Załącznik nr 3

do wniosku dr Jarosława Ruczkowskiego
o przeprowadzenie postępowania habilitacyjnego

Autoreferat (w języku angielskim)

Contents

1 First name and surname

Jarosław Ruczkowski

2 Diplomas and research degrees possessed

- M.Sc. in Physics, specialisation: Applied Physics

  Nicolaus Copernicus University in Toruń, Faculty of Mathematics, Physics and Chemistry, 1988.

  Title of Master's thesis : *Properties of layer carbons* (in Polish)

  Supervisor : Dr Jerzy Wieczorek

- Ph.D. of Physical Sciences in Physics

  Adam Mickiewicz University in Poznań, Faculty of Physics, 2000.

  Title of Ph.D. thesis : *Quantitative determination of configuration interactions effects in the fine and hyperfine structure of praseodymium* (in Polish)

  Professor conferring the degree : Prof. Ewa Stachowska (in the framework of research grant, degree with distinction)

3 Information on the hitherto employment in research institutions

- 01.10.1988 – 30.09.1989 – Trainee Assistant

  Division of Atomic Physics, Institute of Physics, Poznan University of Technology,

- 01.10.1989 – 30.06.1990 – Assistant

  Division of Atomic Physics, Institute of Physics, Poznan University of Technology,

- 01.01.1991 – 30.09.1991 – Senior Technical Assistant

  Division of Atomic Physics, Institute of Physics, Poznan University of Technology,

- 01.10.1991 – 31.01.2000 – Assistant

  Division of Atomic Physics, Institute of Physics, Poznan University of Technology,

  after the establishment of Faculty of Technical Physics in 1997 - Chair of Atomic Physics

- 01.02.2000 – 28.02.2014 – Assistant Professor

  Chair of Atomic Physics, Faculty of Technical Physics, Poznan University of Technology,

  in 2006 Chair of Atomic Physics changed its name to: Chair of Quantum Engineering and Metrology,

- from 01.03.2014 – Assistant

  Division of Control Engineering and Robotics, Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznan University of Technology

4 The course of scientific work

4.1 Before obtaining a Ph.D. degree

In October 1988 I started working in Division of Atomic Physics at Institute of Physics, Poznan University of Technology, headed by Prof. Jerzy Dembczyński. The subject of my scientific activity from the very beginning was the study, by means of semi-empirical methods, of the fine and hyperfine structure of complex atoms and quantitative determination of the effects of the interactions occurring there. In these studies, I cooperated directly with the staff of the Division of Atomic Physics : Prof. Jerzy Dembczyński, Prof. Ewa Stachowska, Dr Magdalena Elantkowska and Dr Gustaw Szawioła. Furthermore, in cooperation with Arleta Stachowska, MSc. Eng., I joined a team developing software for semi-empirical analysis of atomic structure, and after her leaving from the Division, I completely took over the role of the person responsible for this task.

In 1991-93 I participated in the research related to the interpretation of the results of the hyperfine structure and isotope shift measurement for europium atom [1].

In the mid-90s I began the implementation of an original idea of developing an integrated program package used for research in the Division. This resulted from the extension of previously used programs for fine structure analysis with new interactions, for which the relevant angular coefficients formulas, based on the Racah algebra, were derived by Dr M. Elantkowska. The existing separate programs realising calculations for different types of configurations, including entirely new routines for the calculation of interconfiguration interactions, were included as procedures to a single program that generating fine structure angular coefficients matrix. Operating the program was maximally simplified and the dominant role was taken over by appropriately developed algorithms. Part of this study was realised under the research project No 0T11F01008p01 and was associated with implementing the package into the high power computers at Poznan Supercomputing and Networking Center. The analytical formulas and the results of package applications were successively published [2–5]. In the later period, an analogous program for angular coefficients of the hyperfine structure matrix was developed.

At the same time, together with academic staff of the Division, I began cooperation with Dr Safa Bouazza, from the University of Reims. During his stay in Poznan, and in the later period, the joint papers concerned the fine and hyperfine structure analysis of hafnium and zirconium atoms [6, 7]. Dr Bouazza received, used at this time by us, a program package for the fine and hyperfine structure analysis, which he utilised in subsequent years in their independent research.

Together with the entire Division team I participated in the research, which resulted in the world's first observation of praseodymium ions in the Paul trap [8].

In the subsequent years, in collaboration with the research center in Dubna, I took part in the work connected with the fine and hyperfine structure of europium atom [9, 10].

The collaboration with Prof. G.H. Guthöhrleinem from University of the Armed Forces in Hamburg started in the early 90s and resulted in an interest of the analysis of praseodymium atom. This was due to a large amount of unpublished, new data concerning the energy levels and the hyperfine splittings. A semi-empirical analysis of these data provided simultaneously significant help in resolving doubts regarding the interpretation of the experimental results. The observed, at the time, a very high efficiency of a close connection between experimental research and semi-empirical analysis prompted me to appoint research on the structure of the atom praseodymium as the topic of the future doctoral dissertation.

4.2 After obtaining a Ph.D. degree

After obtaining a Ph.D. degree, from February 2000 I was employed as an Assistant Professor in Chair of Atomic Physics at Faculty of Technical Physics.

During that period, I developed an algorithm and created a program for calculations taking into account J-off diagonal effects in the hyperfine structure. It allows the interpretation of very precise experimental results obtained, for example, by means of a optical-microwave double resonance method. The idea of the program is to use an analogy to diagonalization of the fine structure energy matrix. The hyperfine structure matrix contains, besides diagonal elements, also J-off-diagonal elements. Direct diagonalization and the fitting procedure of experimental and calculated hyperfine structure intervals allows analysing results with calculation accuracy of 1 Hz, and thus obtain the so-called corrected hyperfine structure constants (up to magnetic octupole and electric hexadecapole interactions). The program incorporated into the structure of an already existing software is used to derive corrected hyperfine structure constants, qnd is also an effective tool to determine the values of the higher nuclear moments. The first application of the program for the lanthanum atom, was presented in the review work on lanthanum, titanium and hafnium [11].

