%]
Total spin	$S_{Ps} = 0$	$S_{Ps} = 1$
Total spin projections	$s_{Ps} = 0$	$s_{Ps} = -1, 0, +1$
The ground state	1^1S_0	1^3S_1
Half-life	$\tau = 1.244 \cdot 10^{-10}$ s	$\tau = 1.421 \cdot 10^{-7}$ s
Decay mode	$p\text{-Ps} \rightarrow \gamma \gamma + 1022$ keV	$o\text{-Ps} \rightarrow \gamma \gamma \gamma + 1022$ keV

Tabulka 4.1: The overview of the properties of para- and orthopositronium and the common notation.

4.2 Differences between matter and antimatter

The important question is whether the values of electron's and positron's rest masses (m_e and $m_{\bar{e}}$), the absolute values of their charges (q_e and $q_{\bar{e}}$) and their magnetic moments (μ_e and $\mu_{\bar{e}}$) equal (as one would expect) or whether they differ a bit. The experiments have not detected any significant difference [6]:

$$\frac{|m_e - m_{\bar{e}}|}{\langle m_{e\bar{e}} \rangle} = \frac{|m_e - m_{\bar{e}}|}{\frac{m_e + m_{\bar{e}}}{2}} = \frac{2|m_e - m_{\bar{e}}|}{m_e + m_{\bar{e}}} \leq 8 \cdot 10^{-9} \quad (4.5a)$$

$$\frac{||q_e| - |q_{\bar{e}}||}{e} \leq 4 \cdot 10^{-8} \quad (4.5b)$$

$$\frac{||\mu_e| - |\mu_{\bar{e}}||}{\langle \mu_{e\bar{e}} \rangle} = \frac{||\mu_e| - |\mu_{\bar{e}}||}{\frac{\mu_e + \mu_{\bar{e}}}{2}} = \frac{2||\mu_e| - |\mu_{\bar{e}}||}{\mu_e + \mu_{\bar{e}}} \leq 5 \cdot 10^{-13} \quad (4.5c)$$

The same for a proton and an antiproton:

$$\frac{|m_p - m_{\bar{p}}|}{\langle m_{p\bar{p}} \rangle} = \frac{|m_p - m_{\bar{p}}|}{\frac{m_p + m_{\bar{p}}}{2}} = \frac{2|m_p - m_{\bar{p}}|}{m_p + m_{\bar{p}}} \leq 2 \cdot 10^{-9} \quad (4.6a)$$

$$\frac{||q_p| - |q_{\bar{p}}||}{e} \leq 2 \cdot 10^{-9} \quad (4.6b)$$

$$\frac{||\mu_p| - |\mu_{\bar{p}}||}{\langle \mu_{p\bar{p}} \rangle} = \frac{||\mu_p| - |\mu_{\bar{p}}||}{\frac{\mu_p + \mu_{\bar{p}}}{2}} = \frac{2||\mu_p| - |\mu_{\bar{p}}||}{\mu_p + \mu_{\bar{p}}} \leq 3 \cdot 10^{-3} \quad (4.6c)$$

The particular values are:

$$m_e = m_{\bar{e}} = 9.109382 \cdot 10^{-31} \text{ kg} \wedge m_p = m_{\bar{p}} = 1.672622 \cdot 10^{-27} \text{ kg} \quad (4.7a)$$

$$|q_e| = |q_{\bar{e}}| = |q_p| = |q_{\bar{p}}| = e = 1.602177 \cdot 10^{-19} \text{ C} \quad (4.7b)$$

$$|\mu_e| = |\mu_{\bar{e}}| \approx \frac{m_p}{m_e} |\mu_p| = \frac{m_{\bar{p}}}{m_{\bar{e}}} |\mu_{\bar{p}}| \approx 9.274009 \cdot 10^{-24} \frac{\text{Cm}^2}{\text{s}} \quad (4.7c)$$

5 Charge exchange kinematics

In a charge exchange reaction, an antiproton replaces an electron in a positronium and as a result a neutral antihydrogen atom is obtained. It is the only mechanism of antihydrogen production in AEGIS. Symbolically:



The general energy levels of a positronium is referred as n_{Ps} and that of an antihydrogen as n .

Only the instantaneous velocity vectors at the time of the reaction are considered¹.

In this chapter, the focus is on the charge exchange kinematics. The main goal is to derive an identity putting following quantities together: the magnitudes of initial velocities of an antiproton and of a positronium ($v_{\bar{p}}$ and v_{Ps}), the magnitude of an antihydrogen's final velocity ($v_{\bar{\text{H}}}$), the angles between these velocity vectors (θ_{Ps} and $\theta_{\bar{\text{H}}}$) and the energy levels of the initial positronium and the final antihydrogen². The derivation will be performed in a relativistic way, more accurate in comparison with classical mechanics approach³.

All the mentioned variables are scalars and therefore are the same in any non-rotating coordinate system attached to an inertial frame of reference where the laboratory stays at rest. One is therefore allowed to choose a coordinate system for each charge exchange reaction event separately. The following choice proves to be very useful:

For a chosen charge exchange event, all the derivation of the reaction kinematics in this chapter will take place in a non-rotating Cartesian coordinate system attached to the laboratory with the origin in the charge exchange reaction point. The vectors of incipient particles unambiguously form a plane where the X_1 -axis and X_2 -axis find themselves; since every $A + B \rightarrow C + D$ reaction takes place in a plane due to the energy and linear momentum conservation laws, the X_3 -axis is irrelevant. The X_1 -axis is set so that the vector of the antiproton velocity points in its positive direction and this half-axis defines the zero angle for the associated polar coordinates.

This is exactly the setting in the Figure 5.1.

The advantage is that one angle (that of the antiproton) is always zero by definition and, moreover, the sense of $\theta_{\bar{\text{H}}}$ is antihydrogen's deviation from antiproton's direction which one may be interested in.

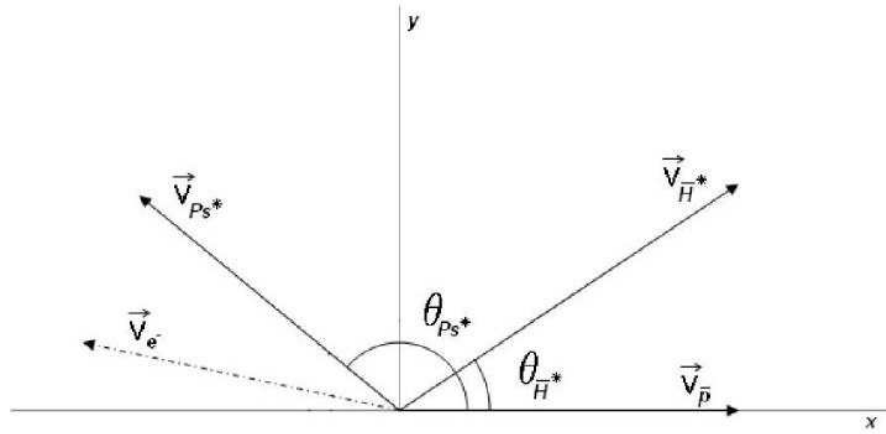
The instantaneous velocity vectors of all the four particles attending the charge exchange are simply $\vec{v} = (v_1, v_2, v_3) = (v_1, v_2, 0)$ in the chosen Cartesian coordinate system. The two Cartesian parameters v_1 and v_2 can be in the common way transformed into polar v and θ ; v is never negative and the values of θ ranges in $[0, 2\pi)$ interval.

The velocity magnitude of the antiproton is denoted as $v_{\bar{p}}$. For the positronium, the velocity and the angle are v_{Ps} and θ_{Ps} , for the antihydrogen $v_{\bar{\text{H}}}$ and $\theta_{\bar{\text{H}}}$ and for the electron v_e and θ_e .

¹No matter whether the initial and final particles are forced to accelerate, decelerate or turn – at the reaction instance, their instantaneous velocities are well defined. The instantaneous velocity of the rising antihydrogen atom serves as the initial conditions in its equation of motion in the crossed fields.

²It will be showed that the variables linked to the electron play almost no role.

³The relativistic derivation was chosen even though the real velocities in the experiment hardly top $\frac{c}{10^4}$



Obrázek 5.1: The setting of the charge exchange reaction. The θ_e angle is missing, however, it is well-defined in the text and its placing is intuitive. The excitations of the positronium and the antihydrogen are reminded by asterisk signs but not used in the text anymore. Taken from [1].

In a chosen charge exchange event, if n_{Ps} stands for the principal quantum number of the positronium and $n_{\bar{H}}$ refers to the principal number of the antihydrogen, one may take the following quantity (defined in two equivalent ways) into consideration:

$$Q = ((m_{\bar{p}} + m_{Ps}) - (m_{\bar{H}} + m_e)) c^2 \quad (5.2a)$$

$$Q = R_{\bar{H}} \left(\frac{1}{n_{\bar{H}}^2} - \frac{1}{2n_{Ps}^2} \right) \quad (5.2b)$$

The sense of Q is the difference between the binding energies of the antihydrogen and of the positronium; the R quantity is the Rydberg constant of antihydrogen.

The energy of a relativistic body and its Taylor power series expansion to the fourth order in $v = |\vec{v}|$ equal

$$E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} \approx mc^2 + \frac{1}{2}mv^2 + \frac{3}{8}m\frac{v^4}{c^2}. \quad (5.3)$$

Similarly for the particle's linear momentum:

$$\vec{p} = \frac{m\vec{v}}{\sqrt{1 - \frac{v^2}{c^2}}} \approx m\vec{v} + \frac{1}{2}m\frac{v^2}{c^2}\vec{v} \quad (5.4)$$

$$p = \frac{mv}{\sqrt{1 - \frac{v^2}{c^2}}} \approx mv + \frac{1}{2}m\frac{v^3}{c^2} \quad (5.5)$$

Besides the derivation of the kinematic identity further, this formula is important for one more reason: It shows (in its strict vector form (5.4) that the linear momentum of a body and its velocity are always parallel. Therefore all the reasoning about a frame of reference and a coordinate system in the beginning of this chapter applies to linear momentums as well as to velocities⁴.

⁴The velocity model for the definition of the frame of reference and of the coordinate system was introduced because it illustrates the motivation of the kinematics. However, the linear momentum is much more suitable as the starting point of the identity's derivation since it is very often conserved in a reaction in contrast to the velocity.

Without a doubt, the energy conservation holds in a charge exchange:

$$E_{\bar{p}} + E_{P_s} = E_{\bar{H}} + E_e \quad (5.6)$$

Because of the outlined relativistic approximations and the way how the Q quantity has been defined, the previous equation could be written as

$$\frac{1}{2}m_e v_e^2 + \frac{3}{8}m_e \frac{v_e^4}{c^2} = \frac{1}{2}m_{\bar{p}} v_{\bar{p}}^2 + \frac{3}{8}m_{\bar{p}} \frac{v_{\bar{p}}^4}{c^2} + \frac{1}{2}m_{P_s} v_{P_s}^2 + \frac{3}{8}m_{P_s} \frac{v_{P_s}^4}{c^2} - \frac{1}{2}m_{\bar{H}} v_{\bar{H}}^2 - \frac{3}{8}m_{\bar{H}} \frac{v_{\bar{H}}^4}{c^2} + Q. \quad (5.7)$$

If both terms containing the electron velocity are exclusively moved on the left-hand side of the equation and the whole right-side is then denoted as P_1 , one gets a biquadratic equation for the electron velocity v_e :

$$v_e^4 + \left(\frac{4}{3}c^2\right)v_e^2 - \left(\frac{8c^2 P_1}{3m_e}\right) = 0 \quad (5.8)$$

There is only one physical solution (that is a positive one if squared) to the equation (5.8):

$$v_e^2(P_1) = \frac{2}{3}c^2 \left(\sqrt{1 + \frac{6P_1}{m_e c^2}} - 1 \right) \quad (5.9)$$

The argument P_1 denotes the connection to the (5.8) equation.

Now one can apply the same procedure to the linear momentum conservation law which is of course also valid. However, the linear conservation law is 2-dimensional and the components are:

$$p_{\bar{p}} + p_{P_s} \cos \theta_{P_s} = p_{\bar{H}} \cos \theta_{\bar{H}} + p_e \cos \theta_e \quad (5.10a)$$

$$p_{P_s} \sin \theta_{P_s} = p_{\bar{H}} \sin \theta_{\bar{H}} + p_e \sin \theta_e \quad (5.10b)$$

The terms including $p_{\bar{H}}$ (and $\theta_{\bar{H}}$ as well) can be easily transferred onto the other sides in each of the equations. Then, by squaring the both equations, summing them and by using the Pythagorean identity, one gets a single equation instead of two, with the θ_e angle completely eliminated.

$$p_{\bar{p}}^2 + p_{P_s}^2 + p_{\bar{H}}^2 - 2p_{\bar{p}}p_{\bar{H}} \cos \theta_{\bar{H}} + 2p_{\bar{p}}p_{P_s} \cos \theta_{P_s} - 2p_{P_s}p_{\bar{H}} \cos(\theta_{P_s} - \theta_{\bar{H}}) = p_e^2 \quad (5.11)$$

Although the proper Taylor series expansion of linear momentum has been already introduced, a bit more is necessary to know in this phase of derivation – expansion of a product of two momentums. Using the equation (5.5) and keeping the terms to the fourth order in v , this is obtained:

$$p_{APB} \approx m_A m_B v_A v_B + \frac{1}{2} m_A m_B \frac{v_A v_B}{c^2} (v_A^2 + v_B^2) \quad (5.12)$$

Substituting these into the formula (5.11), another biquadratic equation for v_e is obtained, this time within the linear momentum conservation law,

$$v_e^4 + (c^2) v_e^2 - \left(\frac{c^2 P_2}{m_e^2} \right) = 0, \quad (5.13)$$

where P_2 is defined as

$$\begin{aligned} P_2 = & m_{\bar{p}}^2 v_{\bar{p}}^2 + m_{\bar{p}}^2 \frac{v_{\bar{p}}^4}{c^2} + m_{\text{Ps}}^2 v_{\text{Ps}}^2 + m_{\text{Ps}}^2 \frac{v_{\text{Ps}}^4}{c^2} + m_{\text{H}}^2 v_{\text{H}}^2 + m_{\text{H}}^2 \frac{v_{\text{H}}^4}{c^2} \\ & - 2m_{\bar{p}}m_{\text{H}}v_{\bar{p}}v_{\text{H}} \left(1 + \frac{v_{\bar{p}}^2 + v_{\text{H}}^2}{2c^2} \right) \cos \theta_{\text{H}} \\ & + 2m_{\bar{p}}m_{\text{Ps}}v_{\bar{p}}v_{\text{Ps}} \left(1 + \frac{v_{\bar{p}}^2 + v_{\text{Ps}}^2}{2c^2} \right) \cos \theta_{\text{Ps}} \\ & - 2m_{\text{H}}m_{\text{Ps}}v_{\text{H}}v_{\text{Ps}} \left(1 + \frac{v_{\text{H}}^2 + v_{\text{Ps}}^2}{2c^2} \right) \cos(\theta_{\text{Ps}} - \theta_{\text{H}}). \end{aligned} \quad (5.14)$$

Like the first one (following from the energy conservation), this biquadratic equation has only one physical solution, too, which is

$$v_e^2(P_2) = \frac{1}{2}c^2 \left(\sqrt{1 + \frac{4P_2}{m_e^2 c^2}} - 1 \right). \quad (5.15)$$

Setting the two solutions $v_e(P_1)$ and $v_e(P_2)$ equal, the whole kinematics is expressed by a single identity. However, any information about the electron (that is v_e and θ_e) has been lost. On the other hand, mathematically, one can get it by return if necessary and the little mass of the electron compared to the antihydrogen suggests its negligible role in the reaction's kinematics. The identity in the terms of P_1 and P_2 is

$$\frac{64P_1^2}{m_e^2 c^4} + \frac{9P_2^2}{m_e^4 c^4} + \frac{8P_1}{m_e c^2} - \frac{48P_1 P_2}{m_e^3 c^4} - \frac{4P_2}{m_e^2 c^2} = 0. \quad (5.16)$$

Both P_1 and P_2 have already been defined and the last step of the derivation is to substitute the two definitions into (5.16) but now keeping only the terms to second order in velocities⁵. The process is very long and error-prone. However, after some algebra, the result is:

$$\begin{aligned} & \left(1 + \frac{m_e}{m_{\text{H}}} + 16\frac{Q}{m_{\text{H}}c^2} + 12\frac{Q}{m_e c^2} \right) v_{\text{H}}^2 + \left(1 - \frac{m_e}{m_{\bar{p}}} - 16\frac{Q}{m_{\bar{p}}c^2} + 12\frac{Q}{m_e c^2} \right) \left(\frac{m_{\bar{p}}}{m_{\text{H}}} \right)^2 v_{\bar{p}}^2 \\ & + \left(1 - \frac{m_e}{m_{\text{Ps}}} - 16\frac{Q}{m_{\text{Ps}}c^2} + 12\frac{Q}{m_e c^2} \right) \left(\frac{m_{\text{Ps}}}{m_{\text{H}}} \right)^2 v_{\text{Ps}}^2 - 2 \left(1 + 12\frac{Q}{m_e c^2} \right) \left(\frac{m_{\bar{p}}}{m_{\text{H}}} \right) v_{\bar{p}}v_{\text{H}} \cos \theta_{\text{H}} \\ & + 2 \left(1 + 12\frac{Q}{m_e c^2} \right) \left(\frac{m_{\bar{p}}m_{\text{Ps}}}{m_{\text{H}}^2} \right) v_{\bar{p}}v_{\text{Ps}} \cos \theta_{\text{Ps}} \\ & - 2 \left(1 + 12\frac{Q}{m_e c^2} \right) \left(\frac{m_{\text{Ps}}}{m_{\text{H}}} \right) v_{\text{Ps}}v_{\text{H}} - 2 \left(1 + 8\frac{Q}{m_e c^2} \right) \left(\frac{m_e}{m_{\text{H}}^2} \right) Q = 0 \end{aligned} \quad (5.17)$$

⁵The fourth order terms served in the biquadratic equation making and are no more required.

It is reasonable now to use these approximations:

$$\frac{Q}{m_{\bar{H}}c^2}, \frac{Q}{m_{\bar{p}}c^2}, \frac{Q}{m_{P_s}c^2}, \frac{Q}{m_e c^2}, \frac{m_e}{m_{\bar{H}}}, \frac{m_e}{m_{\bar{p}}} \ll 1 \quad (5.18a)$$

$$m_{P_s} \approx 2m_e, m_{\bar{H}} \approx m_{\bar{p}} \quad (5.18b)$$

The last two approximations do not apply to the Q quantity. After the implementation of all these approximations, the final identity can be written and understood in the form of a quadratic equation for the antihydrogen velocity:

$$\begin{aligned} v_{\bar{H}}^2 - 2 \left(v_{\bar{p}} \cos \theta_{\bar{H}} + 2 \frac{m_e}{m_{\bar{p}}} v_{P_s} \cos(\theta_{P_s} - \theta_{\bar{H}}) \right) v_{\bar{H}} + \\ + 2 \left(\frac{m_e^2}{m_{\bar{p}}^2} v_{P_s}^2 + 2 \frac{m_e}{m_{\bar{p}}} v_{\bar{p}} v_{P_s} \cos \theta_{P_s} - \frac{m_e Q}{m_{\bar{p}}} \right) = 0 \end{aligned} \quad (5.19)$$

Exactly the same formula is the result of the fully non-relativistic approach, too. The conservation laws are:

$$\frac{1}{2} m_{P_s} v_{P_s}^2 + \frac{1}{2} m_{\bar{p}} v_{\bar{p}}^2 = \frac{1}{2} m_e v_e^2 + \frac{1}{2} m_{\bar{H}} v_{\bar{H}}^2 - Q \quad (5.20a)$$

$$m_{\bar{p}} v_{\bar{p}} + m_{P_s} v_{P_s} \cos \theta_{P_s} = m_e v_e \cos \theta_e + m_{\bar{H}} v_{\bar{H}} \cos \theta_{\bar{H}} \quad (5.20b)$$

$$m_{P_s} v_{P_s} \sin \theta_{P_s} = m_e v_e \sin \theta_e + m_{\bar{H}} v_{\bar{H}} \sin \theta_{\bar{H}} \quad (5.20c)$$

The derivation is very similar, just the solutions of two quadratic equations are set equal instead of two biquadratic equations' solutions. The result is the same. This can serve as a control.

