

# **INSTITUTE OF THEORETICAL PHYSICS AND ASTRONOMY**

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**Director** - Dr. Habil. *Gražina Tautvaišienė*

## ***STAFF***

64 research fellows (12 habilitated doctors, 2 doctors with the habilitation procedure, 37 doctors) and 11 doctoral students. Full staff comprises 84 people.

## ***MAIN RESEARCH TRENDS OF THE INSTITUTE***

Structure and Evolution of Galactic, Interstellar Matter and Galaxies.

Physics of Atoms, Molecules and Condensed Matter.

New Materials, Nano-structures and Surfaces: Synthesis, Characterization, Technologies.

## ***DOCTORAL DISSERTATIONS MAINTAINED IN 2010***

Rytis Juršėnas. Algebraic Development of Many-Body Perturbation Theory in Theoretical Atomic Spectroscopy.

Viačeslavas Nelkinas. Investigation of the Electronic Structure and XPS Band Form of Chalcogenides Crystals

## ***CONFERENCES AND SEMINARS ORGANIZED IN 2010***

Seventh International Conference “Atomic and Molecular Data and Their Applications” (ICAMDATA 2010), Vilnius, 21-24 September 2010.

Humboldt Forum on Science and Society in Modern Europe, Vilnius, 23-26 September 2010 (organized jointly with the Department of Quantum Electronics of Faculty of Physics and Faculty of Philosophy).

## ATRONOMICAL OBSERVATORY

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**Head** – Dr. Habil. *Gražina Tautvaišienė*

### **STAFF**

**Chief Researchers:** Prof. Habil. Dr. A. Bartkevičius, Habil. Dr. G. Tautvaišienė, Prof. Habil. Dr. V. Straižys, Habil. Dr. K. Zdanavičius.

**Senior Researchers:** Dr. K. Černis, Dr. R. Janulis, Dr. A. Kazlauskas, Dr. A. Kučinskas.

**Research fellows:** Dr. Y. Chorniy, Dr. V. Laugalys, Dr. E. Pakštienė, J. Zdanavičius.

**Junior Researchers:** G. Barisevičius (part time), A. Ivanauskas (part-time), M. Maskoliūnas (part time), Š. Mikolaitis, D. Prakupavičius (part-time), E. Puzeras, E. Stonkutė (part time).

**Doctoral students:** G. Barisevičius, V. Čepas, M. Maskoliūnas, Š. Mikolaitis, D. Prakupavičius, E. Stonkutė, R. Ženovienė.

**Lecturers:** S. Lovčikas, M. Masaitis.

**Engineers:** A. Černiauskas (part-time), G. Valiauga, R. Ženovienė.

**Technicians:** J. Klevas (part-time), V. Milkus (part-time).

**Administrator:** V. Kakarienė.

**Operator:** R. Mikutavičienė.

### **RESEARCH INTERESTS**

Galactic structure and chemical evolution

Stellar photometry, stellar classification, multicolour photometric systems

Interstellar reddening and extinction

Chemical analysis of stellar atmospheres, mixing in stellar atmospheres

Stellar asteroseismology

Star formation histories in galaxies of the Local Group

Search and positional observations of comets, asteroids and near-Earth objects

### **RESEARCH PROJECTS CARRIED OUT IN 2010**

#### **Project Supported by University Budget**

**Chemical Composition and Evolution of Stellar Atmospheres.** Dr. Habil. G. Tautvaišienė. 2005–2010.

The Hipparcos orbiting observatory has revealed a large number of helium-core-burning "clump" stars in the Galactic field. These low-mass stars exhibit signatures of extra-mixing processes that require modeling beyond the first dredge-up of standard models. The  $^{12}\text{C}/^{13}\text{C}$  ratio is the most robust diagnostic of deep mixing, because it is insensitive to the adopted stellar parameters. In this work for the first time we determined  $^{12}\text{C}/^{13}\text{C}$  isotope ratios in a sample of 34 Galactic clump stars as well as abundances of nitrogen, carbon and oxygen. Comparisons to evolutionary models show that the stars fall into two groups: the one is of first ascent giants with carbon isotope ratios altered according to the first dredge-up prediction, and the other one is of helium-core-burning stars with carbon isotope ratios altered by extra mixing. The stars investigated fall to these groups in approximately equal numbers.

The main atmospheric parameters and abundances of the iron group elements were determined for 62 red giant "clump" stars revealed in the Galactic field by the Hipparcos orbiting observatory. A Gaussian fit to the [Fe/H] distribution produced the mean [Fe/H] =  $-0.01 \pm 0.08$ . The near-solar metallicity with so small dispersion of clump stars of the Galaxy obtained in this work confirmed the theoretical model of the Hipparcos suggesting that the nearby clump stars are (in the mean) relatively young objects, reflecting mainly the near-solar metallicities developed in the local disk during the last few Gyrs of its history.