In subsequent years, I participated in research related to the analysis of the fine and hyperfine structure of praseodymium ion [12] and europium atom [13]. The availability of new data on the fine structure and hyperfine atomic praseodymium allowed me to continue the work related to this topic [14]. These papers were also related to the extension of the computational capabilities of the program package by the inclusion of interactions with configurations up to four open shells and more complete consideration of the second order effects, both in the fine and the hyperfine structure. The modified package was used in the paper on the analysis of the fine and hyperfine structure of atomic scandium in a broad configuration basis [15], which also includes the expected values of hyperfine structures constants for the levels in a wide energy range as a significant help in the planning and the interpretation of experimental studies. In the research on precise measurements of atomic chromium, by knowing the experimental hyperfine structure intervals, diagonalization of the hyperfine structure matrix was completed and the "corrected" values of hyperfine structure constants were derived, including magnetic octupole interactions constants [16]. In 2008, I participated in a semi-empirical analysis of the experimental results concerning the hyperfine structure of lanthanum ion [17, 18].

In the years 2003-2014 I was the main investigator or investigator of research projects founded by Ministry of Science and Higher Education (MNiSW) and National Science Centre (NCN) entitled "Revision of the model of hyperfine interactions in the atom, including the hypotheses of the significant influence of the entanglement of nucleus states and electronic shell" (MNiI 2 P03B 056 24) and "A complete software package to describe the structure of complex atoms and to determine its attributes on the basis of the experimental databases" (MNiSW N519 033 32/4065). These projects contributed to the further development of the program package, in particular the calculation procedures for the hyperfine structure. In the paper concerning the lanthanum atom, it was demonstrated that the direct diagonalization of the hyperfine structure matrix enables the correct partition of the observed hyperfine splittings into the contributions of successive ranks of interactions (magnetic dipole, electric quadrupole, etc.) [19]. An analogy between the methods of parameterization including "closed shell → open shell" and "open shell → empty shell" excitations was also analysed. Implementation of the project "The procedure of computer design of the nuclear frequency standard" (NCN N519 650740) was a continuation of the development of software and applications for different elements [20, 21]. In the paper, which was the summary of the project, a method of searching the thorium nuclear isomeric state as a potential candidate for the nuclear frequency standard, by means of the hyperfine structure studies, was proposed [22].

In 2012, I proposed the application of precisely defined wave functions to describe the electric dipole radiative transitions. A series of publications related to this issue [23–30] is my achievement which is the basis for applying for assistant-professorship and will be presented in section 5.2.

In 2014, I had a short-term research visit at the invitation of Prof. Safa Bouazza from Reims University, during which I presented the above-mentioned method of oscillator strengths parametrization and provided the program package for that purpose. Apart from the papers resulting from the renewal of cooperation with Prof. S. Bouazza [25, 26], this package was used in other articles, with Prof. Bouazza as a co-author [31–33].

Years of study related to the development of author's software for atomic structure analyzis resulted in a unique a worldwide scale package. During the "Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data" conference in 2015, Alexander Kramida from the National Institute of Standards and Technology (NIST) during his lecture mentioned our programs beside the COWAN CODE and other recognised packages [34]. A very valuable is my own concept of consistency of the package, so that data entered once into the input file, along with results obtained at any stage of the calculations are communicated between the different programs, minimising the possibility of errors, simultaneously improving the analysis process in a meaningful way up to the presentation of results in a form ready for publication. Invaluable here is the role of many small auxiliary programs developed independently of the main elements of the package. It should be emphasised that this is the result of teamwork, where the main ideas related to the description of the atomic structure were suggested by Prof. Jerzey Dembczyński and Dr Magdalena Elantkowska, analytical formulas were derived by Dr Magdalena Elantkowska, whereas the algorithms and the creation of the program package is my original contribution. The workload associated with testing the correctness of formulas and programs was also our joint effort. The correctness of the formulas describing the parameters of the first-order perturbation theory was tested by comparing them with the results of calculations obtained by means of COWAN CODE package, which uses a different coupling scheme between electrons [35, 36]. In the case of parameters describing the interactions of the second order perturbation theory, I developed a number of programs making appropriate summations of the products of first-order parameters, the correctness of which was confirmed earlier.

Recently, a detailed description of the parameterization methods of the fine and hyperfine structure, together with the explicit presentation of analytical formulas used in the calculation of the angular coefficient was presented in a series of papers [37–42]. The results of studies on the structure of tantalum ion were also published [43].

In 2014, I started a collaboration with Dr Andrzej Sikorski from Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznan University of Technology, regarding the optimization of wave function determination procedures (theATOM program). This cooperation resulted in a significant acceleration of calculations, which was partly used in the analysis of the fine and hyperfine structure of atomic terbium [44]. In 2016, Dr Sikorski received Microsoft Azure for Research grant whose research plan foreseeing large-scale calculations for the rare earths elements was developed with my participation. Optimization of procedures and their adaptation to Microsoft Azure architecture will allow, for the first time, to conduct the calculations without the limitation of the number of SL states for $4f^N$ core. It will also make it possible to reply the question how the restrictions applied thus far affected the results of the fine and hyperfine structure calculations.

In 2016, I started a cooperation with Ruohong Li and Jens Lassen, from the TRIUMF Canada's National Laboratory for Particle and Nuclear Physics in Vancouver. In 2017 the paper concerning the laser resonance ionization spectroscopy of antimony was published [45].