To demonstrate that (5.19) gives reasonable outcomes, let the antiproton and the positronium fly on the same line (the faster positronium following the antiproton) with these sample velocities and principal quantum numbers:

$$v_{\bar{p}} = 45 \text{ m/s}, v_{P_s} = 300 \text{ m/s}, \theta_{P_s} = 0, \theta_{\bar{H}} = 0, n_{P_s} = 29, n_{\bar{H}} = 41 \quad (5.21)$$

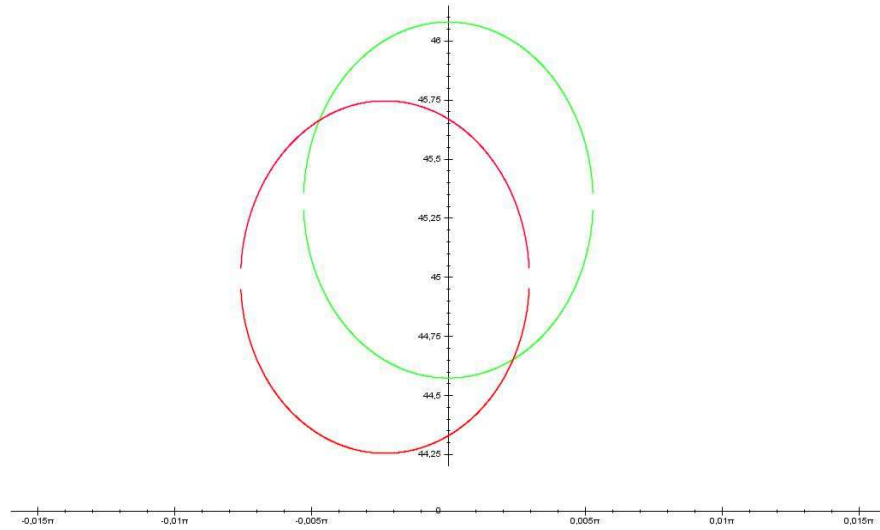
For the chosen pair $n_{P_s} = 29$ and $n_{\bar{H}} = 41$, the absolute value of Q quantity is the smallest up to $n_{P_s} = 43$ and $n_{\bar{H}} = 60$. Therefore its influence to (5.19) is very weak.

Then, according to the positive solution of the formula (5.19), the antihydrogen velocity just after the reaction is 45.3 ± 0.2 m/s.

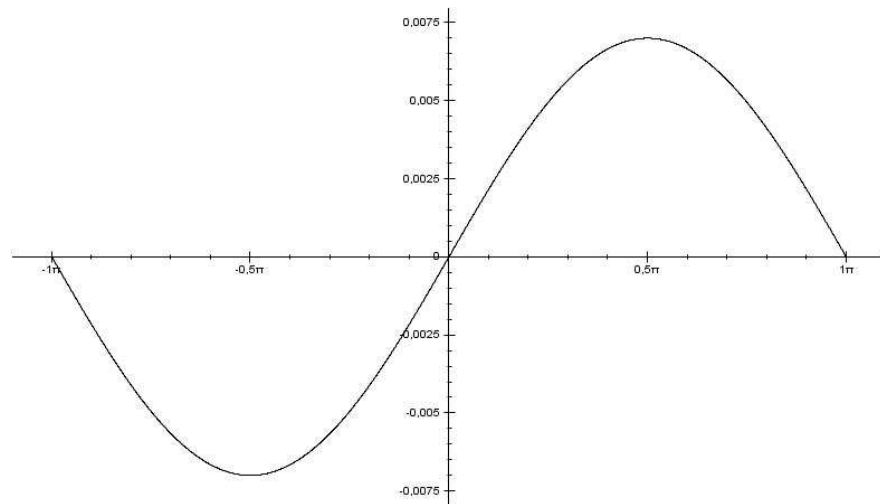
Furthermore, the vector of the final antihydrogen cannot be known precisely since all the information about the electron has been eliminated – there is a class of possible vectors $(v_{\bar{H}}, \theta_{\bar{H}})$ solving the identity. However, the effect of the electron is very small. In the Figure 5.2, it is shown (still with the previous values) how the class of the solutions looks like (the green curve) and how it looks like if the angle of the positronium is changed to perpendicular $\theta_{P_s} = \frac{\pi}{2}$ (the red curve):

The maximum relative difference is 1.3 %. For the same values, if one is interested what is the functional dependence of the deviation of the curve centres (from the previous figure) on the θ_{P_s} angle, the answer is in the Figure 5.3.

The deviation $|\theta_{\bar{H}}|$ (still the effect of the elimination of the information concerning the electron) of the antihydrogen velocity vector from the original antiproton's direction is therefore very small.



Obrázek 5.2: Two classes of solutions of the identity – the green curve for $\theta_{Ps} = 0$ and the red curve for $\theta_{Ps} = \frac{\pi}{2}$. The antihydrogen velocity magnitude is on the vertical axis and the polar angle of the antihydrogen velocity vector on the horizontal axis.



Obrázek 5.3: The dependence of the deviation of the antihydrogen velocity solutions' class centre on the polar angle of the positronium velocity. The horizontal axis refers to that angle and the vertical means the velocity deviation.

Now, for the rising antihydrogen, the direction of its velocity vector may be set equal to that of antiproton ($\frac{\vec{v}_{\bar{H}}}{|\vec{v}_{\bar{H}}|} \approx \frac{\vec{v}_{\bar{p}}}{|\vec{v}_{\bar{p}}|}$) and the velocity magnitude is a solution of (5.19):

$$v_{\bar{H}} = v_{\bar{p}} \cos \theta_{\bar{H}} + 2 \frac{m_e}{m_{\bar{p}}} v_{Ps} \cos(\theta_{Ps} - \theta_{\bar{H}})$$

$$\pm \sqrt{\left(v_{\bar{p}} \cos \theta_{\bar{H}} + \frac{2m_e v_{Ps}}{m_{\bar{p}}} \cos(\theta_{Ps} - \theta_{\bar{H}}) \right)^2 - 2 \frac{m_e^2 v_{Ps}^2}{m_{\bar{p}}^2} - 4 \frac{m_e v_{\bar{p}} v_{Ps}}{m_{\bar{p}}} \cos \theta_{Ps} + \frac{2m_e Q}{m_{\bar{p}}^2}} \quad (5.22)$$

6 Deexcitation

As mentioned in the chapter Experimental facts, it is the nature of a Rydberg hydrogen (or antihydrogen) atom to get rid of the extra internal energy. The effect happens in this reaction:

$$\bar{H}(n, l, m, s) \rightarrow \bar{H}(n', l', m', s') + \gamma \quad (6.1)$$

$$1 \leq n' < n \quad (6.1a)$$

$$n, n' \in N \quad (6.1b)$$

In words: An antihydrogen atom on an energy level given by n switches to a lower energy level labelled with n' ("deexcites") which leads to a single photon radiation¹.

Definition: The reaction (6.1) is called deexcitation and the photon in (6.1) is referred as the deexcitation photon.

The quantities linked to the final antihydrogen have usually a prime aside. The quantities linked to the deexcitation photon have γ subscript.

All the possible energy states are discrete and they are all unambiguously labelled with a natural number (n or n') called the principal quantum number; the rest quantum numbers have no effect on the energy of an antihydrogen². The final state is not necessary the ground state. To make things simpler, only certain transitions are considered, namely those when only the principal quantum number changes:

$$\bar{H}(n, l, m, s) \rightarrow \bar{H}(n', l, m, s) + \gamma \quad (6.2)$$

The condition (6.2) enforces that $l < n'$.

Intuitively, the effect of a deexcitation may suddenly change the kinematic properties of an antihydrogen atom. The magnitude of the effect is about to find in this chapter. The derivation is very similar to that of a Compton scattering but there are two differences: First, a photon is only on the right-hand side of (6.1), and second, an antihydrogen (in contrast to an electron in the Compton scattering) changes its internal state.

The rest energy of an antihydrogen is given by the sum of the rest energies of both its components (an antiproton and a positron) reduced by an amount of the system's binding energy:

$$E_0(n) = m_{\bar{p}}c^2 + m_{\bar{e}}c^2 - \frac{R}{n^2} \quad (6.3a)$$

$$E_0(n') = m_{\bar{p}}c^2 + m_{\bar{e}}c^2 - \frac{R}{n'^2} \quad (6.3b)$$

In this sense, the rest masses of antihydrogen are simply:

$$m_0(n) = m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n^2c^2} \quad (6.3c)$$

$$m_0(n') = m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n'^2c^2} \quad (6.3d)$$

¹More-photon radiation is also possible but very rare [4].

²This statement is not strictly valid. In fact, there is a dependence of the energy level on more quantum numbers which follows from the Dirac equation or from the corrective fine structure terms in the Schrödinger equation. However, due to its weak effect, it is not taken into account in this thesis.

Both rest energy and rest mass of an antihydrogen depend on the principal quantum number only. However, the total antihydrogen energy in a frame of reference depends in addition on its velocity and it is then given by a product of its rest energy and its Lorentz factor ("gamma-factor"):

$$E(v, n) = E_0(n)\gamma(v) = \frac{m_{\bar{p}}c^2 + m_{\bar{e}}c^2 - \frac{R}{n^2}}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{m_0(n)c^2}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (6.4a)$$

$$E(v', n') = E_0(n')\gamma(v') = \frac{m_{\bar{p}}c^2 + m_{\bar{e}}c^2 - \frac{R}{n'^2}}{\sqrt{1 - \frac{v'^2}{c^2}}} = \frac{m_0(n')c^2}{\sqrt{1 - \frac{v'^2}{c^2}}} \quad (6.4b)$$

For sure, there is a frame of reference in which the initial antihydrogen stays at rest. One can write the conservation laws of the deexcitation in this frame of reference quite easily; in fact, the conservation equations take their simplest forms there (since $p(v, n) = 0$):

$$m_0(n)c^2 = E(v', n') + E_\gamma \quad (6.5)$$

$$p(v', n') \cos \theta_{\bar{H}'} = p_\gamma \cos \theta_\gamma \quad (6.6a)$$

$$p(v', n') \sin \theta_{\bar{H}'} = p_\gamma \sin \theta_\gamma \quad (6.6b)$$

The meanings of the symbols in the first equation (energy conservation) was shown in the beginning of this chapter. Like in any other double-particle decays, the three linear momentum vectors form a plane. If the polar coordinates are chosen in that plane, the $p(v', n')$ and p_γ quantities refer to linear momentum magnitudes of the final antihydrogen and the deexcitation photon respectively (both never negative). The $\theta_{\bar{H}'}$ quantity³ is the polar angle of the final antihydrogen in the polar coordinates system and θ_γ is defined for the deexcitation photon in the same way. The inertial frame of reference, where the initial antihydrogen stays at rest and where the polar coordinates are defined, will be used for most of this chapter.

Like in the previous chapter, a proper frame of reference is chosen for each deexcitation event separately – only scalars are expected to figure in what one aims to find in this chapter and therefore the results have a general meaning.

Anyway, the chosen frame of reference is the centre-of-mass one. Then it should be clear that

$$p(v', n') = p_\gamma. \quad (6.7)$$

Since the linear momentum of the initial antihydrogen is always zero, the linear momentums of the two final particles have to be equal in magnitudes (and opposite in directions). The justification is that the (6.7) information follows from the laws (6.6a) and (6.6b) – squaring them, summing and using of Pythagorean identity finally result in the same equation for linear momentum conservation.

Any photon's energy and linear momentum satisfy

$$p_\gamma = \frac{E_\gamma}{c}. \quad (6.8)$$

Setting this and the previous linear momentum information equal, one gets

$$\frac{E_\gamma}{c} = p_\gamma = p(v', n'). \quad (6.9)$$

³The dash stresses that the angle refers to the final antihydrogen in (6.1) and it is therefore distinguished from $\theta_{\bar{H}}$ in the chapter Charge exchange kinematics.

Hence the energy of the deexcitation photon can be expressed as a multiple of the final antihydrogen linear momentum magnitude:

$$E_\gamma = p(v', n')c \quad (6.10)$$

This can be substituted into the energy conservation equation:

$$m_0(n)c^2 = E(v', n') + p(v', n')c \quad (6.11)$$

Now, the final antihydrogen's energy is transferred onto the opposite side of the equation:

$$p(v', n')c = m_0(n)c^2 - E(v', n') \quad (6.12)$$

Squaring of this formula leads to

$$(p(v', n')c)^2 = (m_0(n)c^2 - E(v', n'))^2. \quad (6.13)$$

Now the $(p(v', n')c)^2$ term is expressed. Furthermore, there is one more general way of how the quantity can be found – the Lorentz invariant of the final antihydrogen – it says that

$$(p(v', n')c)^2 = E^2(v', n') - (m_0(n')c^2)^2. \quad (6.14)$$

Setting the two previous expressions equal

$$m_0^2(n)c^4 - 2m_0(n)c^2E(v', n') + E^2(v', n') = E^2(v', n') - m_0^2(n')c^4 \quad (6.15)$$

and eliminating the $E^2(v', n')$ terms give

$$2m_0(n)c^2E(v', n') = m_0^2(n')c^4 + m_0^2(n)c^4. \quad (6.16)$$

Now it is easy to find $E(v', n')$. Moreover, an independent definition of $E(v', n')$ is what the equation (6.4) presents. Now these two expressions of the $E(v', n')$ quantity can be set equal:

$$\frac{m_0^2(n')c^4 + m_0^2(n)c^4}{2m_0(n)c^2} = E(v', n') = \frac{m_0(n')c^2}{\sqrt{1 - \frac{v'^2}{c^2}}} \quad (6.17)$$

If both sides are multiplied with $\frac{1}{m_0(n')c^2}$, the Lorentz factor of the final antihydrogen stands on its side of the equation alone as

$$\frac{1}{\sqrt{1 - \frac{v'^2}{c^2}}} = \frac{m_0^2(n')c^4 + m_0^2(n)c^4}{2m_0(n')m_0(n)c^4}. \quad (6.18)$$

Setting the both fractions reciprocal

$$\sqrt{1 - \frac{v'^2}{c^2}} = \frac{2m_0(n)m_0(n')c^4}{m_0^2(n')c^4 + m_0^2(n)c^4} \quad (6.19)$$

and squaring lead to

$$1 - \frac{v'^2}{c^2} = \left(\frac{2m_0(n)m_0(n')c^4}{m_0^2(n')c^4 + m_0^2(n)c^4} \right)^2. \quad (6.20)$$

Now the goal is to find the value of v' or $\frac{v'}{c}$.

$$\begin{aligned}
\frac{v'^2}{c^2} &= 1 - \left(\frac{2m_0(n)m_0(n')c^4}{m_0^2(n')c^4 + m_0^2(n)c^4} \right)^2 = \\
&= \frac{m_0^4(n')c^8 + 2m_0^2(n)m_0^2(n')c^8 + m_0^4(n)c^8 - 4m_0^2(n)m_0^2(n')c^8}{(m_0^2(n')c^4 + m_0^2(n)c^4)^2} = \\
&= \frac{m_0^4(n')c^8 - 2m_0^2(n)m_0^2(n')c^8 + m_0^4(n)c^8}{(m_0^2(n')c^4 + m_0^2(n)c^4)^2} = \left(\frac{m_0^2(n)c^4 - m_0^2(n')c^4}{m_0^2(n')c^4 + m_0^2(n)c^4} \right)^2 \quad (6.21)
\end{aligned}$$

Hence the result is

$$v' = \frac{m_0^2(n)c^4 - m_0^2(n')c^4}{m_0^2(n')c^4 + m_0^2(n)c^4} c. \quad (6.22)$$

The just derived velocity of the final antihydrogen is linked to the final antihydrogen's linear momentum and possesses analogical qualities – the velocity, like the momentum, is one of the polar coordinates and it is therefore never negative.

The fraction is appropriate to abbreviate even though the reason is just aesthetic.

$$v' = \frac{m_0^2(n) - m_0^2(n')}{m_0^2(n') + m_0^2(n)} c \quad (6.23)$$

The rest masses of the initial and final antihydrogen atoms has been already introduced and now they will be replaced with their definitions (6.3c) and (6.3d) in the previous expression:

$$\begin{aligned}
v' &= \frac{\left(m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n^2 c^2}\right)^2 - \left(m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n'^2 c^2}\right)^2}{\left(m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n^2 c^2}\right)^2 + \left(m_{\bar{p}} + m_{\bar{e}} - \frac{R}{n'^2 c^2}\right)^2} c = \\
&= \frac{(m_{\bar{p}} + m_{\bar{e}})^2 - 2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{n^2 c^2} + \frac{R^2}{n^4 c^4} - (m_{\bar{p}} + m_{\bar{e}})^2 + 2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{n'^2 c^2} - \frac{R^2}{n'^4 c^4}}{(m_{\bar{p}} + m_{\bar{e}})^2 - 2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{n^2 c^2} + \frac{R^2}{n^4 c^4} + (m_{\bar{p}} + m_{\bar{e}})^2 - 2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{n'^2 c^2} + \frac{R^2}{n'^4 c^4}} c = \\
&= \frac{-2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{c^2} \left(\frac{1}{n^2} - \frac{1}{n'^2}\right) + \frac{R^2}{c^4} \left(\frac{1}{n^4} - \frac{1}{n'^4}\right)}{2(m_{\bar{p}} + m_{\bar{e}})^2 - 2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{c^2} \left(\frac{1}{n^2} + \frac{1}{n'^2}\right) + \frac{R^2}{c^4} \left(\frac{1}{n^4} + \frac{1}{n'^4}\right)} c \quad (6.24)
\end{aligned}$$

It follows that the velocity of the final antihydrogen depends on the initial and final states' principal numbers only – the rest in (6.24) are constants, namely: the rest mass of an antiproton, the rest mass of a positron, the Rydberg constant of an antihydrogen and the speed of light in vacuum. They are all known with a very high accuracy. A brief analysis of the equation (6.24) indicates that the fraction is dimensionless since the dimension of the rightmost speed of light corresponds with the final antihydrogen velocity's dimension on the left-hand side of the equation. In SI units [3]:

$$m_{\bar{p}} = 1.672622 \cdot 10^{-27} \text{ kg} \wedge m_{\bar{e}} = 9.109382 \cdot 10^{-31} \text{ kg}$$

$$R = 2.179872 \cdot 10^{-18} \text{ J}$$

$$c = 299792458 \frac{\text{m}}{\text{s}}$$

Only the principal numbers and the rightmost c constant will be untouched:

$$v = \frac{-8.118 \cdot 10^{-62} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right) + 5.883 \cdot 10^{-70} \left(\frac{1}{n^4} - \frac{1}{n'^4} \right)}{5.601 \cdot 10^{-54} - 8.118 \cdot 10^{-62} \left(\frac{1}{n^2} + \frac{1}{n'^2} \right) + 5.883 \cdot 10^{-70} \left(\frac{1}{n^4} + \frac{1}{n'^4} \right)} c \quad (6.25)$$

This should help to simplify the expression of the final velocity a bit since the magnitude of the terms in the numerator and the denominator can be compared.

In the denominator, the second and the third term are limited since $\left(\frac{1}{n^2} + \frac{1}{n'^2} \right) \leq 2$ and $\left(\frac{1}{n^4} + \frac{1}{n'^4} \right) \leq 2$ for all possible pairs of natural numbers n and n' . So there is no need to discuss the particular values of the second and the third term - they form less than one ten-millionth of the denominator.