We have made an analysis of high-resolution spectra of core-helium-burning "clump" stars and giants in the open clusters NGC 6134 and IC 4651. In this study we presented abundances of  $^{12}\text{C}$ ,  $^{13}\text{C}$ , N, O and up to 24 other chemical elements. A comparison of the observational data with theoretical models of stellar evolution showed that processes of extra-mixing in stars of 2–3  $M_{\text{Sun}}$  turn-off masses are larger than predicted.

Photospheric parameters and chemical composition were determined for the single-lined chromospherically active RS CVn-type stars Lambda Andromedae and 29 Draconis. From the high resolution spectra obtained on the Nordic Optical Telescope, abundances of 22 chemical elements and isotopes, including such key elements as  $^{12}\text{C}$ ,  $^{13}\text{C}$ , N and O, were investigated. The carbon isotope ratios for these stars of the RS CVn-type were determined for the first time, and their low values gave a hint that extra-mixing processes may start acting in low-mass chromospherically active stars below the bump of the luminosity function of red giants.

We presented the preliminary results of a project aimed at high resolution spectral analysis of stars in a kinematically identified stellar group, suspected to belong to a remnant of a disrupted satellite galaxy. The 16 stars analysed by now have a metallicity around -0.7 dex, an average isochrone age of about 12 Gyr, their chemical composition is homogeneous and distinct from the Galactic disk dwarfs. This provides further evidence of their common and extragalactic origin.

Quadruple stellar system WDS J00047+3416 was analysed. For a component D (F8 dwarf) a spectroscopic orbit was determined. From 42 Coravel-type radial velocity measurements with 0.8 km/s error of one observation, orbital elements were determined. The spatial distance between AB and D components is very large  $\sim 24000$  AU (0.12 pc). The optical component C is situated at over 600 pc distance. It was found that Hipparcos observations for the component C are not correct. Instead of the Hipparcos high proper motion  $\mu = 137.17 \pm 29.97$  mas/yr, a very small proper motion  $\mu = 3.619 \pm 0.58$  mas/yr was determined.

### **Investigation of star-forming regions and dust clouds in the 2nd Galactic quadrant.**

Prof. V. Straizys. 2006–2010.

Spectral energy distributions are determined for 140 YSOs in the region of dark clouds of Camelopardalis.

Interstellar extinction in the direction of open cluster IC 361 is investigated on the grounds of CCD photometry of 1420 stars in the Vilnius photometric system and their two-dimensional classification. Parameters of the cluster are determined.

A method for the photometric identification of red clump giants and the stars of spectral classes A-F is developed. It uses photometry data from the 2MASS, MegaCam and IPHAS surveys. This method is applied for the investigation of extinction and distance of the interstellar dust cloud LDN 1525 in the direction of Aur OB1 association. (V. Straizys, V. Laugalys);

The investigation of stars and dust clouds was continued in the region of the Cepheus Flare. CCD frames in the Vilnius system were obtained in two 1.5 square degree fields, their reductions are in progress (M. Maskoliūnas, K. Zdanavičius, J. Zdanavičius);

V. Straizys and K. Zdanavičius participated in the working group for stellar classification of the ESA Gaia project. They proposed a new method for determining the decontamination corrections for the Gaia low-dispersion spectra.

CCD photometry in the Vilnius system, two-dimensional spectral types, interstellar extinctions and distances were determined for 1549 stars in the vicinity of open cluster King 7 (J. Zdanavičius, V. Čepas, K. Zdanavičius).

### **Positional Astrometry of Unusual Asteroids and Comets.** Dr. K. Černis. 2005–2010.

74 new asteroids have been discovered (at Molėtai Astronomical Observatory 68 asteroids). We succeeded to discover a new NEO Amor group asteroid 2010 BT3 (period about 4.14 years) with the diameter of more than 200 meters. The astronomical observations were carried out with 0.35/0.51-m f/3.5 Maksutov reflector (we observed 32 nights, from January till November, 2010). 3200 CCD images of good quality have been obtained and processed. During the sky survey about 700 square degrees of the sky have been covered.

The results of NEO Aten group asteroid 2008 OS9 astrometric and photometric observations at the Moletai and Baldone observatories have been published. From the brightness variation with the 0.27 mag amplitude, a rotation period of 8.43 h was determined. The mean values of secular differences in the semi-major axis, eccentricity and inclination were computed with and without the Yarkovsky and YORP effects. The orbit of the asteroid was computed from 499 observations from 2008 July to 2009 May with an rms error of 0.519". The calculated ephemerides of the asteroid show that its nearest close approach to Earth is expected on 2085-08-14 at 0.07 AU distance with the positional uncertainty of about 0.5 deg.

The asteroid project together with the Vatican Observatory has been prosecuted. During the search for new asteroids with the 1.8 m reflector at Mount Graham observatory (observer R. P. Boyle) three asteroids have been discovered: 2010 VC199, 2010 VD199 ir 2010 VE199 (8

nights of observations in the period of May-November, 2010, limiting detection magnitude of moving objects was about 23 mag).