5 Indication of the achievement constituting the basis for the habilitation procedure

As a scientific achievement corresponding to article 16, sec. 2 of the act of March 14th 2003 on research degrees and the research title (Journal of Laws No 65, item 595 with further amendments) I hereby indicate the single-topical series of research articles entitled ***Semi-empirical determination of the parameters of radiative transitions in an atom.***

5.1 List of works constituting the single-topical series of research articles:

Impact Factor for the year of publication was given, with the exception of papers published after 2015

H1) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
An alternative method for determination of oscillator strengths: The example of Sc II,
J. Quant. Spectrosc. Radiat. Transfer **145** (2014) 20-42; IF=2.645

H2) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Semi-empirical calculations of oscillator strengths and hyperfine constants for Ti II,
J. Quant. Spectrosc. Radiat. Transfer **149** (2014) 168-183; IF=2.645

H3) **J. Ruczkowski**, S. Bouazza, M. Elantkowska, J. Dembczyński,
Semi-empirical analysis of oscillator strengths for Nb II,
J. Quant. Spectrosc. Radiat. Transfer **155** (2015) 1-9; IF=2.859

H4) S. Bouazza, **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Hyperfine structure, lifetime and oscillator strength of V II,
J. Quant. Spectrosc. Radiat. Transfer **166** (2015) 55-63; IF=2.859

H5) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Semi-empirical analysis of the fine structure and oscillator strengths for atomic strontium,
J. Quant. Spectrosc. Radiat. Transfer **170** (2016) 106-116; IF(2015)=2.859

H6) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Semi-empirical determination of radiative lifetimes for Sc II and Ti II,
J. Quant. Spectrosc. Radiat. Transfer **176** (2016) 6-11; IF(2015)=2.859

H7) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Semi-empirical determination of radiative parameters for Ag II,
Mon. Not. R. Astron. Soc. **459** (2016) 3768-3782; IF(2015)=4.952

H8) **J. Ruczkowski**, M. Elantkowska, J. Dembczyński,
Semi-empirical determination of radiative parameters for atomic nickel,
Mon. Not. R. Astron. Soc. **464** (2017) 1127–1136; IF(2015)=4.952

5.2 Description of the scientific objective of the above mentioned works and discussion of the results achieved, and their possible application

5.2.1 Introduction

The observed spectral lines, emitted by atoms or ions, are described by three quantities: frequency, intensity and shape [46]. They are directly connected with the quantities describing the atomic structure. The energy difference between electronic levels defines a transition frequency (linewidth). The transition probabilities (oscillator strengths) have an effect on the observed line intensities. The lifetimes of excited levels determine the natural linewidths. They are also related to the transition probabilities. At the same time, external environment of the emitter has an influence on the spectral lines. The frequency of the transition may be altered by a shift of the energy levels in the presence of electric and magnetic fields. The line intensity depends on the states population, which undergoes changes due to collisions or the presence of radiation. The line shapes may be broadened due to emitter motion. Therefore, spectroscopic studies provide information necessary to describe the atomic structure and are used for various types of diagnostics. In recent years, research related to plasma diagnostics in thermonuclear fusion reactors is of particular interest [47].

Accurate data on the transition probabilities (oscillator strengths) and radiative lifetimes are of particular importance in astrophysics, for reliable determinations of chemical abundances in stellar atmospheres. Abundance of elements in the Universe depends on the processes that led to their formation. The most abundant hydrogen is the result of primary nucleosynthesis in the early stages of Universe evolution. Heavier elements, including the iron group elements, were formed by the processes occurring in the stars. Other elements were created as a result of neutron capture processes at different stages of stellar evolution, and as a result of supernova explosions [48, 49]. Determination of the element abundance compared to hydrogen, and their analysis for various elements, enables the verification of both the models of stellar atmosphere and their evolution, as well as the evolution of galaxies and the whole Universe.

5.2.2 Semi-empirical description of atomic structure

The way to obtain the information regarding the structure of the atom, mechanisms of interactions between the electrons and the interactions of electron shell with the nucleus, is finding the most accurate possible wave function describing the state of the atom. Knowledge of the exact wave function allows specifying, according to the quantum mechanics rules, the expected values of observables, i.e.

attributes of the atomic structure that are measurable, and therefore their experimental verification is possible.

The wavefunctions describing the individual atoms, or ions, in accordance with the laws of quantum physics are presented as functions dependent on the angular coordinates (quantum numbers) and the radial coordinates. Separability of the wave function into the angular dependent part and the radial part allows the strict calculation of the angular part based on the quantum physics rules, i.e. the theory of angular momentum in complex atom. Whereas, the radial part, in *ab initio* theoretical calculations requires the assumption of an appropriate model eg. as a potential of the electric field in which electrons are moving. An alternative to the *ab initio* theoretical calculations is the application of semi-empirical methods that utilize existing experimental databases.

According to Schrödinger's equation, the total energy of electronic state $|\gamma J\rangle$ is the eigenvalue of Hamiltonian operator

$$\hat{H} \left|\gamma J\right\rangle = E \left|\gamma J\right\rangle , \tag{1}$$

This Hamiltonian describes the interactions of the first- and higher-orders perturbation theory, predicted by quantum mechanics

The eigenfunctions are a linear combination of all states of interacting configurations:

$$|\gamma J\rangle = \sum_i c_i \left|\psi_i \; SLJ\right\rangle \tag{2}$$

where c_i are the eigenfunction amplitudes.

After having defined the basis functions and Hamiltonian, the elements of energy matrix are specified as follows:

$$H_{ij} = \left\langle\psi_i \; SLJ\right| \hat{H} \left|\psi_j \; S'L'J\right\rangle \tag{3}$$

Matrix elements of all operators are diagonal in J quantum number, therefore the energy matrix can be divided into submatrices corresponding to possible values of J. The rank of each submatrix is determined by the number of states with the same value of the total angular momentum J. For each submatrix a secular determinant is constructed:

$$\begin{vmatrix} H_{11}-E_J & H_{12} & H_{13} & \dots & H_{1j} \\ H_{21} & H_{22}-E_J & \dots & \dots & H_{2j} \\ H_{31} & H_{32} & H_{33}-E_J & \dots & H_{3j} \\ \dots & \dots & \dots & \dots & \dots \\ H_{i1} & \dots & \dots & \dots & H_{ij}-E_J \end{vmatrix} = 0 \tag{4}$$

The above mentioned determinant, after expansion, is a polynomial of degree i of unknown E_J. Every root of the polynomial approximates one of the possible eigenvalues of the Hamiltonian. In an iterative fitting procedure of experimental and calculated energy values, the radial parameters and the eigenfunctions amplitudes c_i are determined. The wave functions obtained by this method can be used, for example, for parameterization of the hyperfine structure or transition probabilities.