In the numerator, one can see that $0 \leq \frac{1}{n^2} \leq 1$, $0 \leq \frac{1}{n'^2} \leq 1$, $0 \leq \frac{1}{n^4} \leq 1$ and $0 \leq \frac{1}{n'^4} \leq 1$ which leads to $-1 \leq \frac{1}{n^2} - \frac{1}{n'^2} \leq 1$ and $-1 \leq \frac{1}{n^4} - \frac{1}{n'^4} \leq 1$.

Furthermore, $\frac{1}{n^4} - \frac{1}{n'^4} = \frac{n'^4 - n^4}{n^4 n'^4} = \frac{(n'^2 + n^2)(n'^2 - n^2)}{n^2 n'^2} = \left(\frac{1}{n^2} + \frac{1}{n'^2} \right) \left(\frac{1}{n^2} - \frac{1}{n'^2} \right)$. It was mentioned in the analysis of the denominator that $\left(\frac{1}{n^2} + \frac{1}{n'^2} \right) \leq 2$ and now it follows that the term $\frac{1}{n^4} - \frac{1}{n'^4}$ cannot be more than twice as higher than $\frac{1}{n^2} - \frac{1}{n'^2}$. Therefore the second term in the numerator can be neglected, too.

These sensible approximations simplify the formula for the final antihydrogen velocity:

$$v' = \frac{-2(m_{\bar{p}} + m_{\bar{e}}) \frac{R}{c^2} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right)}{2(m_{\bar{p}} + m_{\bar{e}})^2} c = \frac{R}{m_{\bar{p}} c^2 + m_{\bar{e}} c^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) c \quad (6.26)$$

The fully non-relativistic approach can serve as a control. The proper energy and linear momentum conservation laws are:

$$-\frac{R}{n^2} = -\frac{R}{n'^2} + \frac{1}{2}(m_{\bar{p}} + m_{\bar{e}}) v'^2 + E_{\gamma} \quad (6.27)$$

$$0 = (m_{\bar{p}} + m_{\bar{e}}) v' - \frac{E_{\gamma}}{c} \rightarrow E_{\gamma} = (m_{\bar{p}} + m_{\bar{e}}) c v' \quad (6.28)$$

Substituting the second equation into the first one, the result is a quadratic equation for the final antihydrogen velocity.

$$v'^2 + 2c v' - \frac{2R}{m_{\bar{p}} + m_{\bar{e}}} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) = 0 \quad (6.29)$$

Its positive solution is

$$v' = \frac{-2c + \sqrt{4c^2 + 4c^2 \frac{2R}{m_{\bar{p}} c^2 + m_{\bar{e}} c^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)}}{2}. \quad (6.30)$$

The Taylor series of the solution to the first order equal

$$v' \approx \left(-1 + 1 + \frac{1}{2} \cdot 2 \cdot \frac{\frac{R}{c^2}}{m_{\bar{p}} c^2 + m_{\bar{e}} c^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \right) c = \frac{R}{m_{\bar{p}} c^2 + m_{\bar{e}} c^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) c. \quad (6.31)$$

The results of two different approaches, that of the special relativity (6.26) and that of the classical mechanics (6.31) are the same.

Some of the characteristics of the result are simple to find. For $1 \leq n' \leq n$, the v' value is positive, naturally, and for $n' = n$ (nothing happens to the antihydrogen), the velocity is zero, as expected – note the frame of reference where the initial antihydrogen stays at rest has not been abandoned yet.

The result depends on four constants: R , $m_{\bar{p}}$, $m_{\bar{e}}$ and c . If the values are used instead of symbols, this is obtained:

$$v' = 4.345 \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \left[\frac{\text{m}}{\text{s}} \right] \quad (6.32)$$

The number 4.345 (with its proper SI unit metre per second) also means the theoretically maximum velocity which the final antihydrogen can gain in the centre-of-mass frame of reference.

If one would like now to work with quantities in the laboratory frame of reference, they had to transfer the v' result into that frame. According to the fact that the values of the initial antihydrogen velocity in the laboratory frame of reference would not be greater than 1000 metres per second, the classical Galilean velocity transformation can be used – the possible relative difference to the "slow Lorentz transformation" [7] would be approximately 10^{-11} . As the direction of the deexcitation photon is random and isotropic, so it is in the laboratory frame of reference after the transformation.

Finally, one can try to evaluate v' for certain pairs of n and n' :

$$n = 25, n' = 24 \rightarrow v' = 5.914 \cdot 10^{-4} \left[\frac{\text{m}}{\text{s}} \right] \quad (6.33a)$$

$$n = 25, n' = 1 \rightarrow v' = 4.338 \left[\frac{\text{m}}{\text{s}} \right] \quad (6.33b)$$

Evidently, the effect of the deexcitation can reach the order of metres per second and the smaller the deexcitaion difference in the principal numbers is, the smaller is the velocity change effect. Note the chapter Experimental facts where the dependence of the n level lifetime on the magnetic field strength was mentioned.

In fact, only one deexcitation of $n - n' = 1$ or $n - n' = 2$ is expected to happen to an antihydrogen atom during his whole life in the AEGIS experiment measurement. Generally:

$$v' = 4.345 \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \left[\frac{\text{m}}{\text{s}} \right] = 4.345 \frac{n^2 - n'^2}{n'^2 n^2} \left[\frac{\text{m}}{\text{s}} \right] = 4.345 \frac{(n + n')(n - n')}{n'^2 n^2} \left[\frac{\text{m}}{\text{s}} \right] \quad (6.34)$$

For $n - n' = 1$, (6.34) becomes $v' = 4.345 \frac{2n-1}{(n-1)^2 n^2} \left[\frac{\text{m}}{\text{s}} \right]$, whereas $v' = 4.345 \frac{2n-2}{(n-2)^2 n^2} \left[\frac{\text{m}}{\text{s}} \right]$ is obtained for $n - n' = 2$. For Rydberg antihydrogens close to $n = 25$, both outcomes become approximately:

$$v' \approx \frac{8.7}{n^3} \left[\frac{\text{m}}{\text{s}} \right] \quad (6.35)$$

The magnitude of (6.35) for the expected Rydberg levels is of the order $5 \cdot 10^{-4} \left[\frac{\text{m}}{\text{s}} \right]$ which forms less than one millionth of the initial velocity in the laboratory frame of reference. Therefore it would not be a rough approximation at all to neglect the deexcitation kinematics effects completely; on the other hand, the deexcitation itself has to be taken into account all the time since the instantaneous quantum numbers are variables in the antiatoms' dynamics in external crossed fields as it will be showed.

The same result and the same reasoning hold for a hydrogen atom when $m_{\bar{e}}$ and $m_{\bar{p}}$ are switched to m_e and m_p .

7 Elementar dipoles

As it was showed in the chapter Theoretical facts, the unperturbed spectrum of a hydrogen atom is discrete. The same quantum character can be expected for the perturbed spectrum as well, that is for an atom in non-zero crossed fields. This chapter does not examine the quantisation itself; its aim is to find the macroscopic dynamics if the spectrum is known. The analysis will be naturally presented within the field of classical mechanics.

First, the following Ansatz is stated: *The spectral energy shift W_1 of a hydrogen atom in crossed fields is its potential energy and the macroscopic (net) force acting on such an atom is given as*

$$\vec{F} = -\vec{\nabla}W_1. \quad (7.1)$$

The W_1 symbol does not mean the total energy $W = W_0 + W_1$ of the particular state (that is the particular energy level, for instance) but refers to the difference between such a total energy and the corresponding unperturbed energy W_0 , even though when confused, (7.1) would give the same results. This Ansatz will be a heuristic principle. However, this chapter will provide a few examples, where the Ansatz can be directly justified, and therefore supports its extrapolation (or interpolation) for an arbitrary dipole in arbitrary crossed fields.

If the dipole terms at the most are taken into account in the multipole expansion of the system (here of a hydrogen atom), the spectrum is said to have a dipole-like character (when computing or when interpreting the measurements results).

It has to be stressed that although a magnetic field is not conservative, the magnetic potential energy of a magnetic *dipole* (instead of a charged particle) in a magnetic field is well-defined quantity. Therefore the Ansatz handles well-defined quantities as well since, in fact, all types of dipoles discussed in this thesis are similar in this sense.

Consider a set of charges and currents. In the case of sole charges it holds that the scalar potential is formed by another non-Coulomb terms – the multipole expansion terms.

In the distance of R from the charge set, the scalar potential ϕ is given [7] as

$$\phi(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left(\frac{Q}{R} + \frac{d}{R^2} + \frac{\kappa_E}{R^3} + \dots \right), \quad (7.2)$$

where Q , d and κ_E symbols refer to the total electric monopole moment (electric charge) of the set, the total electric dipole moment (electric dipole) of the set and the total electric quadrupole moment (electric quadrupole) of the set. Similarly, in the case of sole currents, one obtains the vector potential as

$$\vec{A}(\vec{R}) = \frac{\mu_0}{4\pi} \left(\frac{\tilde{Q}\vec{R}}{R^2} + \frac{\vec{\mu} \times \vec{R}}{R^3} + \frac{\vec{f}(\kappa_M, \vec{R})}{R^4} + \dots \right), \quad (7.3)$$

where \tilde{Q} , μ and κ_M refer to the total magnetic monopole moment (magnetic charge) of the set – which is always zero –, the total magnetic dipole moment (magnetic dipole) of the set and the total magnetic quadrupole moment (magnetic quadrupole) of the set. For a not-ionised hydrogen atom, both Q and \tilde{Q} equal zero and $\frac{\kappa_E}{R^3}$ and $\frac{\kappa_M}{R^3}$ are very small when compared to $\frac{d}{R^2}$ and $\frac{m}{R^2}$ in this thesis' model.

What remains are $\phi(\vec{R}) = \frac{1}{4\pi\epsilon_0} \frac{d}{R^2}$ and $\vec{A}(\vec{R}) = \frac{\mu_0}{4\pi} \frac{\vec{\mu} \times \vec{R}}{R^3}$. These terms correspond to the terms in the Hamiltonian (3.4) which was formed in the dipole approximation already. In other words, the spectrum of a hydrogen atom corresponds to the (3.4) Hamiltonian, both when computing and when measuring.

It was briefly indicated that there are two types of dipoles – electric and magnetic; however, this is not the only division. According to the crossed fields' strength (or dependence on quantum numbers or the form of a potential energy), both dipoles may be classified as not-induced or induced. An example of a

system with a not-induced electric dipole is a water molecule; an induced electric dipole is observable on a hydrogen atom in the ground state; a not-induced magnetic dipole is evinced by a neutron, for instance; and one can encounter an induced magnetic dipole when studying a parapositronium.

7.1 Not-induced electric dipole – a water molecule

In an experiment, it can be measured that a water molecule evinces an electric dipole moment [3]:

$$d = 6.2 \cdot 10^{-30} \text{ C} \cdot \text{m} \quad (7.4)$$

Its value almost does not depend on the strength of an external electric field, therefore it is called not-induced. It is a quality of the internal structure of the molecule itself – the charge is distributed non-uniformly. The positions \vec{r}_- and \vec{r}_+ of the centres of the negative and positive charge distributions can be defined; the charge values corresponding to them are simply $q_+ = -q_- = 2e$.

The relative position of the previous two charge centres is

$$\vec{l} = \vec{r}_+ - \vec{r}_-. \quad (7.5)$$

The relation of this quantity to the not-induced electric dipole moment is simply $\vec{d} = q\vec{l}$ where $q = |q_+| = |q_-|$. Aside the vector \vec{l} in (7.5), another important vector associated with the molecule is the centre of mass position:

$$\vec{R} = \frac{m_+\vec{r}_+ + m_-\vec{r}_-}{m_+ + m_-} \quad (7.6)$$

The m_- and m_+ symbols could be understood as the parts of the molecule's total mass which are concentrated about the \vec{r}_- and \vec{r}_+ points.

The equations (7.5) and (7.6) together form simultaneous linear equations for \vec{r}_- a \vec{r}_+ to be found. The solution is:

$$\vec{r}_+ = \vec{R} + \frac{m_-}{m_+ + m_-} \vec{l} \quad (7.7a)$$

$$\vec{r}_- = \vec{R} - \frac{m_+}{m_+ + m_-} \vec{l} \quad (7.7b)$$

Now consider the water molecule placed into an external electric field. According to the phenomenological fact, the absolute value of the molecule's dipole is invariant, therefore only the spatial orientation may vary – like an elementary rigid body. The total macroscopic force on the molecule is given as the vector sum of the forces experienced separately by both charge centres as

$$\begin{aligned} \vec{F} = \vec{F}_+ + \vec{F}_- &= q \left(\vec{E}(\vec{r}_+) - \vec{E}(\vec{r}_-) \right) = q \left(\vec{E} \left(\vec{R} + \frac{m_-}{m_+ + m_-} \vec{l} \right) - \vec{E} \left(\vec{R} - \frac{m_+}{m_+ + m_-} \vec{l} \right) \right) \approx \\ &\approx q \left(\vec{E}(\vec{R}) + \frac{m_-}{m_- + m_+} (\vec{l} \cdot \nabla) \vec{E}(\vec{R}) - \vec{E}(\vec{R}) + \frac{m_+}{m_- + m_+} (\vec{l} \cdot \nabla) \vec{E}(\vec{R}) \right) = \\ &= q (\vec{l} \cdot \nabla) \vec{E}(\vec{R}). \end{aligned} \quad (7.8)$$

The separation of the charge centres was treated to be very small when compared to the distances of the molecule's macroscopic motion, that is $|\vec{l}| \ll |\vec{R}|$. In the expansion, a $\vec{l}\vec{\nabla}$ operator (as a kind of an extrapolation of a usual derivative into three dimensions) was introduced and it is defined as

$$\vec{l}\vec{\nabla} = \sum_{j=1}^3 l_j \frac{\partial}{\partial X_j} = l_1 \frac{\partial}{\partial X_1} + l_2 \frac{\partial}{\partial X_2} + l_3 \frac{\partial}{\partial X_3}. \quad (7.9)$$

If the $\vec{d} = q\vec{l}$ relation is substituted into (7.8), one obtains

$$\vec{F} = \left(\vec{d}\vec{\nabla} \right) \vec{E} \left(\vec{R} \right). \quad (7.10)$$

Written by Cartesian coordinates, it is

$$F_i = \sum_{j=1}^3 d_j \frac{\partial E_i}{\partial X_j}. \quad (7.11)$$

Now an alternative derivation of (7.11) will be presented – not in the language of Newtonian mechanics but with the help of a potential energy. The potential energy of a water molecule in an external electric field [7] is

$$W_1 = -\vec{d}\vec{E} = -\tilde{d}E, \quad (7.12)$$

where \tilde{d} means the projection of \vec{d} into the \vec{E} direction (with respect to the sign). The force on the molecule in an external electric field is then (according to the Ansatz) given as

$$\vec{F} = -\vec{\nabla}W_1 = -\vec{\nabla} \left(-\tilde{d}E \right) = \tilde{d}\vec{\nabla}E, \quad (7.13)$$

where a usual gradient operator $\vec{\nabla} = \left(\frac{\partial}{\partial X_1}, \frac{\partial}{\partial X_2}, \frac{\partial}{\partial X_3} \right)$ is present instead of (7.9). Written by Cartesian coordinates it holds that

$$\begin{aligned} F_i &= \tilde{d} \frac{\partial}{\partial X_i} E = \tilde{d} \frac{\partial}{\partial X_i} \left| \vec{E} \left(\vec{R} \right) \right| = \tilde{d} \frac{\partial}{\partial X_i} \sqrt{\sum_{j=1}^3 E_j E_j} = \tilde{d} \frac{2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i}}{2 \sqrt{\sum_{j=1}^3 E_j E_j}} = \\ &= \frac{\tilde{d}}{\sqrt{\sum_{j=1}^3 E_j E_j}} \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} = \tilde{d} \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}. \end{aligned} \quad (7.14)$$

Regardless the factors, the two outcomes (7.14) and (7.11) differ in the derivatives and indices – even though they look similar, the analytical difference is significant. However, the discrepancy can be explained and rectified. In fact, the constant magnitude of the electric dipole in the case of a water molecule means a holonomic constraint which reduces the six degrees of freedom (of the pair of the point-like charges) to five. The equation (7.11) establishes the system's dynamics only for three of these five degrees of freedom – another two have not been determined yet.

In accordance with the rules of dynamics, the total force on a rigid body has to be supplemented with the total torque on it. The torque on a water molecule is given as a cross product of the electric dipole vector and the electric intensity vector [7] as

$$\vec{N} = \vec{d} \times \vec{E} \left(\vec{R} \right). \quad (7.15)$$

In fact, the equation (7.15), which deals with the remaining two degrees of freedom, means that the electric dipole vector is being turned towards the electric intensity vector's direction. The detailed description of the orientation plays no role in the macroscopic dynamics – one is actually interested

only in the three degrees of freedom associated with \vec{R} . Hence the equations (7.11) and (7.15) can be transformed into a single one so that the orientation given by (7.15) is introduced into (7.11).

If the space orientation act of a dipole according to (7.15) is very quick, the previous Newtonian derivation is modified so that one takes only those electric field gradients into account which are parallel to the local electric field intensity vector (more in the section about a not-induced magnetic dipole). In this case, the (7.11) equation takes this form:

$$F_i = \tilde{d} \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} \quad (7.16)$$

The two alternative derivations are quite different – when starting from the potential energy, the molecule is considered point-like (that is its electric dipole is not defined by the separation of two charge centres but understood as a fundamental concept); when starting from the Newtonian mechanics, the knowledge of the molecule's size is necessary in the very beginning and it has to be taken into account that the field varies at least in the first order on this scale. However, both outcomes are the same.

7.2 Induced electric dipole – a hydrogen atom in the ground state

In an experiment, the electric dipole of a hydrogen atom in the ground state proves itself to be variable (contrary to the water molecule case) – it depends on the strength of an external electric field. This dependence is linear and the proportionality constant α is called the polarizability of a hydrogen atom (in the ground state¹) [8].

$$\vec{d} = \alpha \vec{E} \quad (7.17)$$

$$\alpha = \alpha(1, 0, 0) = 7.2 \cdot 10^{-41} \frac{\text{C}^2 \text{s}^2}{\text{kg}} \quad (7.18)$$

The electric dipole of a hydrogen atom in the ground state is naturally called induced since it is really induced by an external electric field and it is not a quality of a hydrogen atom itself. In a zero external electric field, the electric dipole of a hydrogen atom in the ground state is zero as well; on the contrary, in non-zero external electric field, the electric dipole is non-zero, too.

If the induced electric dipole is understood within the same model like a water molecule as a pair of separated charges (and if the distance is variable this time) and if (7.17) is understood as a holonomic constraint as well, the number of the degrees of freedom is reduced to three – (7.17) determines not only the magnitude of the electric dipole of a hydrogen atom but the orientation of the dipole's vector at the same time as well.

A hydrogen atom in the ground state possesses only three degrees of freedom in this thesis model and the torque equation is trivial and not necessary to be considered at all. The force equation can be found in the same way like in the case of a water molecule with the different holonomic constraint (7.17). By the Cartesian coordinates it is

$$F_i = \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i}. \quad (7.19)$$

There is an alternative of how to derive (7.19), too. The potential energy of a hydrogen atom in an external electric field is known:

$$W_1 = -\frac{1}{2} \alpha \vec{E}^2 \quad (7.20)$$

¹The polarizability is well defined for every state of a hydrogen atom, that is $\alpha = \alpha(n, l, m)$. In this section it is $\alpha(1, 0, 0)$.

In the sense of the Ansatz from the beginning of this chapter, the force on a hydrogen atom in the ground state should be a negative gradient of its potential energy. Really:

$$\vec{F} = -\vec{\nabla}W_1 \rightarrow F_i = -\frac{\partial}{\partial X_i}W_1 = -\frac{\partial}{\partial X_i}\left(-\frac{1}{2}\alpha\vec{E}^2\right) = \frac{1}{2}\alpha \cdot 2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} = \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} \quad (7.21)$$

Again, the same force was found by two different approaches – a pure Newtonian and that following from the Ansatz.

7.3 Not-induced magnetic dipole – a neutron

A neutron evinces a magnetic dipole moment [3]:

$$\mu = |\vec{\mu}| = 5.050783 \cdot 10^{-27} \frac{\text{Cm}^2}{\text{s}} \quad (7.22)$$

Like in the case of a water molecule, this magnetic dipole of a neutron does not depend on the strength of an external field (a magnetic one in this case, of course) and is naturally called not-induced – it is an intrinsic property of the particle.

Although the not-induced electric and magnetic dipoles are of a different nature, they are similar when their own lines of force are concerned (that is the lines induced by themselves, not by any external field) and they are also similar in the form of the potential energy when placed into an external field – for the not-induced magnetic dipole in a magnetic field it is

$$W_1 = -\vec{\mu}\vec{B}, \quad (7.23)$$

where the orientation of $\vec{\mu}$ is general for now but its magnitude is fixed (see (7.22)). Due to the formal sameness of (7.23) and (7.12), the equations of motion for the two dipoles have to be formally the same as well. First, the torque equation is

$$\vec{N} = \vec{\mu} \times \vec{B}. \quad (7.24)$$

It has to be stressed that (7.24) is (contrary to the analogical case of a not-induced electric dipole) analytically solvable. To the left-hand side, the Euler's second law can be substituted – the total torque of external forces on an object equals the total time derivative of the system's total angular momentum [9]:

$$\vec{N} = \frac{d\vec{L}}{dt} \quad (7.25)$$

Since the magnetic dipole of a particle is proportional to its (mechanical) angular momentum, the right-hand side of (7.25) can be rewritten to

$$\vec{N} = \frac{d\left(\frac{1}{g}\vec{\mu}\right)}{dt}. \quad (7.26)$$

The constant of proportionality μ in (7.26) connecting the dipole and the angular momentum is called a gyromagnetic ratio. Due to (7.25) and (7.26), the equation (7.24) becomes

$$\frac{d\vec{\mu}}{dt} = g\vec{\mu} \times \vec{B}. \quad (7.27)$$

Written by Cartesian coordinates and without loss of generality with $\vec{B} = (0, 0, B)$, one obtains:

$$\frac{d\mu_1}{dt} = gB\mu_2 \quad (7.28a)$$

$$\frac{d\mu_2}{dt} = -gB\mu_1 \quad (7.28b)$$

$$\frac{d\mu_3}{dt} = 0 \quad (7.28c)$$

The third equation is trivial to solve – its meaning is that the $\vec{B} = (0, 0, B)$ direction is significant in the space for the orientation of a particle possessing a magnetic dipole – the third coordinate μ_3 is invariant. The other two form simultaneous differential equations of the first order which is best to solve in its matrix representation

$$\frac{d}{dt} \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \begin{pmatrix} 0 & +gB \\ -gB & 0 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad (7.29)$$

and the solution is

$$\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \begin{pmatrix} -\frac{\mu_1^0}{gB} \cos(gBt) + \frac{\mu_2^0}{gB} \sin(gBt) \\ +\frac{\mu_1^0}{gB} \cos(gBt) + \frac{\mu_2^0}{gB} \sin(gBt) \end{pmatrix}, \quad (7.30)$$

where μ_1^0 and μ_2^0 are Cartesian coordinates of the magnetic dipole vector's initial conditions in the plane perpendicular to the $(0, 0, B)$ direction. In fact, this is equivalent to an initial condition for an angle between the $\vec{\mu}$ and \vec{B} vectors. It will be shown in the following chapter that the cosine of this angle is quantised and therefore that the initial condition is given by an appropriate quantum number.

It is also important that the direction of the local magnetic field \vec{B} is significant² – (7.30) gives then an information that the orientation of the magnetic dipole vector is determined by the \vec{B} direction and about this direction, the precession motion of the magnetic dipole takes place.

This precession is called the Larmor precession. Since the time scale of its period is incomparably smaller than the scale of the macroscopic motion of the system, on which is the focus in this thesis, it is possible (in a model) to replace the precession motion by simple ignoring (self-cancelling) the coordinates of the magnetic dipole vector which are perpendicular to the \vec{B} direction (time averaging of a high frequency motion) and to take only that coordinate parallel to the \vec{B} into account.

So now consider a not-induced magnetic dipole which is automatically oriented to the $\vec{B} = (0, 0, B)$ direction and which is quantised. In the case of an electric dipole, a model of a pair of separated charges is the most appropriate. In the classical electromagnetism, the most suitable model for a magnetic dipole is an elementary current loop. If one is interested in the force on the magnetic dipole in an external magnetic field, the classical electromagnetism provides a way of how to find a force on such a current loop.

In a uniform magnetic field, all the forces on any two sides of a current loop would cancel each other (according to the Amper law, for instance) – it is necessary to introduce gradients, that is quantities like $\partial B_j / \partial X_i$. Let the loop be a square. The total external force in the local field's direction (that is in the X_3 -axis direction here) equals the sum of the forces on all four sides of the square current loop with respect to the signs [10]:

$$F_3 = F_{B1}^+ + F_{B1}^- + F_{B2}^+ + F_{B2}^- \quad (7.31)$$

²In the analysis, the vector $\vec{B} = (0, 0, B)$ was considered but the outcomes can be easily transformed to any general case of a local magnetic field $\vec{B} = (B_1, B_2, B_3)$ since $(0, 0, B)$ can be achieved by an appropriate axes rotation.

The $F_{B_j}^\pm$ symbols refer to magnetic forces on the particular sides of the current loop in the X_j directions (as they are understood in a common Amper law) with the current flowing in the positive or negative sense. It is

$$\begin{aligned} F_3 &= +I\Delta_1 B_2 - I\Delta_1 \left(B_2 + \Delta_2 \frac{\partial B_2}{\partial X_2} \right) + I\Delta_2 B_1 - I\Delta_2 \left(B_1 + \Delta_1 \frac{\partial B_1}{\partial X_1} \right) = \\ &= -I\Delta_1 \Delta_2 \left(\frac{\partial B_1}{\partial X_1} + \frac{\partial B_2}{\partial X_2} \right), \end{aligned} \quad (7.32)$$

where Δ_1 and Δ_2 refer to the dimensions of the current loop's square. Therefore, a conventional magnetic dipole (its magnitude³) of the loop can be introduced as $\mu = I\Delta_1 \Delta_2$. It is

$$F_3 = -\mu \left(\frac{\partial B_1}{\partial X_1} + \frac{\partial B_2}{\partial X_2} \right). \quad (7.33)$$

Finally, the Gauss law for a magnetic field can be implemented and it gives that

$$\vec{\nabla} \cdot \vec{B} = \frac{\partial B_1}{\partial X_1} + \frac{\partial B_2}{\partial X_2} + \frac{\partial B_3}{\partial X_3} = 0. \quad (7.34)$$

This finding will help to simplify (7.33) since it holds that $\frac{\partial B_1}{\partial X_1} + \frac{\partial B_2}{\partial X_2} = -\frac{\partial B_3}{\partial X_3}$. The coordinate of the external force in the X_3 direction is

$$F_3 = \mu \frac{\partial B_3}{\partial X_3}. \quad (7.35)$$

In the same manner, the F_1 and F_2 coordinates of the \vec{F} force can be found (although much easily due to the symmetry of the problem):

$$F_1 = F_{B_1}^+ + F_{B_1}^- = -I\Delta_2 B_3 + I\Delta_2 \left(B_3 + \Delta_1 \frac{\partial B_3}{\partial X_1} \right) = I\Delta_1 \Delta_2 \frac{\partial B_3}{\partial X_1} = \mu \frac{\partial B_3}{\partial X_1} \quad (7.36a)$$

$$F_2 = F_{B_2}^+ + F_{B_2}^- = -I\Delta_1 B_3 + I\Delta_1 \left(B_3 + \Delta_2 \frac{\partial B_3}{\partial X_2} \right) = I\Delta_1 \Delta_2 \frac{\partial B_3}{\partial X_2} = \mu \frac{\partial B_3}{\partial X_2} \quad (7.36b)$$

The three outcomes can be summed up as

$$F_i = \mu \frac{\partial B_3}{\partial X_i}. \quad (7.37)$$

The reason of the presence of B_3 in (7.37) is due to the special choice of the Cartesian axes. The current loop takes its orientation to the $\vec{B} = (0, 0, B)$ direction automatically and immediately. In fact, (7.37) is not harmed when rewritten as

$$F_i = \mu \frac{\partial B}{\partial X_i}, \quad (7.38)$$

which means that the derivative is taken on $B = |\vec{B}|$ instead of B_3 . It is not necessary to distinguish the B_1 , B_2 and B_3 coordinates in a particular coordinates system anymore since the loop automatically points in the \vec{B} direction. The (7.38) equation therefore represents the most natural generalisation of (7.37) into an arbitrary Cartesian coordinate system, not only that where $\vec{B} = (0, 0, B)$.

³The orientation of the magnetic dipole vector is perpendicular to the plane of the square current loop and points in the direction of tangential lines of field.

When expanded:

$$F_i = \mu \frac{\partial B}{\partial X_i} = \mu \frac{\partial}{\partial X_i} |\vec{B}| = \mu \frac{\partial}{\partial X_i} \sqrt{\sum_{j=1}^3 B_j^2} = \mu \frac{\sum_{j=1}^3 2B_j \frac{\partial B_j}{\partial X_i}}{2\sqrt{\sum_{j=1}^3 B_j^2}} = \mu \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \quad (7.39)$$

This is how the classical electromagnetism solves the problem. When the potential energy of an elementary not-induced magnetic dipole in an external magnetic field is concerned, according to (7.23) and (7.30), it is given as

$$W_1 = -\tilde{\mu}B = -\tilde{\mu} |\vec{B}|. \quad (7.40)$$

According to the Ansatz from the beginning of the chapter, the force on such a dipole should equal a negative gradient of its potential energy.

$$F_i = -\frac{\partial W_1}{\partial X_i} = -\frac{\partial}{\partial X_i} (-\tilde{\mu}B) = \tilde{\mu} \frac{\partial B}{\partial X_i} \quad (7.41)$$

The (7.41) outcome completely agrees with (7.38) and the total force (7.39) is found in two independent ways again. The Ansatz holds in another special case.

The same technique, which was just showed for a not-induced magnetic dipole, can be used in the case of a not-induced electric dipole as well. One would have to use the Gauss law for an electric field which is

$$\vec{\nabla} \vec{E} = \frac{\rho}{\epsilon_0}, \quad (7.42)$$

where ρ means the electric charge density of the system. However, for an electric dipole it holds that $Q = 0$ as it is stated in the beginning of this chapter and therefore:

$$\vec{\nabla} \vec{E} = 0 \quad (7.43)$$

The fact, that the Gauss law has the same formal shape for the both not-induced dipoles (electric and magnetic), is supported by the sameness of their lines of field or their potential energies.

7.4 Induced magnetic dipole – a parapositronium

The potential energy of a parapositronium in an external magnetic field is

$$W_1 = -\frac{1}{2}\beta B^2, \quad (7.44)$$

where β refers to the so called magnetic polarizability of a parapositronium⁴. By comparing (7.44) and (7.40), it is clear that the magnetic dipole of a parapositronium is proportional to the (external) magnetic induction and the particle's dipole is therefore called induced.

By comparing (7.44) and (7.20), one sees the analogy of the induced magnetic dipole of a parapositronium and an induced electric dipole of a hydrogen atom in the ground state. It was suitable to substitute a hydrogen atom in the ground state by a pair of charges with a separation proportional to an external electric field; a similar model is appropriate for a positronium, too – a current loop with an area proportional to an external magnetic field.

⁴The magnetic polarizability of an orthopositronium is the same but for an orthopositronium it does not play a significant role in an external magnetic field which is not extremely strong.

With the same derivation technique like in the case of a not-induced magnetic dipole, the $\Delta_1\Delta_2$ quantity is explicitly proportional to the magnetic induction B – it is reduced with the same quantity in the denominator of (7.39) and the factor can be identified as the polarizability β . The result is

$$F_i = \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}. \quad (7.45)$$

Starting from the Ansatz and knowing the potential energy of a parapositronium in an external magnetic field, one obtains

$$F_i = -\frac{\partial W_1}{\partial X_i} = -\frac{\partial}{\partial X_i} \left(-\frac{1}{2}\beta B^2 \right) = \frac{1}{2}\beta \frac{\partial}{\partial X_i} \sum_{j=1}^3 B_j^2 = \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}. \quad (7.46)$$

Again, the Ansatz is supported by an alternative approach in another special case.

7.5 Summary

In this chapter, four different systems were analysed – a not-induced electric dipole in an external electric field, an induced electric dipole in an external electric field, a not-induced magnetic dipole in an external magnetic field and an induced magnetic dipole in an external magnetic field. A macroscopic force on each of the systems was found by two different approaches. One of them was always based on the Ansatz and its validity in these special cases was successfully tested.

It is therefore reasonable to trust its validity in all cases which are "combinations" of the four ones – for instance when an electric and a magnetic fields are present at the same time (that is for general crossed fields), when a system possesses more kinds of dipoles at the same time etc.

Type of a dipole	Potential energy of a dipole	Force on a dipole
Not-induced electric dipole in electric field	$W_1 = -\tilde{d}E$	$F_i = \tilde{d} \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}$
Induced electric dipole in electric field	$W_1 = -\frac{1}{2}\alpha E^2$	$F_i = \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i}$
Not-induced magnetic dipole in magnetic field	$W_1 = -\tilde{\mu}B$	$F_i = \tilde{\mu} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}$
Induced magnetic dipole in magnetic field	$W_1 = -\frac{1}{2}\beta B^2$	$F_i = \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}$

Tabulka 7.1: The summary of the chapter's finding. All the forces in the last column were found independently but they follow from the second column (due to the Ansatz $F_i = -\frac{\partial}{\partial X_i}W_1$) as well. The symbols with a tilde (\tilde{d} and $\tilde{\mu}$) refer to the projections of not-induced dipoles into the fields' directions.

8 Stark and Zeeman effect

In the previous chapter, an Ansatz of how to find the macroscopic force on a dipole-like object in an electromagnetic field was presented and justified. However, it was necessary to know the object's potential energy.

Now the focus is on a hydrogen atom only. It was predicted that its potential energy (that is its spectrum) is quantised in crossed fields – dependent on atom's quantum numbers. In special cases of a pure electric field (Stark effect) and pure magnetic field (Zeeman effect) it will prove itself that these spectra known from experiments are in accordance with their dipole characters and their analytical form will be found.

The spin (an intrinsic not-induced magnetic dipole) of an electron (or a hydrogen atom) is completely ignored in this chapter.

As already mentioned, the hydrogen spectrum in zero crossed fields, which is called unperturbed, is the solution of the $\hat{H}_0\psi = W_0\psi$ equation and equals

$$W_0 = -\frac{R}{n^2}. \quad (8.1)$$

It depends only on the so called principal quantum number n . The "0" indices the zero crossed fields configuration. The unperturbed spectrum is degenerated since, for a given n , more eigenstates ψ_0 correspond to the same eigenenergy W_0 - there are n^2 of them¹ and can be expressed like this:

$$\psi(n, l, m) = \psi_{nlm} = R_{nl}Y_{lm} = R(n, l)Y(l, m) \quad (8.2)$$

The notation means that it is possible to write all the eigenfunctions $\psi_{nlm} = \psi(n, l, m)$ as a product of a radial function $R_{nl} = R(n, l)$ and a spherical harmonic $Y_{lm} = Y(l, m)$. In this thesis, the second "parenthesis" notation is preferred.

The sets of possible values for the quantum numbers are dependant. The principal quantum number n equals one if a hydrogen atom is in the ground state or equals 2, 3, 4, ... (and effectively up to $+\infty$) if the atom is in an excited state.

For a given n , the azimuthal quantum number l is an element of the set $\{0, +1, +2, \dots, +n - 1\}$ and a magnetic quantum number m is an element of the set $\{-l, -l + 1, \dots, -1, 0, +1, \dots, +l - 1, +l\}$. The total number of different eigenstates for a given n really is

$$\sum_{l=0}^{n-1} \sum_{m=-l}^{+l} 1 = \sum_{l=0}^{n-1} (2l + 1) = 2 \sum_{l=0}^{n-1} l + \sum_{l=0}^{n-1} 1 = 2 \cdot \frac{n(n-1)}{2} + n = n^2 - n + n = n^2. \quad (8.3)$$

In zero crossed fields, there are also n^2 different eigestates with the same energy and their spectral lines are identical – this is sometimes called the accidental degeneracy. However, the number of different spectral lines for the same n increases in non-zero crossed fields and the number of different eigestates with the same energy therefore decreases at the same time.

The Hamiltonian of a hydrogen atom in crossed fields is

$$\hat{H} = \hat{H}_0 + \hat{P}(\vec{E}, \vec{B}), \quad (8.4)$$

where H_0 denotes the atom's Hamiltonian in zero crossed-fields (see (3.3)) and $\hat{P}(\vec{E}, \vec{B})$ refers to the perturbation operator of the non-zero crossed fields.

¹If the spin is ignored.

According to (3.6), this operator equals²

$$\hat{P}(\vec{E}, \vec{B}) = -e\vec{E}\hat{r} + \frac{e}{2m_e}\vec{B}\hat{L}, \quad (8.5)$$

where e is the (positive) elementary charge, m_e the rest mass of an electron, \hat{r} is an operator of electron's position in the atom and \hat{L} is an operator of electron's orbital angular momentum³. The model described in the section 2.1 is used – an adiabatic motion of a hydrogen atom, that is where the crossed fields are locally uniform and the macroscopic motion of a hydrogen atom is sufficiently slow so that the spectrum can always stabilise.

The two special cases will be analysed in two different approaches – by a "modern" quantum mechanics and by an "old" quantum mechanics. For both of them, the energy of an atom in crossed fields is the starting point.

This classical energy is continuous which does not agree with experiments and therefore a quantisation is necessary to introduce – the first method transforms the energy into the Hamiltonian by the correspondence principle and the discrete spectrum is the solution of the Schrödinger equation; the second method directly introduces so called Sommerfeld's quantum conditions.

The case of $(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = (\vec{E}(\vec{R}), 0)$ is called a pure electric field to which (linear⁴) Stark effect (Stark spectrum) corresponds; the case of $(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = (0, \vec{B}(\vec{R}))$ is called a pure magnetic field to which a (linear⁵) Zeeman effect (Zeeman spectrum) corresponds. The quantisation is most demonstrative to show in these two crossed fields examples.

8.1 Perturbation theory

The perturbation theory is a common approximate method of how to find a spectrum of a system. It explains how the known spectrum of a system in a medium is changed when the medium undergoes a small change (a perturbation).

The "small change" is understood in the language of Hamiltonians. Let the system (a hydrogen atom, for example) to be described by \hat{H}_0 in the original state (before the perturbation is applied) and the perturbation (crossed fields, for instance) to be described by \hat{H}_1 Hamiltonian – the system's Hamiltonian responding to the perturbation is $\hat{H}_0 + \hat{H}_1$. The presence (or absence) of the perturbation and system's description by $\hat{H}_0 + \hat{H}_1$ (or \hat{H}_0) Hamiltonians are therefore equivalent. If the \hat{H}_1 Hamiltonian is time-independent, the appropriate perturbation theory is also called time-independent.

The requirement to use the perturbation theory is

$$\|\hat{H}_0\| \gg \|\hat{H}_1\| \quad (8.6)$$

and it is assumed that one knows unperturbed spectrum of the \hat{H}_0 Hamiltonian as a solution of the equation

$$\hat{H}_0\psi_0(i) = W_0(i)\psi_0(i), \quad (8.7)$$

where i denotes different⁶ solutions of the Schrödinger equation (8.7). The motivation of the (8.6) requirement is that the spectral lines which were identical in the original unperturbed case are in the presence of the perturbation still distinguishable from those with different original spectral lines.

²The Darwin term, relativistic kinetic terms and all terms including electron or proton spins were dropped for now.

³For an electron in a hydrogen atom, there are two angular momentums – an orbital (an analogy to $\vec{L} = \vec{r} \times \vec{p} = m\vec{r} \times \dot{\vec{r}}$ from the classical mechanics) and a spin angular momentum (with no classical analogy). In this chapter, the spin is ignored.