5.2.3 Parametrization of the radiative transitions in an atom

For the electric dipole transitions between the levels $|\gamma J\rangle$ i $|\gamma' J'\rangle$, the relationship between transition probability A, line strength $\mathbf{S}$ and weighted oscillator strength gf is as follows [35, 50]:

$$A_{\gamma\gamma'} = 2.0261 \times 10^{-6} \, \frac{\sigma^3}{g_\gamma} \, \mathbf{S} = 0.667 \times \frac{\sigma^2}{g_\gamma} \, gf, \tag{5}$$

where $\sigma = \left|E(\gamma) - E(\gamma')\right| / hc$ is the wavenumber (in cm^{-1}); $g_\gamma = (2J+1)$ and $g = (2J'+1)$ refer to the initial and final states, respectively. The transition probability is expressed in s^{-1}, line strength - in atomic units, while the oscillator strength is dimensionless.

The line strength is described by the reduced element $\mathbf{P^1}$ representing the electric dipole moment:

$$\mathbf{S} = \left|\left\langle\gamma J \left\| \mathbf{P^1} \right\| \gamma' J'\right\rangle\right|^{\mathbf{2}}, \tag{6}$$

In many configuration approximation, the wave functions $|\gamma J\rangle$ i $|\gamma' J'\rangle$ are a linear combination of basis functions $|\psi\ SLJ\rangle$ and $|\psi'\ S'L'J'\rangle$:

$$|\gamma J\rangle = \sum_i c_i \left|\psi\ SLJ\right\rangle, \quad \left|\gamma' J'\right\rangle = \sum_j c'_j \left|\psi'\ S'L'J'\right\rangle. \tag{7}$$

Therefore, the line strength can be written as:

$$\mathbf{S}_{\gamma\gamma'} = \Big|\sum_i \sum_j c_i c'_j \left\langle\psi\ SLJ \left\| \mathbf{P^1} \right\| \psi'\ S'L'J'\right\rangle\Big|^2, \tag{8}$$

where the reduced matrix element of tensorial operator $\mathbf{P^1}$ can be written as a product of angular and radial parts. The radial part is defined as: $\int_0^\infty R_{nl}(r) r R_{n'l'}(r) \mathrm{d}r$.

The matrix element of a transition operator can be written in two forms: "in length" or "in velocity" [51], which are applied in *ab initio* theoretical calculations [52–54]. It is also possible to provide a strict definition of the angular part and calculation of the radial part by means of eg. Thomas-Fermi-Dirac potential [55, 56].

In 1963, Mendlowitz proposed a semi-empirical method for determination of the relative line strengths for vanadium ion V III [57]. The angular coefficients of the transition matrix in pure LS coupling were calculated by means of straightforward Racah algebra and then transformed into the actual intermediate coupling by means of wave functions obtained in a semi-empirical fine structure analysis. Due to the application of one-configuration approximations, only one radial parameter appeared in the calculations, the value of which for simplicity was assumed equal to unity. This allowed, therefore to determine only the relative values of the line strength and the transition probability. An analogous approach was applied for Ni II, Ti II and Ti III ions [58–60].

In the mid-70s, Kurucz [55] and Biemont [56] presented a method for determining the absolute oscillator strengths using semi-empirical wave functions and radial parameters calculated theoretically by means of scaled Thomas-Fermi-Dirac method [61, 62].

In 2012, I proposed the use of precise wave functions, calculated by our own program package, to describe the electric dipole transitions [23]. The angular coefficients of matrix elements $\left\langle\psi\ SLJ \left\| \mathbf{P^1} \right\| \psi'\ S'L'J'\right\rangle$ are precisely calculated, on the basis of formulas contained in the monograph of B.G. Wybourne [63] or derived by Dr M. Elantkowska. The radial integrals were treated as free parameters in the least squares fit to the experimental values of oscillator strengths gf. In contrast to the approach applied by Mendlowitz, this procedure allows to determine the values of radial parameters and the absolute values of line strengths transition probabilities. The proposed method also differs from Kurucz's and Biemont's approach by the way of radial integrals determination. It should also be noted that despite the fact that the wave functions are derived by the same semi-empirical method, the results obtained are closely dependent on the assumed model of interactions.

By introducing a new quantity SR_{gf}, where $(SR_{gf})^2 = gf$, we can express the SR_{gf} values as a linear combination:

$$SR_{gf} = \sum_{nl,n'l'} \left(303.76\ \sigma \times 10^{-8}\right)^{1/2} \sum_i \sum_j c_i c'_j \left\langle\psi\ SLJ \left\| \mathbf{P^1} \right\| \psi'\ S'L'J'\right\rangle, \tag{9}$$

where the sum $nl, n'l'$ extends over all possible transitions.

In the calculation procedure, it is assumed that the SR_{gf} values can be either positive or negative, depending on the transition integrals having dominant contribution. It should be noted that due to the application of many configurations approximation, in the summation over basis states i, j in equation (9) there are factors related to many transition parameters which can give the contributions of different signs. Therefore, the so-called "cancellation effects" described by Cowan [35, 64] are particularly important and the correct description of radiative transitions is only possible by using the appropriate wavefunctions.

In the first step of calculation procedure, only the transitions with the most accurate gf-values, between the levels with pure eigenvector composition, were taken into consideration. This enables for precise determination of the main transition parameters. From the analysis of the transitions for which the contributions of two parameters are comparable, it is possible to determine their relative sign. In the next steps of the fitting procedures, the calculations are performed for the transitions between the levels with considerable configuration mixing. At every stage of the calculation, it is possible to fix the value of the previously determined radial parameter and the analysis of the contributions of individual parameters to the calculated value of oscillator strength.