⁴If the crossed fields are not extremely strong, the dependence of the energy splitting on the field's magnitude (and on the quantum numbers as well) is linear – therefore the "linear" attribute.

⁵The reason why "linear" is the same as in the case of Stark effect; Zeeman spectrum is sometimes called "paramagnetic", too.

⁶The solutions of a Schrödinger equation are different if the eigenstates are different (not necessarily the eigenenergies).

The energy spectrum is then the spectrum of this matrix

$$W_1^{ij} = \int \psi_0^*(i) \hat{H}_1 \psi_0(j) dV. \quad (8.8)$$

Its eigenvalues $W_1(i)$ can be labelled with the i index and the eigenenergies of the $\hat{H} = \hat{H}_0 + \hat{H}_1$ Hamiltonian approximately are

$$W(i) = W_0(i) + W_1(i). \quad (8.9)$$

Although the original spectrum (with no perturbation) and the new spectrum (with the perturbation) are labelled by the same i , their numbers does not have to be the same, for instance when it for some i and j holds $W_0(i) = W_0(j)$ and $W_1(i) \neq W_1(j)$ at the same time.

Note that $W_1(i)$ in (8.9) is exactly that W_1 standing in (7.1) Ansatz.

It is not possible to evaluate the unperturbed spectrum of a hydrogen atom since there is no reasonable way of how to define a "vacuum" Hamiltonian for which H_0 would be a perturbation. However, this unperturbed spectrum is the starting point for many other perturbations applied to the atom.

8.2 Sommerfeld's quantum conditions

In the past, before the Schrödinger equation was postulated, the discrete spectra were explained as a consequence of the fact that only certain motions of the system are allowed while the classical description remained. The requirement for this method is that the system evinces a periodicity.

If the classical Hamiltonian of the system is $H = H(p_i, q_i)$, where p_i a q_i are the canonical conjugates of momentum and position, then the i th Sommerfeld's quantum condition (where n_i denotes an integer and T_i denotes the corresponding system's period) is

$$\oint_{T_i} p_i dq_i = 2\pi n_i \hbar. \quad (8.10)$$

The integral on the left-hand side is an action and therefore it should not be surprising that there is the (reduced) Planck's constant on the right-hand side as an "elementary action". To find the set of possible values for n_i is an independent problem.

The accuracy (or usability) of this method is much more limited that the accuracy (or usability) of the perturbation theory although both methods often give the same results. Sometimes when the perturbation theory fails, it is possible to accept the outcomes of this second method – if the limits are possible to evaluate with the perturbation theory, they serve as a control.

Aside (8.10), there is one more equivalent way of implementing the Sommerfeld's quantum conditions – if the classical Hamiltonian takes the form of a product of canonical conjugated actions (J_i) and frequencies (f_i) as $H_1 = \sum_i J_i f_i$ then the spectrum is [11]

$$W_1 = \sum_i 2\pi n_i \hbar f_i, \quad (8.11)$$

where $n_i \hbar$ stands for the J_i action with the Sommerfeld's quantum conditions applied on it. The n_i symbols are still integers (or half-integers).

The spectrum of a hydrogen atom in the ground state is possible to evaluate with this method – these conditions are the starting points:

$$\oint p_r dr = 2\pi n_r \hbar \quad (8.12a)$$

$$\oint p_\phi d\phi = 2\pi n_\phi \hbar \quad (8.12b)$$

When substituted into the classical Hamiltonian, the two conditions imply [11]

$$W_0 = -\frac{e^4 m_e}{32\pi^2 \hbar^2 \epsilon_0^2 (n_r + n_\phi)^2} = -\frac{R}{n^2}. \quad (8.13)$$

Also the Sommerfeld's quantum conditions give the same result as (8.1) which is the solution to the Schrödinger equation (8.7).

8.3 Zeeman effect

The Zeeman effect is the energy spectrum splitting (ground energy shifts) of a hydrogen atom placed in a pure external magnetic field, that is the crossed fields are $(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = (0, \vec{B}(\vec{R}))$. The time dependence of the field has already been excluded and the magnetic field is within the same model still considered as locally uniform (uniform in the atom's volume, for instance). With no loss of generality, one can choose the Cartesian axes so that

$$(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = ((0, 0, 0), (0, 0, B)). \quad (8.14)$$

Such a Cartesian system surely exist, where five of the six crossed fields' vectors coordinates equal zero – the sixth is simply the magnitude of the magnetic field in the local area. The problem is best solved in this coordinate system.

The electron spin is still ignored for simplicity. Then the classical Hamiltonian of the hydrogen atom in locally uniform magnetic field equals

$$H = \frac{\vec{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m_e} \vec{B} \vec{L}. \quad (8.15)$$

The correspondence principle gives the energy operator

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 \hat{r}} + \frac{e}{2m_e} \vec{B} \hat{L}, \quad (8.16)$$

which (according to (8.14)) takes a special form

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 \hat{r}} + \frac{e}{2m_e} B \hat{L}_3. \quad (8.17)$$

In (8.17), it is easy to identify $\hat{H}_0 = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 \hat{r}}$ which has been already analysed. The third term in (8.17) is therefore the perturbation:

$$\hat{H}_1 = \hat{P}(\vec{E}, \vec{B}) = +\frac{e}{2m_e} B \hat{L}_3 \quad (8.18)$$

This expression will be used in the perturbation theory to find the perturbed spectrum. As (8.8) suggests, one examines a matrix which in the Zeeman case take the form

$$W_1^{(l'm')(lm)} = \int R_{n'l'}^* Y_{l'm'}^* \left(+\frac{e}{2m_e} B \hat{L}_3 \right) R_{nl} Y_{lm} dV. \quad (8.19)$$

The matrix (as already mentioned in the section 8.1) is compiled for each n separately and the order of its columns (or rows) is given by the l and m numbers so that the pair (l_1, m_1) precedes (l_2, m_2) if $l_1 > l_2$ or if $m_1 > m_2$ in the case of $l_1 = l_2$ (analogically for the rows).

The problem can be solved analytically [12] and the outcome (where m denotes the magnetic quantum number) is

$$W_1 = W_1(m) = \frac{e\hbar}{2m_e}mB. \quad (8.20)$$

The $W_1^{(l'm')(lm)}$ matrix's dimension is $n^2 \times n^2$ but the number of their different eigenvalues $W_1(m)$ equals the number of possible values of m , that is $2n - 1$ (since $m \in \{-n + 1, \dots, +n - 1\}$).

The expression (8.20) is the solution to the problem of finding the perturbed spectrum of a hydrogen atom placed in a locally uniform magnetic field according to the perturbation theory. The same problem can be solved with the help of the Sommerfeld's quantum conditions starting from (8.15) again:

$$H = H_0 + H_1 = H_0 + \frac{e}{2m_e}BL_3 \quad (8.21)$$

For the implementation of the Sommerfeld's quantum conditions for H_0 , just the particular frequency $f_i = \frac{1}{2\pi} \frac{e}{2m_e}B$ and action $J_i = 2\pi L_z$ in the sense of (8.11) are necessary to identify. Then

$$W_1 = W_1(m) = 2\pi \left(\frac{1}{2\pi} \frac{e}{2m_e}B \right) (m\hbar) = \frac{e\hbar}{2m_e}mB. \quad (8.22)$$

The outcome perfectly agrees with (8.20) and the Zeeman effect is also one of the problems for which both perturbation theory and Sommerfeld's quantum conditions lead to the same result. For $n = 3$, for instance, m is an element of $\{-2, -1, 0, +1, +2\}$ so there are $2 \cdot 3 - 1 = 5$ of possible values. The single unperturbed energy level $W_0(n = 3) = -\frac{R}{9}$ splits into five new levels (labelled with m) symmetrically around the $W_0(n = 3)$:

$$\begin{aligned} W(n = 3, m = -2) &= -\frac{R}{9} + (-2) \cdot \frac{e\hbar}{2m_e}B = -\frac{R}{9} - \frac{e\hbar}{m_e}B \\ W(n = 3, m = -1) &= -\frac{R}{9} + (-1) \cdot \frac{e\hbar}{2m_e}B = -\frac{R}{9} - \frac{e\hbar}{2m_e}B \\ W(n = 3, m = 0) &= -\frac{R}{9} + (0) \cdot \frac{e\hbar}{2m_e}B = -\frac{R}{9} \\ W(n = 3, m = +1) &= -\frac{R}{9} + (+1) \cdot \frac{e\hbar}{2m_e}B = -\frac{R}{9} + \frac{e\hbar}{2m_e}B \\ W(n = 3, m = +2) &= -\frac{R}{9} + (+2) \cdot \frac{e\hbar}{2m_e}B = -\frac{R}{9} + \frac{e\hbar}{m_e}B \end{aligned}$$

The magnetic quantum numbers therefore realize the symmetrical outcome but it is the magnitude of the magnetic induction what determines the amount of the splitting – due to the linear proportionality, the difference between the $W(n = 3, m = -2)$ and $W(n = 3, m = +2)$ levels doubles if the magnetic field strength doubles, for example.

Like $n = 3$ level splits into five lines in a magnetic field, $n = 2$ splits into three lines in the same field, $n = 4$ level is splitted into seven lines, always symmetrically around the unperturbed $W_0(n)$ and always respecting the $2n - 1$ rule. The fields' magnitudes are limited in AEGIS and therefore the lines of different n do not cross and at least the n number is well-defined for every single (anti)hydrogen atom.

Because of the known properties of an electron and because of the form of (8.20), the spectrum of a hydrogen atom in an external magnetic field is dipole-like – it is a not-induced magnetic dipole spectrum. The example of a neutron in a magnetic field corresponds to it in the previous chapter⁷ – the not-induced orbital magnetic dipole of an electron (and of the hydrogen atom at the same time) precesses around the \vec{B} direction and the cosine of the angle between the two vectors is quantised by m .

⁷The difference is that the not-induced magnetic dipole of a neutron is spin-like. However, the dynamics is the same.

The macroscopic force on the hydrogen atom in an arbitrary state n by Cartesian coordinates is

$$F_i = -\frac{\partial}{\partial X_i} W_1 = -\frac{\partial}{\partial X_i} \left(\frac{e\hbar}{2m_e} m B \right) = -\frac{e\hbar}{2m_e} m \frac{\partial}{\partial X_i} B = -\frac{e\hbar}{2m_e} m \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}, \quad (8.23)$$

where m is an element of $\{-n + 1, \dots, n - 1\}$ ⁸.

8.4 Stark effect

The Stark effect is an analogy to the Zeeman effect in the case of a pure electric field. With no loss of generality, like in the Zeeman case, one can work in a particular Cartesian coordinate system where the crossed fields are

$$(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = ((0, 0, E), (0, 0, 0)). \quad (8.24)$$

The classical Hamiltonian for a hydrogen atom in an electric field and by the correspondence principle the Hamiltonian operator (with (8.24)) are

$$H = \frac{\vec{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} - eEx_3, \quad (8.25)$$

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 \hat{r}} - eE\hat{x}_3. \quad (8.26)$$

Like in the Zeeman case, the first two terms in (8.26) form the unperturbed Hamiltonian \hat{H}_0 and the third term is the electric field's perturbation:

$$\hat{H}_1 = \hat{P}(\vec{E}, \vec{B}) = -eE\hat{x}_3 \quad (8.27)$$

To find the spectrum W_1 by the perturbation theory, one examines this matrix (with the order of columns and rows like in (8.19)):

$$W_1^{(l'm')(lm)} = \int R_{nl'}^* Y_{l'm'}^* (-eE\hat{x}_3) R_{nl} Y_{lm} dV \quad (8.28)$$

The analytical solution of the spectrum [12] can be written in the form of

$$W_1 = W_1(p) = \frac{3}{2} a_0 e n p E. \quad (8.29)$$

In (8.29), a_0 denotes the Bohr radius and p the so called parabolic quantum number which is (for a given n) an element of $\{-n + 1, -n + 2, \dots, n - 2, n - 1\}$. The number of allowed values for p equals $2n - 1$ of allowed m 's in the Zeeman effect for the same n . Again, expressing the set by n leads to the lost of the information about degeneracy.

However, like in the Zeeman case (where l was a good quantum number), there is an alternative of how to express the set – instead for a given n , it is possible to write the energy splitting for a given n and m at the same time. The (8.29) then takes the form of

$$W_1(m, k) = \frac{3}{2} a_0 e n k E, \quad (8.30)$$

⁸The set of allowed m 's is given by l and the set of allowed l by n . However, it is possible to express the set for m by n as well, just the information of the degeneracy is lost.

where k is a new quantum number (different from p)⁹ going from $-n + 1 + |m|$ to $n - 1 - |m|$ by the steps of two. If the difference $n - |m|$ is odd, the number of elements in the set is odd, too; if the difference is even, the number of the elements is even as well. In both cases, the number equals $n - |m|$.

The number of energy levels distinguished by this approach is

$$\sum_{|m|=0}^{n-1} (n - |m|) = 2 \sum_{m=1}^{n-1} (n - m) + n = 2n(n - 1) - 2 \cdot \frac{n(n - 1)}{2} + n = n(n - 1) + n = n^2. \quad (8.31)$$

The result is n^2 like in (8.3).

Hence the set of n^2 eigenfunctions ψ_0 can be represented in two different ways – using l and m appropriate for the Zeeman effect or using k and $|m|$ more suitable for the Stark effect.

Consider $n = 3$ again. Then p is one of the $2 \cdot 3 - 1 = 5$ elements of the set $\{-2, -1, 0, 1, 2\}$. These are like in the Zeeman case symmetrically aligned around the unperturbed $W_0(n = 3) = -\frac{R}{9}$ and they represent the splitting due to the electric field.

$$\begin{aligned} W(n = 3, p = -2) &= -\frac{R}{9} + 3 \cdot (-2) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} - 9 a_0 e E \\ W(n = 3, p = -1) &= -\frac{R}{9} + 3 \cdot (-1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} - \frac{9}{2} a_0 e E \\ W(n = 3, p = 0) &= -\frac{R}{9} + 3 \cdot (0) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} \\ W(n = 3, p = +1) &= -\frac{R}{9} + 3 \cdot (+1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} + \frac{9}{2} a_0 e E \\ W(n = 3, p = +2) &= -\frac{R}{9} + 3 \cdot (+2) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} + 9 a_0 e E \end{aligned}$$

The splitting pattern is described by p and the amount of the shifts is proportional to the magnitude E of the electric field – the difference $W(n = 3, p = +2) - W(n = 3, p = -2)$ doubles if the electric field's strength doubles, very similarly to the Zeeman effect.

If the spectrum is expressed by k and $|m|$, not by p , there are nine outcomes of (8.30) but some of them are identical:

$$\begin{aligned} W(n = 3, m = 0, k = -2) &= -\frac{R}{9} + 3 \cdot (-2) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} - 9 a_0 e E \\ W(n = 3, m = -1, k = -1) &= -\frac{R}{9} + 3 \cdot (-1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} - \frac{9}{2} a_0 e E \\ W(n = 3, m = +1, k = -1) &= -\frac{R}{9} + 3 \cdot (-1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} - \frac{9}{2} a_0 e E \\ W(n = 3, m = -2, k = 0) &= -\frac{R}{9} + 3 \cdot (0) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} \\ W(n = 3, m = 0, k = 0) &= -\frac{R}{9} + 3 \cdot (0) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} \\ W(n = 3, m = +2, k = 0) &= -\frac{R}{9} + 3 \cdot (0) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} \\ W(n = 3, m = -1, k = +1) &= -\frac{R}{9} + 3 \cdot (+1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} + \frac{9}{2} a_0 e E \\ W(n = 3, m = +1, k = +1) &= -\frac{R}{9} + 3 \cdot (+1) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} + \frac{9}{2} a_0 e E \\ W(n = 3, m = 0, k = +2) &= -\frac{R}{9} + 3 \cdot (+2) \cdot \frac{3}{2} a_0 e E = -\frac{R}{9} + 9 a_0 e E \end{aligned}$$

⁹Their allowed values are different.

In this thesis, the quantum number p is preferred.

The Sommerfeld's quantum conditions for the evaluation of W_1 have to be applied to the classical Hamiltonian ((8.27) is its analogy):

$$H_1 = -eEx_3 \quad (8.32)$$

The outcome (8.29) taken from [12] was by the authors achieved by solving the problem in a parabolic coordinate system, instead of a Cartesian. The system is also more appropriate for the Sommerfeld's quantum conditions. The conversion $(x_1, x_2, x_3) \rightarrow (\xi, \eta, \phi)$ from the original Cartesian coordinate system is:

$$x_1 = \xi\eta \cos \phi \quad (8.33a)$$

$$x_2 = \xi\eta \sin \phi \quad (8.33b)$$

$$x_3 = \frac{1}{2} (\xi^2 - \eta^2) \quad (8.33c)$$

The generalised momentums are $p_\xi = m_e \dot{\xi} (\xi^2 + \eta^2)$, $p_\eta = m_e \dot{\eta} (\xi^2 + \eta^2)$ and $p_\phi = m_e \dot{\phi} \xi^2 \eta^2$; the Sommerfeld's quantum conditions are $\oint p_\xi d\xi = 2\pi n_\xi \hbar$, $\oint p_\eta d\eta = 2\pi n_\eta \hbar$ and $\oint p_\phi d\phi = 2\pi n_\phi \hbar$ respectively.

The solution of the problem according to [11] is

$$W_1 = \frac{3a_0 e E}{8\pi^2 \hbar^2} \cdot 2\pi (n_\xi + n_\eta + n_\phi) \hbar \cdot 2\pi (n_\eta - n_\xi) \hbar = \frac{3}{2} a_0 e n p E. \quad (8.34)$$

The result (8.34) again matches (8.29) and the Stark effect is another example where the two methods lead to the same outcome.

For $n = 2$, there are three spectral lines, $n = 4$ is splitted into seven spectral lines etc. by the rule $2n - 1$. Like for the Zeeman effect, the possibility of line crossing is excluded by the limits on the fields' strengths and the n number is still well-defined for every (anti)hydrogen atom.

Again, the perturbed Zeeman spectrum is of a dipole character. By Cartesian coordinates, the force on a hydrogen atom in an external electric field is

$$F_i = -\frac{\partial}{\partial X_i} W_1 = -\frac{\partial}{\partial X_i} \left(\frac{3}{2} a_0 e n p E \right) = -\frac{3}{2} a_0 e n p \frac{\partial}{\partial X_i} E = -\frac{3}{2} a_0 e n p \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}. \quad (8.35)$$

8.5 Comments

The just analysed obvious (or linear) Zeeman and Stark effects describe the quantisation of hydrogen atom's not-induced magnetic dipole in an external magnetic field and its not-induced electric dipole in an external electric field (separately).

In fact, a hydrogen atom generally possesses in any state not-induced and induced dipoles (electric and magnetic) at the same time. The influence of not-induced (linear) ones highly exceeds the influence of induced (quadratic) ones. This dominance does not hold if one of the not-induced dipoles equals coincidentally zero – then the induced one dominates and this is what happens for a hydrogen atom in the ground state $\psi(1, 0, 0)$ for instance. The potential energy W_1^{ind} is nonzero (see (7.20)) but one has to prove that $W_1^{\text{not-ind}} = 0$ is determined by (8.29).

The force on a hydrogen atom in the ground state in an external electric field is given by (7.19). In the analysis in the section 7.1, the potential energy of such an atom and the force on it were postulated and it was stressed that it really is an induced electric dipole. To rely on (7.19) and (7.20), the energy (8.29)

of a not-induced electric dipole has to equal zero for such a ground state hydrogen atom: for $n = 1$, p is an element of $\{-n + 1, \dots, n - 1\} = \{0\}$ and $W_1^{\text{not-ind}} = 0$. This makes the findings of this and the previous chapter consistent.