Apart from the comparison of calculated and experimental values of oscillator strengths, it is also possible to determine their values for all possible transitions between the levels in the considered configuration system.

The radiative lifetime of the excited state $|\gamma J\rangle$ can be written as a reciprocal of the sum of probabilities $A_{\gamma\gamma'}$ for all possible transitions to lower levels $|\gamma' J'\rangle$:

$$\tau_\gamma = \frac{1}{\sum_{\gamma'} A_{\gamma\gamma'}}. \tag{10}$$

By making the appropriate summations it is possible to determine the values of the lifetimes for all upper levels studied. The comparison of calculated and experimental values of radiative lifetimes is a test of the correctness of oscillator strengths parametrization and can be executed at any stage of the calculation.

5.2.4 Description of the program package for a semi-empirical analysis of atomic structure and radiative transition

The scheme of the main calculation procedures used in the fine and hyperfine structure analysis is shown on fig. 1.

For the construction of the matrix of angular coefficients of fine structure interaction operators, the EMATRIX program has been used. It consists of a main program, performing control functions, and modules responsible for the calculations for different types of configurations and for the calculation of inter-configuration interactions matrix elements. The program uses standardized sets of input files that should be available in the calculation process. These files are opened automatically and have fixed, reserved names, clearly defining their content. The program consists of 276 subroutines, about 600 formulas and has a total of approximately 130 thousand lines of source code.

In the main program the electron configurations, for which the matrix will be generated, are declared. Configurations are given in accordance with the traditionally accepted spectroscopic descriptions (principal quantum number n, orbital quantum number l and the number of electrons N on electronic sub-shell). The program analyses the above mentioned record, assigning appropriate values of quantum numbers n, l, etc. After reading the designations of all the configurations, for each of them the matrix elements are calculated. In the case of interconfiguration interactions, for each pair of configurations a distinct code, determined by special algorithm, is assigned, which allows to direct computation to appropriate procedures. During the calculations the information about the parameters and electronic states numbering is written to a special file, used by other programs of the package.

After completing the calculations, the sorting procedure in terms of J quantum number is performed and the resulted fine structure matrix is recorded to the main output file. For this file, the descriptions of possible SL states as well as the corresponding calculated Lande g_J factor values are also appended. At the end, a template for the input file to the fine structure matrix diagonalization is created (the ATOM program), to which the initial values of the radial parameters, the experimental energy levels and the corresponding Lande g_J factor as well as the hyperfine structure constant values should be entered.

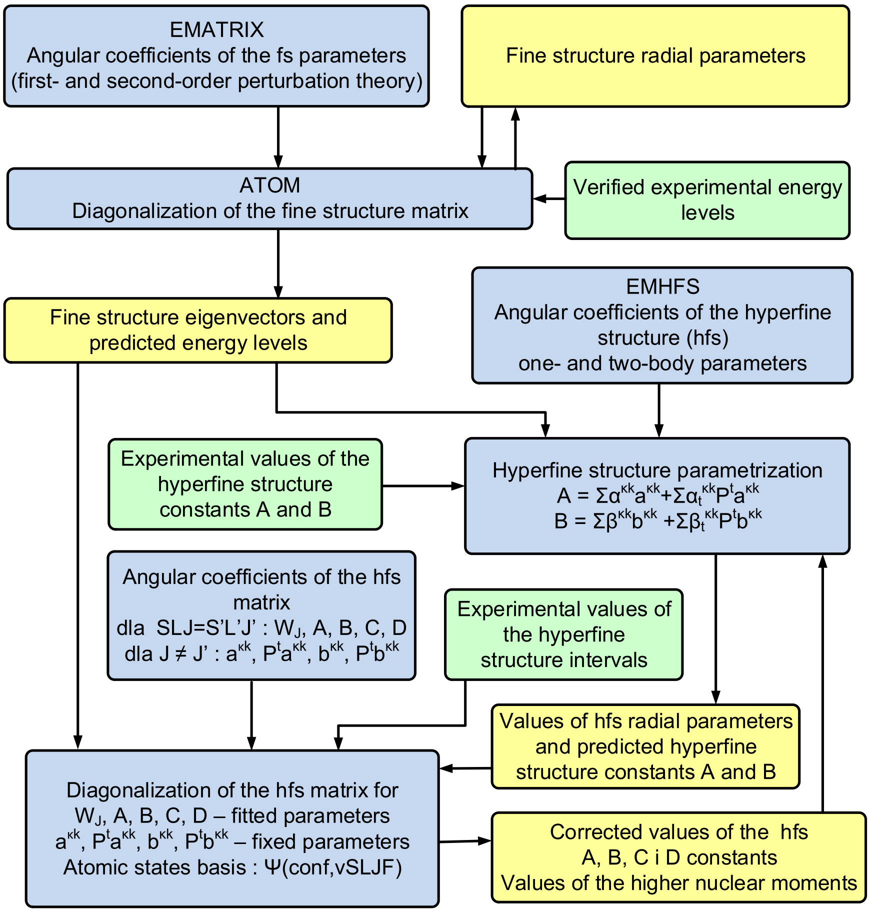

Figure 1: The scheme of the computer procedures of the fine and hyperfine structure analysis

In order to protect the contents against accidental changes and reduce the file size, the matrix elements file is converted into a binary form using FSCONV program.

For the systems containing a large number of configurations, it is assumed that the radial parameters of the interactions of the same type, described by the same quantum numbers are identical. Furthermore, for the electronic configuration of the same type, differing only by principal quantum number (Rydberg series), the relationship between the parameters dependent on the so-called effective quantum numbers can be introduced. This leads to a significant reduction in the number of independent parameters, facilitating the diagonalization procedure of the fine structure matrix. A set of four programs enables reduction of the number of independent parameters, however it is not included in the scheme for clarity reasons. In the case of systems containing several tens of configurations, it is possible to reduce the number of parameters from several thousand to several hundred. This is a necessary condition for the effective fine structure analysis of the investigated system.

For the diagonalization of the energy matrix of the fine structure, the ATOM program is used. As a result of iterative procedure, the values of the radial parameters describing the fine structure and the wave functions are obtained. This allowing the specification of other attributes describing both the electronic levels and radiative transitions between them.

The first stage of the calculation of the hyperfine structure is the generation of matrix angular coefficients of the parameters describing the hyperfine structure interactions (the EMHFS program). The structure of the program is similar to the EMATRIX program. It consists of 76 sub-programs, contains about 250 formulas and has a total of approximately 50 thousand lines of source code. The subsequent procedure, taking into account the wave functions obtained from the fine structure analysis, provides the linear equations describing the experimentally observed hyperfine structure constant. The solution of an overdetermined system of equations, by means of the least squares method, enables obtaining radial parameters and expected hyperfine structure constants.

The hyperfine structure analysis is an important test for the correctness of the wave functions, derived from the fine structure parameterization. Therefore, the ability of quick overall analysis of the results obtained in both these procedures is very important.. For this purpose I developed a program that based on several output files presenting the results in a single table.

A sufficient amount of high precision data concerning hyperfine structure, comprising information on the hyperfine structure intervals, enables the determination of the corrected hyperfine structure constants by means of direct diagonalization of *hfs* matrix. This procedure enables to include the effects of J-off-diagonal interactions on the hyperfine structure intervals. The diagonal part of hfs matrix consists of coefficients corresponding to particular components of the energy of a hyperfine structure sub-level E_F: the centre of gravity of hfs energy W_J and the experimental hfs constants A, B, C and D. These parameters are considered as free in the fitting procedure of the experimental and the calculated energies E_F. The numerical precision of the energy value E_F amounts to 1 Hz. The differences between E_F and $E_{F\pm1}$ values are equal to experimentally determined hyperfine structure intervals. The values of J-off-diagonal parameters are fixed. As a result, we obtain the corrected values of the hyperfine structure constants, which can be used to determine the values of radial hfs parameters and nuclear moments.

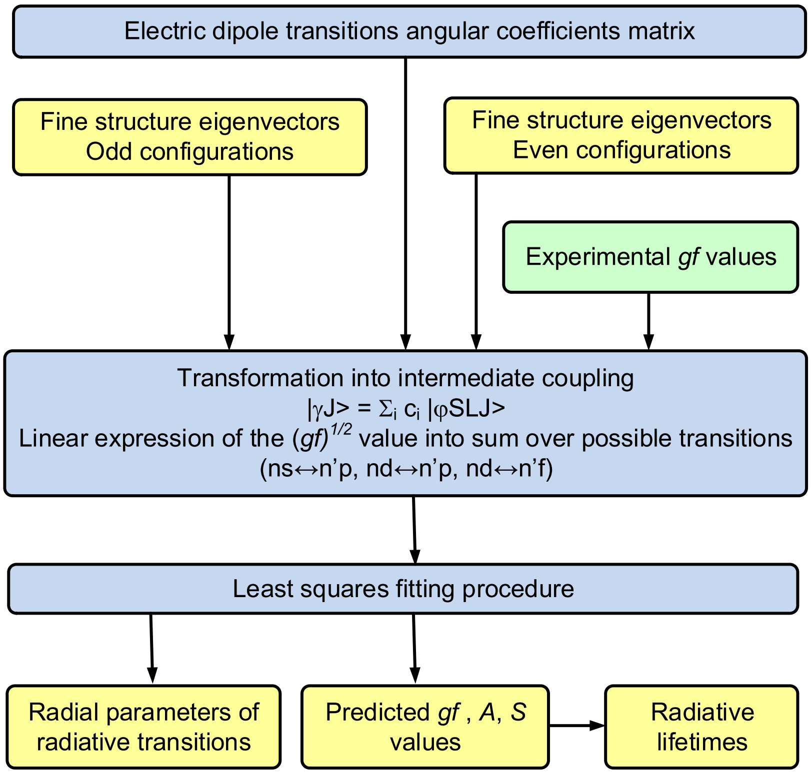

Figure 2: The scheme of computational procedures of radiative transitions parametrization

The algorithms and approximately 90% of source code of all the programs included in the package for the fine and hyperfine structure analysis, whose main elements are shown in fig. 1, except the programs FSCONV and ATOM, are the result of my many years of research.

The scheme of the main computational procedures of the radiative transitions parameterization is shown in fig. 2.

For the generation of the matrix of angular coefficients describing the electric dipole transitions, the EM-TRANSITIONS program is used. The TRANSITIONS-EQ program, using the fine structure wave functions, constructs the linear equations for SR_{gf} values, describing the transitions between the energy levels. The values of the radial transition parameters are determined in the least squares fitting procedure. A number of auxiliary programs used for downloading the values of oscillator strengths from available databases to the input file, for the analysis of the contributions of individual radiative parameters to the SR_{gf} value, for the conversion of calculated values of oscillator strengths to the line strengths, transition probabilities and for the calculations of the radiative lifetimes, were not shown in the diagram.

5.2.5 Description of the papers constituting the single-topical series of research articles

H1) An alternative method for determination of oscillator strengths: The example of Sc II

In this paper, a semi-empirical method of oscillator strengths parametrization for the electric dipole transitions, by means of multiconfiguration approximation, was presented for the first time.

The scandium ion was selected due to its simple electronic structure, in which there are two electrons on the open shells, and the availability of large amounts of data concerning the hyperfine structure constants [65–68] and oscillator strengths [69–71].

The paper presents in detail the method of the fine structure parameterization, aimed at obtaining the wave function describing the electronic states and verify the correctness of these functions on the basis of the hyperfine structure analysis. This is an issue of particular importance, because the description of electronic transitions is the most sensitive test for the wave functions correctness.