Notice the difference between (8.20) and (8.29): The Zeeman spectrum in SI units does not explicitly depend on the principal quantum number n , whereas Stark spectrum does; on the contrary, Stark spectrum is independent of the (reduced) Planck constant, whereas Zeeman spectrum is not. This is not a mistake but a consequence of solving the same problem (8.8) for two different perturbations (8.18) and (8.27).

Simply by the definitions, Zeeman and Stark effects cannot occur at the same time and at the same place. Therefore the quantum number m makes a good sense only for the (limit) Zeeman effect in a pure magnetic field and one can correctly define the quantum number p only in a pure electric field. However, there are some exceptions which will be discussed later. In the perspective of the modern quantum mechanics, the electric and magnetic fields' perturbations do not commute:

$$\begin{aligned}
\left[\frac{e}{2m_e} \vec{B} \hat{L}, e \vec{E} \hat{R} \right] &= \frac{e^2}{2m_e} \sum_{i,j=1}^3 B_i E_j [\hat{L}_i, \hat{X}_j] = \frac{e^2}{2m_e} \sum_{i,j=1}^3 B_i E_j \left[-i\hbar \sum_{a,b=1}^3 \epsilon_{abi} \hat{X}_a \nabla_b, \hat{X}_j \right] = \\
&= -i\hbar \frac{e^2}{2m_e} \sum_{a,b,i,j=1}^3 B_i E_j \epsilon_{abi} \delta_{bj} \hat{X}_a = -i\hbar \frac{e^2}{2m_e} \sum_{a,i,j=1}^3 \epsilon_{aji} B_i E_j \hat{X}_a = \\
&= -i\hbar \frac{e^2}{2m_e} \sum_{a=1}^3 (\vec{E} \times \vec{B})_a X_a = -i\hbar \frac{e^2}{2m_e} (\vec{E} \times \vec{B}) \cdot \vec{R} \quad (8.36)
\end{aligned}$$

Hence the two perturbation operators commute only if one of the fields vanishes or if the \vec{E} and \vec{B} vectors are parallel. These¹⁰ are also the cases when it is possible to define m and p at the same time (that is when they are commensurable).

For the parallel crossed fields, the Stark and Zeeman effects are independent and the spectrum of a hydrogen atom is

$$W_1 = \frac{3}{2} a_0 e n p E + \frac{e\hbar}{2m_e} m B. \quad (8.37)$$

In other cases, Stark and Zeeman effects are not commensurable and the quantum numbers p and m corresponding to both of the effects cannot exist at the same time in one formula.

¹⁰These cases and cases very close to them.

9 Spectrum of a hydrogen atom in crossed fields

In the previous chapter, two important conclusions were drawn - Stark and Zeeman spectra separately in pure electric and magnetic fields.

$$W_1^{\text{Zeeman}} = W_1(m) = \frac{e\hbar}{2m_e}mB \quad (9.1a)$$

$$W_1^{\text{Stark}} = W_1(p) = \frac{3}{2}a_0enpE \quad (9.1b)$$

A pure electric and a pure magnetic fields are limit cases of general locally uniform crossed fields. In this chapter, the spectrum W_1 will be found for the general crossed fields case, that is an interpolation of (9.1a) and (9.1b) for arbitrary $(\vec{E}(\vec{R}), \vec{B}(\vec{R}))$.

One may try to guess such a spectrum and the first what one would try is the simple superposition of (9.1a) and (9.1b), that is:

$$W_1 = \frac{e\hbar}{2m_e}mB + \frac{3}{2}a_0enpE \quad (9.2)$$

Such a guess really satisfies certain requirements (both (9.1a) and (9.1b) are its limits cases, the quantisation is symmetrical around $W_1 = 0$ and $\vec{\nabla}W_1 = 0$ holds in uniform crossed fields) but there are essential deficiencies – for any crossed fields, the numbers p and m are present at the same time and the expression does not depend on the angle γ between the \vec{E} and \vec{B} vectors as it should. Therefore one cannot accept (9.2).

At least the angle dependence could be improved by a simple implementing like:

$$W_1 = \frac{e\hbar}{2m_e}mB + \frac{3}{2}a_0enpE \cos \alpha \quad (9.3)$$

Although this guess depends on the angle, it prefers the direction of \vec{B} for no reason as significant, no matter how strong the electric field is. This is not possible to improve by a simple guess.

The two previous guesses cannot be accepted. The most appropriate method would be the perturbation theory – solving the (8.8) matrix for the operator (8.5) of general crossed fields, that is:

$$W_1^{(l'm')(lm)} = \int R_{nl'}^* Y_{l'm'}^* \left(-e\vec{E}\hat{r} + \frac{e}{2m_e}\vec{B}\hat{L} \right) R_{nl} Y_{lm} dV \quad (9.4)$$

The problem can be simplified if a special Cartesian coordinate system is chosen where the crossed fields $(\vec{E}(\vec{R}), \vec{B}(\vec{R}))$ are expressed only by the fields' magnitudes \vec{E} and \vec{B} and the angle γ between the two vectors, for instance:

$$(\vec{E}(\vec{R}), \vec{B}(\vec{R})) = ((E \sin \gamma, 0, E \cos \gamma), (0, 0, B)) \quad (9.5)$$

Then this matrix should be examined:

$$W_1^{(l'm')(lm)} = \int R_{nl'}^* Y_{l'm'}^* \left(-eE (\sin \alpha \hat{X}_1 + \cos \alpha \hat{X}_3) + \frac{e}{2m_e} B \hat{L}_3 \right) R_{nl} Y_{lm} dV \quad (9.6)$$

The spectrum of this matrix (if the condition (8.6) is satisfied) would be the perturbed spectrum W_1 of a hydrogen atom in general crossed fields. However, it proves itself that the problem cannot be solved analytically.

In the previous chapter, another method was introduced – Sommerfeld’s one – which determines a quantised spectrum of a system with a periodicity. In the Stark and Zeeman effects cases, the results by the two methods were the same. If the perturbation theory fails for a general case, the focus is on the Sommerfeld’s quantum conditions and one can trust their accuracy.

9.1 Hydrogen spectrum by Sommerfeld’s method

The method to find a spectrum for a hydrogen atom in general crossed fields was described by Max Born in [11]. This section briefly reports about it.

The classical potential energy of a hydrogen atom in general crossed fields in the model used in the whole thesis was mentioned in the previous chapter:

$$W_1 = -e\vec{r}\vec{E} + \frac{e}{2m_e}\vec{B}\vec{L} \quad (9.7)$$

To apply the quantum conditions on (9.7), a periodicity has to be revealed in the system’s behaviour and at the same time, all the terms should be factorised to actions and canonical conjugated frequencies.

Since the model is classical (Bohr model), the motion of the electron is considered to be a special case of the Kepler’s problem and its elliptical trajectory is assumed¹. The electron’s equation of motion is

$$m_e\ddot{\vec{r}} = \frac{e^2}{4\pi\epsilon_0}\frac{\vec{r}}{r^3} - e\vec{E} - e\dot{\vec{r}} \times \vec{B}. \quad (9.8)$$

Cross product of \vec{r} applied to (9.8) from the left gives

$$m_e\vec{r} \times \ddot{\vec{r}} = \frac{1}{4\pi\epsilon_0}\vec{r} \times \frac{\vec{r}}{r^3} - e\vec{r} \times \vec{E} - e\vec{r} \times \dot{\vec{r}} \times \vec{B}. \quad (9.9)$$

The left-hand side of (9.9) equals the time derivative of the classical orbital momentum of the electron and the first term on the right-hand side is zero². Instead of a detailed description, one can switch to time averages (that is instead of tracing an electron on the ellipse, to trace the perihelion precession itself). For this purpose, Born introduced so called electrical centre of mass

$$\langle \vec{r} \rangle = \frac{3}{2}a\epsilon, \quad (9.10)$$

where ϵ refers to the eccentricity of the ellipse and a means the semi-major axis. This vector traces the perihelion. It should not be surprising that the modern description of Rydberg atoms by the coherent states theory comes to the elliptic description as well and the Laplace-Runge-Lenz vector, which the theory uses, is a simple multiple of the electrical centre of mass (9.10).

The second term on the right-hand side of (9.9) takes this form:

$$\langle -e\vec{r} \times \vec{E} \rangle = -e\langle \vec{r} \rangle \times \vec{E} = e\vec{E} \times \langle \vec{r} \rangle \quad (9.11)$$

¹One expects perihelion precession as well.

²For any vector \vec{a} it holds that $\vec{a} \times \vec{a} = 0$.

To find the time average of the last term on the right-hand side of (9.9), these two vector identities are useful:

$$\vec{r} \times (\vec{B} \times \dot{\vec{r}}) = \vec{B} \times (\vec{r} \times \dot{\vec{r}}) + \dot{\vec{r}} \times (\vec{B} \times \vec{r}) = \frac{1}{m_e} \vec{B} \times \vec{L} + \dot{\vec{r}} \times (\vec{B} \times \vec{r}) \quad (9.12a)$$

$$\frac{d}{dt} (\vec{r} \times (\vec{B} \times \vec{r})) = \vec{r} \times (\vec{B} \times \dot{\vec{r}}) + \dot{\vec{r}} \times (\vec{B} \times \vec{r}) \quad (9.12b)$$

By combining them, one obtains

$$\langle \vec{r} \times (\vec{B} \times \dot{\vec{r}}) \rangle = \frac{1}{2m_e} \vec{B} \times \vec{L}. \quad (9.13)$$

After time averaging, the total time derivative of the electron's orbital momentum becomes:

$$\dot{\vec{L}} = e\vec{E} \times \langle \vec{r} \rangle + \frac{e}{2m_e} \vec{B} \times \vec{L} \quad (9.14)$$

This vector equation can be understood as simultaneous equations for two triads of the coordinates of \vec{r} and \vec{L} vectors. To complete the simultaneous equations, Born added three more scalar identities:

$$W_1 = e\vec{E} \langle \vec{r} \rangle + \frac{e}{2m_e} \vec{B} \vec{L} \quad (9.15a)$$

$$\vec{L} \langle \vec{r} \rangle = 0 \quad (9.15b)$$

$$\langle \vec{r} \rangle^2 + \left(\frac{3}{2} a_0 n \right)^2 = \left(\frac{3}{2} a \right)^2 \quad (9.15c)$$

After some algebra, the second triad reduces³ to one vector condition

$$\frac{d}{dt} \langle \vec{r} \rangle = e \left(\frac{3a_0 n}{2\hbar} \right)^2 \vec{E} \times \vec{L} + \frac{e}{2m_e} \vec{B} \times \langle \vec{r} \rangle. \quad (9.16)$$

The best way to solve the simultaneous equations (9.14) and (9.16) for \vec{r} and \vec{L} is to switch to new variables $\vec{\rho}_A = \langle \vec{r} \rangle + \frac{3a_0 n}{2\hbar} \vec{L}$ and $\vec{\rho}_B = \langle \vec{r} \rangle - \frac{3a_0 n}{2\hbar} \vec{L}$, that is to the linear combinations. Then the simultaneous equations fall apart into two independent vector differential equations⁴:

$$\dot{\vec{\rho}}_A = \left(+\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right) \times \vec{\rho}_A \quad (9.17a)$$

$$\dot{\vec{\rho}}_B = \left(-\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right) \times \vec{\rho}_B \quad (9.17b)$$

Both of them have the form of $\dot{\vec{\rho}} = \vec{\omega} \times \vec{\rho}$, that is like (7.27) in the seventh chapter. The solution is the precession of the vector $\vec{\rho}$ around the $\vec{\omega}$ direction with the angular velocity $\omega = |\vec{\omega}|$ or (if one is interested in the time average), constant projection of $\vec{\rho}$ into $\vec{\omega}$.

So the vector $\vec{\rho}_A = \langle \vec{r} \rangle + \frac{3a_0 n}{2\hbar} \vec{L}$ precesses around $\vec{\omega}_A = +\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B}$ with the angular velocity $\omega_A = \left| +\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right|$ and the vector $\vec{\rho}_B = \langle \vec{r} \rangle - \frac{3a_0 n}{2\hbar} \vec{L}$ precesses around $\vec{\omega}_B = -\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B}$ with the angular velocity $\omega_B = \left| -\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right|$.

³In the sense of notation – no variable was excluded.

⁴Or to a pair of independent scalar simultaneous equations.

There are also two significant directions in the space $\vec{\omega}_A$ and $\vec{\omega}_B$ and there are two vectors $\vec{\rho}_A$ and $\vec{\rho}_B$ precessing around them (or which have constant projections into the two directions). The Larmor precession is a limit for both of them if $\vec{E} = 0$.

The just found angular frequencies are exactly the periodicities which were necessary to find. The energy (9.7) can be therefore written in the form of actions and canonical conjugated frequencies.

$$\begin{aligned} W_1 &= -e\vec{r}\vec{E} + \frac{e}{2m_e}\vec{B}\vec{L} = J_A f_A + J_B f_B = J_A \frac{\omega_A}{2\pi} + J_B \frac{\omega_B}{2\pi} = \\ &= J_A \frac{\left| +\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right|}{2\pi} + J_B \frac{\left| -\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right|}{2\pi} \end{aligned} \quad (9.18)$$

One may apply the Sommerfeld's quantum conditions (8.11) now and the quantised spectrum of a hydrogen atom is

$$\begin{aligned} W_1 &= 2\pi n_A \hbar \frac{\left| +\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right|}{2\pi} + 2\pi n_B \hbar \frac{\left| -\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right|}{2\pi} = \\ &= \left| +\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right| n_A \hbar + \left| -\frac{3a_0 en}{2\hbar}\vec{E} + \frac{e}{2m_e}\vec{B} \right| n_B \hbar. \end{aligned} \quad (9.19)$$

For Born in [11], this was the final result. However, when the absolute values are expanded, one obtains⁵

$$\begin{aligned} W_1 &= \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2} + 2 \cdot \frac{3}{2}a_0 enE \cdot \frac{e\hbar}{2m_e}B \cdot \cos \alpha \cdot n_A + \\ &+ \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2} - 2 \cdot \frac{3}{2}a_0 enE \cdot \frac{e\hbar}{2m_e}B \cdot \cos \alpha \cdot n_B = \\ &= \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2} + \frac{3a_0 e^2 n \hbar}{2m_e} EB \cos \alpha \cdot n_A + \\ &+ \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2} - \frac{3a_0 e^2 n \hbar}{2m_e} EB \cos \alpha \cdot n_B. \end{aligned} \quad (9.20)$$

For the new quantum numbers n_A and n_B for a given n it holds that both are elements of the same set

$$\left\{ -\frac{n-1}{2}, -\frac{n-1}{2} + 1, \dots, +\frac{n-1}{2} - 1, +\frac{n-1}{2} \right\}. \quad (9.21)$$

So for odd n , (9.21) is made up by integers, and for even n , the set is made up by half-integers only. Their sum and difference (separately) are always elements of $\{-n+1, \dots, +n-1\}$. The set of all combinations of n_A and n_B again contains

$$\sum_{n_A=-\frac{n-1}{2}}^{+\frac{n-1}{2}} \sum_{n_B=-\frac{n-1}{2}}^{+\frac{n-1}{2}} 1 = \left(\sum_{n_A=-\frac{n-1}{2}}^{+\frac{n-1}{2}} 1 \right) \cdot \left(\sum_{n_B=-\frac{n-1}{2}}^{+\frac{n-1}{2}} 1 \right) = n \cdot n = n^2 \quad (9.22)$$

elements and their representation is similar to that of k and $|m\rangle$.

⁵These are still the energy shifts due to the crossed fields.

Now it is important to verify that the Zeeman (9.1a) and Stark (9.1b) outcomes are special cases of (9.20). Really:

$$\begin{aligned} W_1^{\text{Zeeman}} = W_1(E = 0) &= \sqrt{\left(\frac{e\hbar}{2m_e}B\right)^2} \cdot n_A + \sqrt{\left(\frac{e\hbar}{2m_e}B\right)^2} \cdot n_B = \\ &= \frac{e\hbar}{2m_e} (n_A + n_B) B \end{aligned} \quad (9.23a)$$

$$\begin{aligned} W_1^{\text{Stark}} = W_1(B = 0) &= \sqrt{\left(\frac{3}{2}a_0enE\right)^2} \cdot n_A + \sqrt{\left(\frac{3}{2}a_0enE\right)^2} \cdot n_B = \\ &= \frac{3}{2}a_0en (n_A + n_B) E \end{aligned} \quad (9.23b)$$

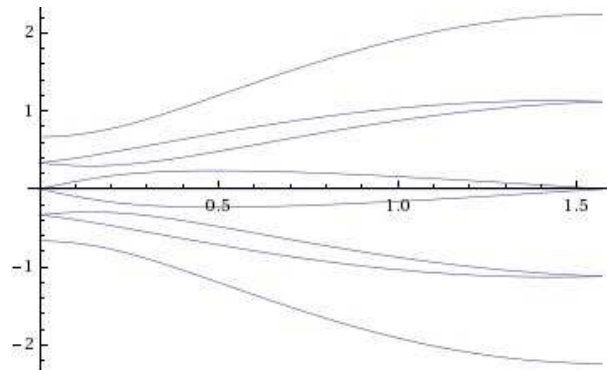
If $(n_A + n_B) = m$ in (9.23a) and $(n_A + n_B) = p$ in (9.23b), then the outcomes perfectly agrees with (8.20) and (8.29) from the previous chapter. One may think that $m = p$ but this is not valid. According to the analysis from the previous chapter, it holds that both m and p are well defined only in the cases of a pure magnetic or a pure electric field. Therefore only in such limit cases it is possible to identify m and p although it seems that Stark and Zeeman effects are quantised by the same number $n_A + n_B$.

$$\vec{E} = 0 \wedge \vec{B} \neq 0 \rightarrow m = n_A + n_B \neq p \quad (9.24a)$$

$$\vec{E} \neq 0 \wedge \vec{B} = 0 \rightarrow p = n_A + n_B \neq m \quad (9.24b)$$

$$\vec{E} \neq 0 \wedge \vec{B} \neq 0 \rightarrow m \neq n_A + n_B \neq p \quad (9.24c)$$

For $n = 3$, the relation between p , m , n_A and n_B is sketched in the Figure 9.1. The diagram stands for the numerical solution of the Hamiltonian (8.5) by the perturbation theory which is not possible to solve analytically. On the horizontal axis, there is $\arctan \frac{B}{E}$ going from 0 to $+\frac{\pi}{2}$ so that the leftmost edge of the diagram represents the Stark splitting and the rightmost edge shows the Zeeman splitting (not to scale). On both edges, the number of the lines is really $2 \cdot 3 - 1 = 5$ with accordance to the theory. In the middle (when the degeneracy is removed), the number of the lines is $3 \cdot 3 = 9$, again with accordance to the theory. The sum $n_A + n_B$ equals p or m only on the edges (or very close). The numerical solution coincides very well with what the formula (9.20) predicts.



Obrázek 9.1: The dependence of W_1 on $\arctan \frac{B}{E}$ for $n = 3$ and $\gamma \approx 63^\circ$ – numerical solution of the spectrum by the perturbation theory.

Now it is important to compare the guess (9.2) with the outcome (9.20) obtained by the Sommerfeld's quantum conditions. The reason why they are different is that one has to comprise the not-induced electric and not-induced magnetic dipole to connect Stark and Zeeman effects. These two dipoles are not independent in general crossed fields since they both concern the same electron (and its trajectory in the Bohr model) – therefore a simple superposition of the Stark and Zeeman outcomes cannot be valid, contrary to the approach described by Born.

The spin of the electron was still ignored. Its influence will be discussed now.

9.2 Electron spin influence

The calculation of Born in fact connects effects of general crossed fields on not-induced electric and not-induced orbital magnetic dipole of the electron in a hydrogen atom. As it was analysed, both electric and magnetic fields influence both of the dipoles at the same time – simple superpositions of limit cases were excluded and Born's alternative was presented.

The same holds in a pure magnetic field for the superposition of a not-induced orbital magnetic dipole and not-induced spin magnetic dipole. The real Hamiltonian of a hydrogen atom in a magnetic field has new terms and it is

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} + \frac{e\hbar}{2m_e}B(\hat{L}_3 + 2\hat{S}_3) - \frac{\hat{p}^4}{8m_e^3c^2} + \frac{e^2\hbar^2}{4\pi\epsilon_0m_e^2c^2r^3}\hat{L} \cdot \hat{S} + \frac{e^2\hbar^2}{8\epsilon_0m_e^2c^2}\delta(\vec{r}). \quad (9.25)$$

The presence of the term $-\frac{e\hbar}{m_e}\hat{S}_3$ demands to introduce a new quantum number s which is independent on the rest n, l, m, n_A and n_B and is an element of the set $\{-\frac{1}{2}, +\frac{1}{2}\}$.

Their names are: $-\frac{e\hbar}{m_e}B\hat{S}_3$ is the spin term; $-\frac{\hat{p}^4}{8m_e^3c^2}$ is the kinetic (relativistic) term; $\frac{e^2\hbar^2}{4\pi\epsilon_0m_e^2c^2r^3}\hat{L} \cdot \hat{S}$ is the spin-orbital term; and $\frac{e^2\hbar^2}{8\epsilon_0m_e^2c^2}\delta(\vec{r})$ is the Darwin term. The sum of the second, third and fourth one is obviously called the fine structure Hamiltonian and the sum of the first (spin) and already introduced term $-\frac{e\hbar}{2m_e}\hat{L}_3$ is called full Zeeman Hamiltonian. The relative "magnitude" of the two Hamiltonians rules how the perturbation theory is used and how the final spectrum looks like.

In the limit of weak magnetic fields, the full Zeeman Hamiltonian dominates over the fine structure Hamiltonian. The perturbation theory is applied in two phases:

$$\hat{H}_0^{(1)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} \quad (9.26a_1)$$

$$\hat{H}_1^{(1)} = \hat{H}_{FS} \quad (9.26a_2)$$

$$\psi^{(1)}(n, l, m) = \psi_0(n, l, m) \quad (9.26a_3)$$

$$\hat{H}_0^{(2)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} + \hat{H}_{FS} \quad (9.26b_1)$$

$$\hat{H}_1^{(2)} = \frac{e}{2m_e}B(\hat{L}_3 + 2\hat{S}_3) \quad (9.26b_2)$$

$$\psi^{(2)} = \psi_1(n, l, m) \quad (9.26b_3)$$

The notation of the eigenfunctions corresponds to $\hat{H}_0^{(1)}\psi_0 = W_0\psi_0$ and $\hat{H}_0^{(2)}\psi_1 = (W_0 + W_1^{(1)})\psi_1$. The second phase (9.26b) can be understood as a redefinition of the vacuum where the magnetic field is present.

The spectrum [13] is

$$W_1 = \frac{e\hbar}{2m_e} B \left(1 + \frac{2s}{2l-1} \right) j, \quad (9.27)$$

where the quantum number j goes by the steps of one from $-l-s$ to $l+s$. The term in the brackets is called Landé g -factor for a hydrogen atom.

In the strong magnetic field limit, the fine structure Hamiltonian dominates over the full Zeeman Hamiltonian. The perturbation theory is applied in two phases again:

$$\hat{H}_0^{(1)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} \quad (9.28a_1)$$

$$\hat{H}_1^{(1)} = -\frac{e\hbar}{2m_e} B \left(\hat{L}_3 + 2\hat{S}_3 \right) \quad (9.28a_2)$$

$$\psi^{(1)}(n, l, m) = \psi_0(n, l, m) \quad (9.28a_3)$$

$$\hat{H}_0^{(2)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} - \frac{e\hbar}{2m_e} B \left(\hat{L}_3 + 2\hat{S}_3 \right) \quad (9.28b_1)$$

$$\hat{H}_1^{(2)} = \hat{H}_{\text{FS}} \quad (9.28b_2)$$

$$\psi^{(2)} = \psi_1(n, l, m) \quad (9.28b_3)$$

The hydrogen atom spectrum is then

$$W_1 = \frac{e\hbar}{2m_e} B (m + 2s). \quad (9.29)$$

The force on such a full Zeeman hydrogen atom is

$$\begin{aligned} F_i &= -\frac{\partial}{\partial X_i} W_1 = -\frac{\partial}{\partial X_i} \left(\frac{e\hbar}{2m_e} B (m + 2s) \right) = -\frac{e\hbar}{2m_e} (m + 2s) \frac{\partial}{\partial X_i} B = \\ &= -\frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \end{aligned} \quad (9.30)$$

The way of connecting the not-induced electric dipole with the not-induced orbital magnetic dipole is known – (9.20) – as well as the way of connecting the not-induced orbital magnetic dipole with the not-induced spin magnetic dipole – (9.27) or (9.30). The connection of all the three together will be postulated. Since the magnetic quantum number m is present both in (9.1a) and in (9.29) and since the differences between (9.27) and (9.29) is not very significant within the model used in this thesis, the spectrum of a hydrogen atom with the three types of not-induced dipoles in general crossed fields equals (9.20) plus the spin term from (9.29):

$$\begin{aligned} W_1 &= \sqrt{\left(\frac{3}{2} a_0 e n E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 + \frac{3a_0 e^2 n \hbar}{2m_e} E B \cos \alpha \cdot n_A +} \\ &+ \sqrt{\left(\frac{3}{2} a_0 e n E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 - \frac{3a_0 e^2 n \hbar}{2m_e} E B \cos \alpha \cdot n_B + \frac{e\hbar}{m_e} s B} \end{aligned} \quad (9.31)$$

In the case of $\vec{E} = 0$, that is a pure magnetic field and Zeeman effect, (9.31) gives (9.29) which is the full Zeeman spectrum:

$$W_1^{\text{Zeeman}} = \frac{e\hbar}{2m_e} B (m + 2s) \quad (9.32)$$

In the case of the parallel crossed fields with the spin taken into account, the formula (8.37) becomes

$$W_1 = \frac{3}{2} a_0 e n p E + \frac{e\hbar}{2m_e} (m + 2s) B \quad (9.33)$$

and, according to the Ansatz, the force on a hydrogen atom in such crossed fields is

$$\begin{aligned} F_i &= -\frac{\partial}{\partial X_i} W_1 = -\frac{\partial}{\partial X_i} \left(\frac{3}{2} a_0 e n p E + \frac{e\hbar}{2m_e} (m + 2s) B \right) = \\ &= -\frac{3}{2} a_0 e n p \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} - \frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}. \end{aligned} \quad (9.34)$$

9.3 Strong fields effects

The induced dipoles (electric and magnetic) can be regarded as independent of the previous not-induced ones. In the case of significantly strong fields, it is possible to simply add the quadratic terms to (9.31). Finally

$$\begin{aligned} W_1 &= \sqrt{\left(\frac{3}{2} a_0 e n E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 + \frac{3a_0 e^2 n \hbar}{2m_e} E B \cos \alpha \cdot n_A} + \\ &+ \sqrt{\left(\frac{3}{2} a_0 e n E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 - \frac{3a_0 e^2 n \hbar}{2m_e} E B \cos \alpha \cdot n_B} + \\ &+ \frac{e\hbar}{m_e} s B - \frac{1}{2} \alpha(n, l, m) E^2 - \frac{1}{2} \beta(n, l, m) B^2, \end{aligned} \quad (9.33)$$

where α and β are hydrogen polarizabilities dependent on n and other quantum numbers as well.

Depending on the formalism, the form of the Ansatz $\vec{F} = -\vec{\nabla} W_1$ may vary in the sign. However, the first three terms in (9.33) are symmetrical in the quantum numbers n_A , n_B and s and the sign difference can be solved by simple redefining of these numbers. The quadratic terms, to the contrary, have to be expressed with the correct signs.

10 Special limit

Consider a case when both fields – electric and magnetic – are present but the influence of the magnetic field is much greater than the influence of the electric field. The spin is ignored again. Then

$$\hat{H}_0 \gg \hat{H}_B \gg \hat{H}_E, \quad (10.1)$$

where $\hat{H}_B = \frac{e}{2m_e} \vec{B} \hat{L}$ and $\hat{H}_E = -e\vec{E}\hat{r}$. In this particular situation, the direction \vec{B} is really significant and the most appropriate Cartesian coordinate system is such where the crossed fields are

$$\left(\vec{E}, \vec{B} \right) = \left((E \sin \gamma, 0, E \cos \gamma), (0, 0, B) \right), \quad (10.2)$$

where γ denotes the angle between the \vec{E} and \vec{B} vectors.

The character of the problem allows using the same two-phase perturbation method like in the previous section to find the spectrum of the system. It is:

$$\hat{H}_0^{(1)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} \quad (10.3a_1)$$

$$\hat{H}_1^{(1)} = \frac{e}{2m_e} B \hat{L}_3 \quad (10.3a_2)$$

$$\psi^{(1)}(n, l, m) = \psi_0(n, l, m) \quad (10.3a_3)$$

$$\hat{H}_0^{(2)} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0\hat{r}} + \frac{e}{2m_e} B \hat{L}_3 \quad (10.3b_1)$$

$$\hat{H}_1^{(2)} = -e\vec{E}\hat{r} = -eE (\hat{x}_1 \sin \gamma + \hat{x}_3 \cos \gamma) \quad (10.3b_2)$$

$$\psi^{(2)} = \psi_1(n, l, m) \quad (10.3b_3)$$

The advantage of the Zeeman effect is that the eigenfunctions ψ_1 equal the eigenfunctions ψ_0 for the perturbation $\hat{H}_1^{(1)}$ – it is a characteristic¹ of the operator $\frac{e}{2m_e} B \hat{L}_3$. The spectrum (from the second phase of the perturbation theory) is the spectrum of the matrix

$$W_1^{(2)} = \int R_{nl'}^* Y_{l'm'}^* (-eE (\hat{x}_1 \sin \gamma + \hat{x}_3 \cos \gamma)) R_{nl} Y_{lm} dV \quad (10.4)$$

the spectrum of which is

$$W_1^{(2)}(p) = \frac{3}{2} a_0 e n p E \cos \gamma \quad (10.5)$$

and the whole energy shifts are

$$W_1 = W_1^{(1)} + W_1^{(2)} = \frac{e\hbar}{2m_e} m B + \frac{3}{2} a_0 e n p E \cos \gamma. \quad (10.6)$$

It is highly interesting that this outcome matches the guess (9.3) which was excluded for its unjustified preference of the \vec{B} direction. Here, however, the condition (10.1) makes the direction given by the

¹It does not hold for the Stark perturbation.

strong magnetic field really significant which was used in the application of the two-step perturbation theory.

The effect of the electron spin can be easily implemented like in the previous chapter. It is

$$W_1 = \frac{e\hbar}{2m_e}mB + \frac{3}{2}a_0enpE + \cos\gamma\frac{e\hbar}{m_e}sB = \frac{e\hbar}{2m_e}(m+2s)B + \frac{3}{2}a_0enpE\cos\gamma. \quad (10.7)$$

The aim of this chapter is to prove that (10.7) is consistent with (9.3) and with (9.31) as well. The condition (10.1) applied to the (9.31) means that

$$\frac{e\hbar}{2m_e}mB \gg \frac{3}{2}a_0enpE. \quad (10.8)$$

One can expand the square roots in (9.31) in the Taylor series:

$$\begin{aligned} W_1 &= \sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0e^2n\hbar}{2m_e}EB\cos\alpha \cdot n_A +} \\ &+ \sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0e^2n\hbar}{2m_e}EB\cos\alpha \cdot n_B + \frac{e\hbar}{m_e}Bs} = \\ &= \frac{e\hbar}{2m_e}B\sqrt{1 + \left(\frac{3a_0m_enE}{\hbar B}\right)^2 + \frac{6a_0m_enE}{\hbar B}\cos\alpha \cdot n_A +} \\ &+ \frac{e\hbar}{2m_e}B\sqrt{1 + \left(\frac{3a_0m_enE}{\hbar B}\right)^2 - \frac{6a_0m_enE}{\hbar B}\cos\alpha \cdot n_B + \frac{e\hbar}{m_e}Bs} = \\ &= \frac{e\hbar}{2m_e}B\sqrt{1 + \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B} + \left(\frac{3a_0m_en}{\hbar}\right)^2 \cdot \left(\frac{E}{B}\right)^2 \cdot n_A +} \\ &+ \frac{e\hbar}{2m_e}B\sqrt{1 - \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B} + \left(\frac{3a_0m_en}{\hbar}\right)^2 \cdot \left(\frac{E}{B}\right)^2 \cdot n_B + \frac{e\hbar}{m_e}Bs} \approx \\ &\approx \frac{e\hbar}{2m_e}B\sqrt{1 + \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B} \cdot n_A +} \\ &+ \frac{e\hbar}{2m_e}B\sqrt{1 - \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B} \cdot n_B + \frac{e\hbar}{m_e}Bs} \approx \\ &\approx \frac{e\hbar}{2m_e}B\left(1 + \frac{1}{2} \cdot \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B}\right) \cdot n_A + \\ &+ \frac{e\hbar}{2m_e}B\left(1 - \frac{1}{2} \cdot \frac{6a_0m_en\cos\alpha}{\hbar} \cdot \frac{E}{B}\right) \cdot n_B + \frac{e\hbar}{m_e}Bs = \\ &= \frac{e\hbar}{2m_e}Bn_A + \frac{3}{2}a_0enE\cos\alpha \cdot n_A + \frac{e\hbar}{2m_e}Bn_B - \frac{3}{2}a_0enE\cos\alpha \cdot n_B + \frac{e\hbar}{m_e}Bs = \\ &= \frac{e\hbar}{2m_e}Bn_A + \frac{e\hbar}{2m_e}Bn_B + \frac{3}{2}a_0enE\cos\alpha \cdot n_A - \frac{3}{2}a_0enE\cos\alpha \cdot n_B + \frac{e\hbar}{m_e}Bs = \\ &= \frac{e\hbar}{2m_e}B(n_A + n_B) + \frac{3}{2}a_0enE\cos\alpha \cdot (n_A - n_B) + \frac{e\hbar}{m_e}Bs \end{aligned} \quad (10.9)$$

In the limit of a pure magnetic field ($E = 0$) it holds that $n_A + n_B = m$. Here, although $E \neq 0$, the magnetic field is so much stronger that the case can be considered as very close to Zeeman limit that the sum of n_A and n_B can be regarded as the magnetic number m again. Moreover, the Hamiltonian \hat{H}_B can be understood as a vacuum redefinition and from this point of view, it is possible to consider the Stark effect on the background of the Zeeman effect and to set $n_A - n_B = p$. The result is

$$\begin{aligned} W &= \frac{e\hbar}{2m_e} Bm + \frac{3}{2} a_0 e n E \cos \alpha \cdot p + \frac{e\hbar}{m_e} B s = \\ &= \frac{e\hbar}{2m_e} (m + 2s) B + \frac{3}{2} a_0 e n p E \cos \gamma, \end{aligned} \quad (10.10)$$

which perfectly agrees with (10.7).

Therefore the cases very close to the Stark and Zeeman limits are those² when m and p can coexist although (strictly) they are both well-defined in the different limits only. The reason is that there are two possibilities of how to construe the vacuum in the perturbation theory – either with no field present or with the presence of the stronger field.

²The another case just mentioned is when the crossed fields are parallel (or almost parallel) – see (8.36).

11 Hydrogen dynamics in crossed fields

Finally, according to the (7.1) Ansatz, the macroscopic force on a hydrogen atom in external crossed fields is

$$\begin{aligned}
F_i &= -\frac{\partial}{\partial X_i} W_1 = -\frac{\partial}{\partial X_i} \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha \cdot n_A} \\
&\quad - \frac{\partial}{\partial X_i} \sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha \cdot n_B} \\
&\quad - \frac{\partial}{\partial X_i} \left(\frac{e\hbar}{m_e} s B\right) - \frac{\partial}{\partial X_i} \left(-\frac{1}{2}\alpha E^2\right) - \frac{\partial}{\partial X_i} \left(-\frac{1}{2}\beta B^2\right) \\
&= -\frac{\left(\frac{3}{2}a_0 en\right)^2 \frac{\partial}{\partial X_i} E^2 + \left(\frac{e\hbar}{2m_e}\right)^2 \frac{\partial}{\partial X_i} B^2 + \frac{3a_0 e^2 n\hbar}{2m_e} \cos \alpha \frac{\partial}{\partial X_i} (EB)}{2\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_A \\
&\quad - \frac{\left(\frac{3}{2}a_0 en\right)^2 \frac{\partial}{\partial X_i} E^2 + \left(\frac{e\hbar}{2m_e}\right)^2 \frac{\partial}{\partial X_i} B^2 - \frac{3a_0 e^2 n\hbar}{2m_e} \cos \alpha \frac{\partial}{\partial X_i} (EB)}{2\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_B \\
&\quad - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} + \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}, \tag{11.1}
\end{aligned}$$

which leads to the thesis finale when the derivatives of the EB product are explicitly written:

$$\begin{aligned}
F_i &= -\frac{\left(\frac{3}{2}a_0 en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_A \\
&\quad - \frac{\frac{3a_0 e^2 n\hbar}{4m_e} \cos \alpha \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_A \\
&\quad - \frac{\left(\frac{3}{2}a_0 en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_B \\
&\quad + \frac{\frac{3a_0 e^2 n\hbar}{4m_e} \cos \alpha \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0 enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0 e^2 n\hbar}{2m_e} EB \cos \alpha}} n_B \\
&\quad - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} + \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} \tag{11.2}
\end{aligned}$$

Now it will be checked whether (11.2) really fulfils the conditions from the fourth chapter.

11.1 Angle dependence

It was stated that the total force on a hydrogen atom in crossed fields should explicitly depend on the angle γ between the crossed fields' constituents, that is between the vectors \vec{E} and \vec{B} .

If $\gamma = 0$, that is if the crossed fields are parallel (and weak enough to neglect the quadratic effects), $\cos \gamma = 1$ and one obtains

$$\begin{aligned}
F_i &= - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} + \frac{3a_0e^2n\hbar}{4m_e} \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \right)}{\frac{3}{2}a_0enE + \frac{e\hbar}{2m_e}B} n_A \\
&\quad - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} - \frac{3a_0e^2n\hbar}{4m_e} \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \right)}{\frac{3}{2}a_0enE - \frac{e\hbar}{2m_e}B} n_B \\
&\quad - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
&= - \frac{\frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} \left(\frac{3}{2}a_0enE + \frac{e\hbar}{2m_e}B \right) + \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \left(\frac{3}{2}a_0enE + \frac{e\hbar}{2m_e}B \right)}{\frac{3}{2}a_0enE + \frac{e\hbar}{2m_e}B} n_A \\
&\quad - \frac{\frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} \left(\frac{3}{2}a_0enE - \frac{e\hbar}{2m_e}B \right) - \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} \left(\frac{3}{2}a_0enE + \frac{e\hbar}{2m_e}B \right)}{\frac{3}{2}a_0enE - \frac{e\hbar}{2m_e}B} n_B \\
&\quad - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
&= - \frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} n_A - \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} n_A - \frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} n_B + \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} n_B \\
&\quad - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
&= - \frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} (n_A + n_B) - \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} (n_A - n_B) - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
&= - \frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} p - \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} m - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
&= - \frac{3}{2}a_0enp \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} - \frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}, \tag{11.3}
\end{aligned}$$

which perfectly matches (9.34).

11.2 Gradients

All terms in (10.2) depend on $\frac{\partial E_j}{\partial X_i}$ or $\frac{\partial B_j}{\partial X_i}$ therefore there is really no force on a hydrogen atom in globally uniform crossed fields.

11.3 Stark and Zeeman limits

For $\vec{B} = 0$, (10.2) takes the form of

$$\begin{aligned}
 F_i &= -\frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} n_A}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2}} - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} n_B}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2}} = \\
 &= -\frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} n_A - \frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} n_B = \\
 &= -\frac{3}{2}a_0en \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} (n_A + n_B) = -\frac{3}{2}a_0enp \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}, \tag{11.4}
 \end{aligned}$$

which is identical to the force on a Stark hydrogen atom (8.35).