In the description of the fine and hyperfine structure, the interactions occurring in both the first- and second order perturbation theory were included. The calculations were performed for 73 odd configurations and the same number of even configurations. In the fine structure analysis for odd configuration, 246 independent parameters were used, of which 36 were considered as free parameters in a fitting procedure to 75 experimental energy levels. In the analogous calculations for even configurations, 516 independent parameters, including 57 free parameters, and 93 experimental energy values were used. The verification of the correctness of the wave functions was carried out by means of simultaneous parametrization of the hyperfine structure for both parities. This approach enabled better determination of the radial parameters and provided a more accurate predictions of the hyperfine structure constants. In the fitting procedure of 97 calculated and experimental oscillator strengths, the values of transition radial parameters were derived. A comparison with the values of oscillator strengths obtained by using the semi-empirical wave functions and theoretically calculated radial parameters was also performed [55, 72]. The calculations confirmed that the main factor determining the compliance of calculated and experimental values of oscillator strengths is the wave function.

The predicted values of the hyperfine structure constants for all the levels in the energy range to around 95 000 cm^{-1}, including those not observed experimentally, were given. The values of oscillator strengths for all possible transitions from the analysed levels were also calculated. The possibility to determine the values of oscillator strengths for transitions from the levels, not previously observed experimentally, was presented.

H2) Semi-empirical calculations of oscillator strengths and hyperfine constants for Ti II

In the paper, a semi-empirical method of oscillator strengths parametrization for the electric dipole transitions in titanium ion was presented. It was another stage of effectiveness verification of the method for configurations system with three electrons on open shells. The most recent data concerning energy levels, transition probabilities and hyperfine structure constants were used [73–77].

The calculations were performed for 61 odd configurations and the same number of even configurations. In the fine structure analysis for odd configuration, 377 independent parameters were used, of which 42 were considered as free parameters in a fitting procedure to the 121 experimental energy levels. In the analogous calculations for even configurations, 488 independent parameters, including 34 free parameters, and 131 experimental energy values were used. The verification of the correctness of the wave functions was carried out by means of simultaneous parameterization of the hyperfine structure for both parity, with the use of the hyperfine structure constants values for 34 energy levels.

In the fitting procedure of 461 calculated and experimental oscillator strengths, the values of 10 independent transition radial parameters were derived. A comparison with the values of oscillator strengths obtained by using the semi-empirical wave functions and theoretically calculated radial parameters was also performed [78, 79]. In the paper, a graphical comparison of the logarithms of calculated and experimental oscillator strengths, in the form commonly accepted in the papers on this subject, was also presented.

In the supplementary materials, available on-line, the predicted values of the hyperfine structure constants for all levels in the energy range to about 84 000 cm^{-1}, even those not observed experimentally, were presented. The predicted values of oscillator strengths for 1340 transitions, sorted by wavenumber, were also included. The expected values of hyperfine structure constants were included by R. Kurucz in their database (`http://kurucz.harvard.edu/atoms/2201/`, `ab220147.dat` and `ab220149.dat` files).

H3) Semi-empirical analysis of oscillator strengths for Nb II

The paper is a result of a short-term research visit at the invitation of Prof. Safa Bouazza at the University of Reims. I suggested therein the use of the wavefunctions for niobium ion, earlier derived and used for the hyperfine structure parameterization [80, 81]. Moreover, this choice was justified by the availability of accurate data on oscillator strengths [82, 83].

The calculations were performed for the system of 11 odd configurations and 17 even configurations. In the fitting procedure of 251 calculated and experimental oscillator strengths, the values of 4 independent transition radial parameters was derived. In the supplementary materials, available on-line, the predicted values of oscillator strengths for 2968 transitions, sorted by wavenumber, were included.

H4) Hyperfine structure, lifetime and oscillator strength of V II

The paper was created in collaboration with Prof. Safa Bouazza at the University of Reims. The wavefunctions for vanadium ion,presented earlier in the papers concerning the fine structure of V II, were utilised [84, 85]. Furthermore, the choice of vanadium ion was justified by the availability of accurate data concerning the hyperfine structure constants and transition probabilities [86–88].

The calculations were performed for the system of 3 odd configurations and 6 even configurations. A comparison of calculated and experimental values of the hyperfine structure constants A for 20 levels was presented. In the fitting procedure of 203 calculated and experimental oscillator strengths, the values of 6 independent transition radial parameters were derived.

The values of radiative lifetimes for 31 odd levels, calculated by means of COWAN CODE program, were given. A comparison with the values of oscillator strengths obtained by using the semi-empirical wave functions and theoretically calculated radial parameters was also performed [78, 79].

In the supplementary materials, available on-line, the predicted values of oscillator strengths for 1093 transitions, sorted by wavenumber, were included.

H5) Semi-empirical analysis of the fine structure and oscillator strengths for atomic strontium

The motivation to undertake the research presented in the paper was the availability of data related to energy levels and transition probabilities for Rydberg configurations with the principal quantum number up to $n = 20$ [89]. This gave an opportunity to analyse the dependence of the radial transition parameters from the n quantum number.

The calculations were performed for 61 odd configurations and 81 even configurations. In the fine structure analysis for odd configurations, 228 independent parameters were used, of which 62 were considered as free parameters in a fitting procedure to the 196 experimental energy levels. In the analogous calculations for even configurations, 792 independent parameters, including 28 free parameters, and 180 experimental energy values were used.

In the fitting procedure of 86 calculated and experimental oscillator strengths, the values of 26 independent transition radial parameters were derived. The paper presented also the results of the radiative lifetimes calculations for 54 levels and their comparison with the values obtained experimentally and by means of theoretical calculations [79, 90–96].

In the supplementary materials, available on-line, the predicted values of oscillator strengths for 728 transitions, sorted by wavenumber, were included.