For $\vec{E} = 0$, (10.2) takes the form of

$$\begin{aligned}
 F_i &= -\frac{\left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} n_A}{\sqrt{\left(\frac{e\hbar}{2m_e}B\right)^2}} - \frac{\left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} n_B}{\sqrt{\left(\frac{e\hbar}{2m_e}B\right)^2}} - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
 &= -\frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} n_A - \frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} n_B - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
 &= -\frac{e\hbar}{2m_e} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} (n_A + n_B) - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} = \\
 &= -\frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}, \tag{11.5}
 \end{aligned}$$

which matches the result (9.30) for the force on a full Zeeman hydrogen atom.

11.4 Antihydrogen

The final formula (10.2) holds for a hydrogen atom, although the motivation of the thesis was to find the force on an antihydrogen atom in the same crossed fields. Some of the antihydrogen's properties differ in sign from that of a hydrogen atom, some do not. However, still referring to the motivation, one is not interested in an equation of motion for one individual atom or antiatom – instead, the focus is on the motion of a cloud of atoms which are most likely in a distribution symmetrical in the quantum numbers. Therefore¹ a simple redefinition of the quantum numbers, in which W_1 is symmetrical, improves all since the quantum numbers distribution of the cloud of particles is symmetrical in these numbers as well.

¹The argumentation is the same like in the section 9.3 where the alternative formulation of the Ansatz was discussed.

12 Summary

The first scientific goal of the AEGIS experiment in CERN is to directly measure the gravitational acceleration of antihydrogen atoms. For this purpose, the antiatoms have to move in crossed fields (the term always denotes electric and magnetic fields present at the same time and point) first before they undergo the pure gravitational motion itself. Therefore it is necessary to know the equation of motion of an antihydrogen atom for successful fitting of the gravitational parabola.

It is more demonstrative to show the analysis for hydrogen atoms, especially when the intermediate and sideline results are necessary to compare with the known laws. The conversion to the language of antimatter is explained at the end.

The model used in this thesis is such that the crossed fields are considered to be locally uniform on the atomic scales. Therefore, the gradients are ignored inside an atom (its spectrum arises in uniform crossed fields) whereas the atom as a whole responds to the fields' gradients outside its volume in its macroscopic motion. There are also limits of the fields' magnitudes to make the principal quantum number n well-defined for every single antiatom and to avoid ionisation.

Antihydrogen atoms are produced artificially in AEGIS in a so called charge exchange reaction when an antiproton replaces a positron in a positronium. For the charge exchange reaction, a kinematic identity was found:

$$v_{\bar{H}}^2 - 2 \left(v_{\bar{p}} \cos \theta_{\bar{H}} + 2 \frac{m_e}{m_{\bar{p}}} v_{Ps} \cos(\theta_{Ps} - \theta_{\bar{H}}) \right) v_{\bar{H}} + 2 \left(\frac{m_e^2}{m_{\bar{p}}^2} v_{Ps}^2 + 2 \frac{m_e}{m_{\bar{p}}} v_{\bar{p}} v_{Ps} \cos \theta_{Ps} - \frac{m_e Q}{m_{\bar{p}}^2} \right) = 0 \quad (12.1)$$

The identity has the form of a quadratic equation in $v_{\bar{H}}$, the coefficients of which are functions of measurable quantities. The identity was derived in two independent ways (the relativistic one and the non-relativistic one) and the results are the same.

On the other hand, (12.1) can be understood as an implicit function for $v_{\bar{H}}$ and $\theta_{\bar{H}}$ (which are the kinematic variables of an antihydrogen atom just leaving the charge exchange). The function stands for the hyperplane of all possible kinematic states of an antihydrogen atom satisfying the conservation laws. The half-width of its diagram then has the meaning of the maximal angle deviation of a just produced antihydrogen atom from the direction given by antiprotons entering the charge exchange.

The outcome (12.1) can very well provide the initial conditions for the equation of motion of antihydrogen atoms which are essential in the dynamics.

Another kinematic identity was found for the effect of antihydrogen deexcitation, that is for the process of

$$\bar{H}(n) \rightarrow \bar{H}(n' < n) + \gamma, \quad (12.2)$$

when the antiatom switches to a lower energy level which is accompanied by a single photon radiation. Such radiation is isotropic in the $\bar{H}(n)$'s rest frame and so is the direction of $\Delta \vec{v} = \vec{v}' - \vec{v}$.

Anyway, the kinematic identity is comprised only of the velocity magnitudes

$$\Delta v = |\Delta \vec{v}| = \frac{R}{m_{\bar{p}} c^2 + m_e c^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) c, \quad (12.3)$$

hence the velocity change is the function just of the initial and final principal numbers of the antihydrogen atom. The typical values for the current experiment design are $\Delta v = 5 \cdot 10^{-4}$ m/s.

Again, the identity was derived in two different ways (non-relativistic and relativistic one) which confirms the result.

There are four types of an elementary dipole – a not-induced electric dipole, an induced electric dipole, a not-induced magnetic dipole and an induced magnetic dipole. For each of them, the force \vec{F} on the dipole and (independently) its potential energy W_1 was found – for the electric dipoles in an electric field and for the magnetic dipoles in a magnetic field. These are summarised in the table:

Type of a dipole	Potential energy of a dipole	Force on a dipole
Not-induced electric dipole in electric field	$W_1 = -\tilde{d}E$	$F_i = \tilde{d} \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}$
Induced electric dipole in electric field	$W_1 = -\frac{1}{2}\alpha E^2$	$F_i = \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i}$
Not-induced magnetic dipole in magnetic field	$W_1 = -\tilde{m}B$	$F_i = \tilde{m} \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}$
Induced magnetic dipole in magnetic field	$W_1 = -\frac{1}{2}\beta B^2$	$F_i = \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}$

Tabulka 12.1: The forces on elementary dipoles and their potential energies. The symbols \tilde{d} and \tilde{m} refer to the projections of not-induced dipoles into the fields' directions.

For all these cases it holds that

$$\vec{F} = -\vec{\nabla}W_1 \quad (12.4)$$

and this principle was postulated (as an Ansatz) to hold for any general dipole in any general crossed fields.

A hydrogen or an antihydrogen atom (in the model used in this thesis) are dipole-like particles. They evince all the four types of dipoles – moreover, one has to distinguish whether the not-induced magnetic dipole is orbital- or spin-like.

There are four special cases of crossed fields for which the potential energy and the net force were found separately: Zeeman effect, Stark effect, parallel fields configuration and a weak electric field on the background of a strong magnetic field.

For the Zeeman effect (when $\vec{E} = 0$ at least locally) it holds that

$$W_1^{\text{Zeeman}} = \frac{e\hbar}{2m_e} (m + 2s) B, \quad (12.5)$$

where m is the magnetic quantum number as an element of $\{-n + 1, \dots, n - 1\}$ and $s = \pm 1$ is the spin quantum number. The force on such a Zeeman (anti)hydrogen atom is

$$F_i = -\frac{\partial}{\partial X_i} W_1^{\text{Zeeman}} = -\frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}. \quad (12.6)$$

In the case of the Stark effect ($\vec{B} = 0$), the spectrum is

$$W_1^{\text{Stark}} = \frac{3}{2} a_0 e n p E, \quad (12.7)$$

where p stands for the parabolic quantum number (separately, an element of the same set like m is for the Zeeman effect). The force on such a Stark (anti)hydrogen atom is

$$F_i^{\text{Stark}} = -\frac{\partial}{\partial X_i} W_1^{\text{Stark}} = -\frac{3}{2} a_0 e n p \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}. \quad (12.8)$$

When the crossed fields are parallel, the corresponding perturbation operators commute and the spectrum is a simple superposition of Zeeman and Stark energies as

$$W_1^{\parallel} = \frac{e\hbar}{2m_e} (m + 2s) B + \frac{3}{2} a_0 enp E \quad (12.9)$$

and the force on an atom in such crossed fields equals vector sum of the previous two forces:

$$F_i^{\parallel} = -\frac{\partial}{\partial X_i} W_1^{\parallel} = -\frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} - \frac{3}{2} a_0 enp \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i}. \quad (12.10)$$

And if a magnetic field significantly exceeds an electric field in the strength, a double-phase perturbation theory (similar for a fine structure Hamiltonian, for instance) implies that

$$W_1^{\text{H}_B \gg \text{H}_E} = \frac{e\hbar}{2m_e} (m + 2s) B + \frac{3}{2} a_0 enp E \cos \gamma, \quad (12.11)$$

where γ denotes the angle between the magnetic induction and the electric intensity vectors. The force on an (anti)atom in such fields is then

$$F_i^{\text{H}_B \gg \text{H}_E} = -\frac{\partial}{\partial X_i} W_1^{\text{H}_B \gg \text{H}_E} = -\frac{e\hbar}{2m_e} (m + 2s) \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} - \frac{3}{2} a_0 enp \sum_{j=1}^3 \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} \cos \gamma. \quad (12.12)$$

For the general local crossed fields, the perturbation theory fails to solve the spectrum analytically¹. One would have to find the spectrum of the matrix $W_1^{(l'm')(lm)} = \int R_{nl'}^* Y_{l'm'}^* \hat{H}_1 R_{nl} Y_{lm} dV$, where $\hat{H}_0(R_{nl} Y_{lm}) = \left(\frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} \right) (R_{nl} Y_{lm}) = -\frac{1}{n^2} (R_{nl} Y_{lm})$ and

$$\begin{aligned} \hat{H}_1 = & -\frac{\hat{p}^4}{8m_e^3 c^2} + \frac{e^2 \hbar^2}{4\pi\epsilon_0 m_e^2 c^2 r^3} \hat{L} \cdot \hat{S} + \frac{e^2 \hbar^2}{8\epsilon_0 m_e^2 c^2} \delta(\vec{r}) + \\ & + \frac{e\hbar}{2m_e} B (\hat{L}_3 + 2\hat{S}_3) + \frac{e^2 B^2}{8m_e} \hat{r}^2 \sin^2 \theta - eE (\hat{x} \sin \gamma + \hat{z} \cos \gamma). \end{aligned} \quad (12.13)$$

However, Max Born succeeded in finding it by applying Sommerfeld's quantum conditions to the classical Hamiltonian after these periodicities were discovered: The vector $\vec{\rho}_A = \langle \vec{r} \rangle + \frac{3a_0 n}{2\hbar} \vec{L}$ precesses around $\vec{\omega}_A = +\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B}$ with the angular velocity $\omega_A = \left| +\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right|$ and the vector $\vec{\rho}_B = \langle \vec{r} \rangle - \frac{3a_0 n}{2\hbar} \vec{L}$ precesses around $\vec{\omega}_B = -\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B}$ with the angular velocity $\omega_B = \left| -\frac{3a_0 en}{2\hbar} \vec{E} + \frac{e}{2m_e} \vec{B} \right|$.

Above, $\langle \vec{r} \rangle$ stands for the so called electric centre of mass of the atom, \vec{L} is the classical orbital momentum of the electron (positron) in the atom (antiatom), a_0 denotes the Bohr radius and \hbar means the reduced Planck constant.

With new quantum numbers n_A and n_B going from $-\frac{n-1}{2}$ to $+\frac{n-1}{2}$ in the steps of one, the potential energy of a hydrogen (antihydrogen) atom in crossed fields is

$$\begin{aligned} W_1 = & \sqrt{\left(\frac{3}{2} a_0 en E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 + \frac{3a_0 e^2 n \hbar}{2m_e} EB \cos \gamma \cdot n_A} + \\ & + \sqrt{\left(\frac{3}{2} a_0 en E \right)^2 + \left(\frac{e\hbar}{2m_e} B \right)^2 - \frac{3a_0 e^2 n \hbar}{2m_e} EB \cos \gamma \cdot n_B} + \frac{e\hbar}{m_e} s B. \end{aligned} \quad (12.14)$$

¹However, special cases were solved numerically for the comparison with further results.

The force on an (anti)hydrogen atom in general local uniform crossed fields equals

$$\begin{aligned}
F_i = & - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_A \\
& - \frac{\frac{3a_0e^2n\hbar}{4m_e} \cos \gamma \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_A \\
& - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_B \\
& + \frac{\frac{3a_0e^2n\hbar}{4m_e} \cos \gamma \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_B \\
& - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}. \tag{12.15}
\end{aligned}$$

The quantum numbers m or p are sensibly defined only in the four previous special cases and they can be linked to n_A and n_B , namely:

$$\vec{E} = 0 \wedge \vec{B} \neq 0 \rightarrow m = n_A + n_B \neq p \tag{12.16a}$$

$$\vec{E} \neq 0 \wedge \vec{B} = 0 \rightarrow p = n_A + n_B \neq m \tag{12.16b}$$

$$\vec{E} \parallel \vec{B} \rightarrow m = \pm (n_A + n_B) \wedge p = \mp (n_A - n_B) \tag{12.16c}$$

$$\frac{e\hbar}{2m_e} B \gg \frac{3}{2} a_0 en E > 0 \rightarrow p = \pm (n_A + n_B) \wedge m = \mp (n_A - n_B) \tag{12.16d}$$

With (12.16) taken into consideration, it was proved that the formula (12.15) gives for the four separately solved special crossed fields the correct results (12.6), (12.8), (12.10) and (12.12) which should be a very good test of its accuracy, at least within the chosen model.

Next, there are some effects in strong crossed fields as well which were also implemented into the dynamics. In the spectrum, these are quadratic terms $\frac{1}{2}\alpha E^2$ and $\frac{1}{2}\beta B^2$ (corresponding with electric and magnetic induced dipoles of an atom). Their derivatives can be simply added to (12.15) due to their independence of the not-induced dipoles.

Finally, the trivial gravitational term Mg_i can be added as well. Note that $g = |\vec{g}|$ is exactly the quantity which the experiment is designed to measure.

Since the velocities of the antiatoms are not expected to exceed 1000 m/s, the non-relativistic left-hand side of the Newton's second law can be used. Therefore:

$$M\ddot{X}_i = F_i \tag{12.17}$$

The goal of the whole thesis is the right-hand side of (anti)hydrogen's equation of motion:

$$\begin{aligned}
F_i = & - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_A \\
& - \frac{\frac{3a_0e^2n\hbar}{4m_e} \cos \gamma \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 + \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_A \\
& - \frac{\left(\frac{3}{2}a_0en\right)^2 \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \left(\frac{e\hbar}{2m_e}\right)^2 \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i}}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_B \\
& + \frac{\frac{3a_0e^2n\hbar}{4m_e} \cos \gamma \sum_{j=1}^3 \left(B \frac{E_j}{E} \frac{\partial E_j}{\partial X_i} + E \frac{B_j}{B} \frac{\partial B_j}{\partial X_i}\right)}{\sqrt{\left(\frac{3}{2}a_0enE\right)^2 + \left(\frac{e\hbar}{2m_e}B\right)^2 - \frac{3a_0e^2n\hbar}{2m_e}EB \cos \gamma}} n_B \\
& - \frac{e\hbar}{m_e} s \sum_{j=1}^3 \frac{B_j}{B} \frac{\partial B_j}{\partial X_i} + \alpha \sum_{j=1}^3 E_j \frac{\partial E_j}{\partial X_i} + \beta \sum_{j=1}^3 B_j \frac{\partial B_j}{\partial X_i} + Mg_i \tag{12.18}
\end{aligned}$$

Not only does the formula (12.15) (or (12.18), respectively) reduce to all the separately solved problems, it also satisfies all the requirements following from the experiment – all the terms are proportional to field's derivatives, all the weak field terms symmetrically depend on the quantum numbers and the formula explicitly depend on the angle γ between the crossed fields.

The very motivation of the problem is not to trace an individual atom but to determine the motion of a cloud of particles. Such a cloud is expected to have symmetrical distribution of quantum numbers. Since the force (12.18) is symmetrical in quantum numbers as well and since CPT can only switch the signs of the terms, the formula (12.18) is valid for symmetrical distribution of antimatter (antihydrogen) particles with no need of modification – just the quantum numbers may (or may not) be redefined.

For the complexity of the problem, it was decided to focus mainly on the theoretical derivation and analysis of the chosen model. The numerical simulation have not been performed yet – they are the goal of the author's next work on the topic which goes beyond the framework of this thesis.

Poděkování

Chtěl bych poděkovat vedoucímu své diplomové práce, doc. RNDr. Vojtěchu Petráčkovi, CSc., za vytrvalou a nevšední pomoc, trpělivost a čas, které mi nezištně věnoval po celou dobu vytváření této práce a díky kterým jsem získal dostatečné znalosti, vědomosti a orientaci. Děkuji mu také za všechny podněty, kterými mě usměrňoval a díky kterým se úroveň textu stále zvyšovala. Pod jeho vedením mě práce velmi těšila.

Také děkuji prom.fyz. Jiřímu Adamovi, CSc. za jeho zájem, pravidelné diskuze a odbornou pomoc s neobvyklými okruhy fyziky, na které si vyhrazoval čas po celý rok, a Ing. Václavu Potočkovi rovněž za jeho zájem, pravidelné konzultace a za pomoc s numerickými řešeními rovnic.

Konečně bych chtěl poděkovat své rodině a přátelům, díky jejichž podpoře jsem měl to správné pracovní zázemí.

13 References

- [1] AEGIS collaboration. *Proposal for the AEGIS Experiment at CERN Antiproton Decelerator : Antimatter Experiment: Gravity, Interferometry, Spectroscopy*. [s.l.] : [s.n.], 2007. 125 s. Dostupný z WWW: <<http://doc.cern.ch/archive/electronic/cern/preprints/spsc/public/spsc-2007-017.pdf>>.
- [2] Goldman, T.; Hughes, R. J.; Nieto, M. M. *Phenomenological Aspects Of New Gravitational Forces: IV. New Terrestrial Experiments*. Phys. Rev. D36, 1254(1987).
- [3] MIKULČÁK, Jiří, CHARVÁT, Jura, MACHÁČEK, Martin, a ZEMÁNEK, František. *Matematické, fyzikální a chemické tabulky a vzorce pro střední školy*. 1. Praha: Prometheus, 2006. ISBN 80-7196-264-3.
- [4] COHEN-TANNOUJDI, Claude, DIU, Bernard, a LALOË, Frank. *Quantum mechanics*. Paris: Collection Enseignement des sciences, 1973. ISBN 0-471-16433-X.
- [5] TOPÇU, Türker, a ROBICHEAUX, Francis. *Radiative cascade of highly excited hydrogen atoms in strong magnetic fields*. Physical Review A 73, 043405 2006. DOI: 10.1103/PhysRevA.73.043405.
- [6] *Particle Physics Booklet*. [s.l.] : Elsevier, 2008. 296 s. Dostupné z WWW: <<http://pdg.lbl.gov/pdgmail>>.
- [7] SEDLÁK, Bedřich; ŠTOLL, Ivan. *Elektřina a magnetismus*. Vydání 2., opravené a rozšířené. Praha : Academia, 2002. 636 s. ISBN 80-200-1004-1.
- [8] ŠTOLL, Ivan. *Elektřina a magnetismus*. Vydání druhé. Praha : Vydavatelství ČVUT, 2003. 216 s. ISBN 80-01-02693-0.
- [9] ŠTOLL, Ivan. *Mechanika*. Vydání druhé. Praha : Vydavatelství ČVUT, 2003. 210 s. ISBN 80-01-02692-2.
- [10] Force and Torque on a Small Magnetic Dipole. *Physics Insights* [online]. [cit. 2012-01-04]. Dostupné z: http://www.physicsinsights.org/force_on_dipole_1.html
- [11] BORN, Max. *Vorlesungen über Atommechanik*. Berlin: Springer, 1925.
- [12] LANDAU, Lev Davidovich; LIFSHITZ, Evgeny Mikhailovich. *Quantum mechanics : Non-relativistic theory*. Third edition, revised and enlarged. [Oxford] : Pergamon Press, 1977. 677 s. ISBN 0-08-020940-8.
- [13] BORN, Max. *Atomic Physics*. New York: Dover Publications, 1989. ISBN 0-486-65984-4.