H6) Semi-empirical determination of radiative lifetimes for Sc II and Ti II

In this paper, the results of oscillator strengths calculations for scandium and titanium ions, published earlier in the papers H1 and H2 [23, 24], were used. Determination of probabilities for all possible transitions allowed the calculation of radiative lifetimes for excited levels. For this purpose, the procedures for conversion of calculated oscillator strengths to transition probabilities and to perform appropriate summations required to determine the radiative lifetimes, were developed. These programs since then have been applied to the current control of the calculation correctness in the oscillator strengths parametrization procedure.

The radiative lifetimes for 38 levels of scandium ion and 75 levels of titanium ion were determined. The calculated values were compared with the available experimental and theoretical results [71, 79, 97–99].

H7) Semi-empirical determination of radiative parameters for Ag II

The motivation to undertake the oscillator strengths calculations for silver ion was a published critical compilation of energy levels and transition probabilities data for Ag II [100].

The calculations were performed in the basis of 16 odd configurations and 24 even configurations. In the fine structure analysis for odd configurations, 445 independent parameters were used, of which 23 were considered as free parameters in a fitting procedure to the 55 experimental energy levels. In the analogous calculations for even configurations, 724 independent parameters, including 26 free parameters, and 43 experimental energy values were used. The mean deviation of 51 cm^{-1} and 14 cm^{-1}, for odd and even configurations, respectively, was achieved. For the odd configurations, this value was comparable, and for the even system - it was approximately four times smaller than the result obtained by Kalus et al. [101]. In the fitting procedure of 237 calculated and experimental oscillator strengths, the values of 13 independent transition radial parameters were derived. In this study, a comparison of experimental and calculated line strength was presented, which from the point of view of quantum mechanics is more relevant than the comparison of logarithms of oscillator strengths.

The paper presented also the results of the radiative lifetimes calculations for 55 odd and 38 even levels. For 15 of these levels, the comparison of calculated radiative lifetimes with the values obtained experimentally and by means of theoretical calculations [102–109] was included.

In the supplementary materials, the predicted values of oscillator strengths and probabilities for 1103 transitions between electronic levels, were included.

H8) Semi-empirical determination of radiative parameters for atomic nickel

The motivation to undertake the oscillator strengths calculations for atomic nickel was the availability of a large number of accurate experimental values of the radiative lifetimes of energy levels [110–114] and transition probabilities [115, 116]. Furthermore, the paper was a continuation of the series devoted to the iron group elements [23, 24, 26, 28], which are of particular interest in the astrophysical studies.

The calculations were performed in the basis of 21 odd configurations and 26 even configurations. In the fine structure analysis for odd configurations, 409 independent parameters were used, of which 38 were considered as free parameters in a fitting procedure to the 153 experimental energy levels. In the analogous calculations for even configurations, 550 independent parameters, including 26 free parameters, and 130 experimental energy values were used. The mean deviation of 59 cm^{-1} and 31 cm^{-1}, for odd and even configuration systems, respectively, was achieved. These values were comparable to the results obtained by [79] and approximately twice smaller than those obtained by [117].

In the fitting procedure of 582 calculated and experimental oscillator strengths, the values of 13 independent transition radial parameters were derived. In order to properly assess the quality of the fit, as in previous papers, the line strengths for the considered transitions were analysed. The comparison of scatter plots of $\log(\mathbf{S}_{\mathrm{exp}}/\mathbf{S}_{\mathrm{calc}})$ as a function of $\mathbf{S}_{\mathrm{calc}}$ for the calculations performed in this paper, and those presented by Kurucz [79] shows that, despite the similar results of fine structure calculations obtained by means of the same semi-empirical method, the results of power oscillator strengths parameterization presented in this paper were better. This is another confirmation of the fact, that the most sensitive test of the wave functions correctness is the analysis of radiative transitions. Moreover, it indicates that our Hamiltonian more completely takes into account the interactions occurring in an atom. This is confirmed also by the comparison of calculated and experimental lifetimes for 75 levels.

In the paper and supplementary materials, the calculated radiative lifetimes for 173 energy levels and the values of oscillator strengths and probabilities for 3044 transitions between electronic levels, were included.

5.2.6 Summary

The correct description of radiative transitions is only possible with the use of precise wavefunctions. In the fine structure analysis, where the wave function amplitudes are determined, depending on the number of available experimental data, the effects of all interactions in an atom should be taken into account as fully as possible. The application of our own, globally unique, integrated software package allows determination of the wavefunction amplitudes necessary for a proper description of a number of attributes describing the energy levels and the transitions between them. The presented studies confirmed the effectiveness of the semi-empirical method description of radiative transitions in an atom, In the case of atoms with many electrons on open shells, a semi-empirical approach yielded, in many cases, better results than the use of other computational methods.

The extensive tables containing the predicted values of the constants of the hyperfine structure, oscillator strengths, transition probabilities and lifetimes, complementary to existing databases will be helpful in the interpretation of the spectra observed in astrophysical research and provide motivation for further experimental and theoretical work.

5.3 Plans for the future research

The confirmation of the effectiveness of a semi-empirical method description of radiative transitions in an atom provides a strong incentive for me to continue the calculations for the iron group elements, for which accurate experimental data concerning transition probabilities and radiative lifetimes were presented in recent years (eg. `http://www.as.utexas.edu/~chris/lab.html`). The same research team published also the data on rare earths elements. The calculations for this group of elements will be undertaken after the optimization of computational procedures for matrices of huge size, initiated recently.

A natural continuation of research concerning the parameterization of radiative transitions will be to develop similar procedures for forbidden transitions. Intensive studies concerning the determination of probabilities for forbidden transitions and lifetimes of metastable levels for the iron group elements are conducted for many years [118].

Another issue worth considering, will be elaboration of a method of simultaneous parameterization of the fine structure for a system containing the configurations of both parities. This will enable a more accurate determination of the values of the parameters for interactions described by the second order of perturbation theory.

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