According to the international collaboration project „On cooperation in scientific investigations of small solar system bodies“ between Institute of Theoretical Physics and Astronomy (TFAI) of Vilnius University and Institute of Astronomy of University of Latvia (representative of project dr. I. Eglitis) three new asteroids have been discovered: 2010 GC158, 2010 JY14 ir 2010 JN76. Astronomical observations have been performed with the Schmidt telescope (0.80/1.20 m, f/3.5) of Baldone Observatory. We obtained and processed 198 high quality CCD images with the limiting magnitude 21 (results are presented in 10 publications).

The results of more than 4000 positions of asteroids and comets have been published (astrometric observations belong to more than 1522 separate objects). Among the 14 observed comets at the Moletai Observatory, the brightest one was the comet 103P/Hartley. Astrometry and photometry of the comet 103P will be published in the International Comet Quarterly journal.

Together with prof. A. Dubietis (VU FF) we finished an analysis of systematic visual and photographic observations of noctilucent clouds seen from Lithuania (in the years from 1973 till 2009). A clear signature of the solar activity cycle was imprinted on the noctilucent cloud occurrence frequency and mean brightness, both showing distinct anti-correlation with the sunspot numbers. The most recent noctilucent cloud observations were linked to variations of local mesospheric temperatures, measured by the Aura satellite. New photographic observations (with small CCD camera) of noctilucent clouds have been performed in summer 2010.

### **Projects Supported by Research Council of Lithuania**

Bilateral Lithuanian-Ukrainian research project „Abundance of the light elements and neutron-capture elements in the atmospheres of the red giants in globular clusters as a probe of the stellar evolution and evolution of the harboring globular clusters“. Dr. A. Kučinskas. 2009-2010

Project: „Extended description of science infrastructure development at Moletai Observatory“. A. Kučinskas. 2010.

Students Summer Practice: R. Chmieliauskaitė, supervisor – Dr. A. Kazlauskas, 2010; M. Macijauskas, supervisor – Prof. Habil.Dr. V. Straižys, D. Mažonas, supervisor – Dr. A. Kučinskas.

### **Projects Supported by FP7**

Baltic Grid II. Dr. Habil. G. Tautvaišienė. 2008–2010.

Researchers' Night in Lithuania 2010 (ReNiLit 2010). Dr. A. Kazlauskas. 2010.

### **Projects Supported from EU Structural Funds**

Science for Business and Society. V. Daniūnas. 2009–2011.

### **Other Projects**

Long-term international project: The Whole Earth Telescope. Dr. R. Janulis, Dr. E. Pakštienė.

Long-term international project: The European Space Agency Satellite GAIA. Prof. V. Straižys, Dr. Habil. G. Tautvaišienė, Dr. Habil. K. Zdanavičius, Dr. A. Kazlauskas, Š. Mikolaitis.

### *EVENTS*

Two big events for wide public were organized at the Moletai Astronomical Observatory. The first one took place on May 7 and was to the 20-th anniversary of Hubble telescope. The big poster with magnificent picture, granted by the European Space Agency, was presented during this event. About 300 visitors attended the event.

The second one took place on September 24 and was a part of the FP7 project “Researchers’ night 2010”. The full staff of the AO was involved in the preparation and performance of this event. About 800 people from all regions of Lithuania listened to the lectures of astronomers and physicists, attended the professional telescopes and admired the objects of the starry sky.

Among other events at MAO it should be mentioned the International exhibition of the aerophotography (October-December), the exhibition of astronomical pictures of the Kaunas art-school students, two nights of equinox-music etc.

Altogether more than 400 groups and about 10000 people visited the Observatory during the year.

### **COOPERATION**

Astrophysical Institute Potsdam (Germany)

Bologna Observatory (Italy)

Copenhagen University (Denmark)

Kiepenheuer Institut für Sonnenphysik (Germany)

National Astronomical Observatory (Japan)

Observatory of Paris Meudon (France)

Padova Observatory (Italy)

Palomar Observatory (USA)

Universidad de Concepción (Chile)

University of Washington (USA)

University of Western Ontario (Canada)

Uppsala Astronomical Observatory (Sweden)

Vatican Observatory (USA)

In the frame of the Whole Earth Telescope (WET) Project, the Astronomical Observatory of the Institute cooperates with astronomical observatories in 15 countries.

## ***OTHER SCIENTIFIC ACTIVITIES***

### **Dr. K. Černis –**

- member of the Lithuanian Astronomical Olympiad Council;
- member of the International Astronomical Union (IAU).

### **Dr. A. Kučinskas –**

- member of Board of Directors of the international journal “Astronomy & Astrophysics”

### **Prof. V. Straizys –**

- editor-in-chief of the international journal “Baltic Astronomy”;
- corresponding member of the Lithuanian Academy of Sciences;
- member of the working group on stellar classification of the ESA Gaia project;
- member of the International Astronomical Union (IAU), since 1967;
- member of the European Astronomical Society, since 1994.

### **Dr. Habil. G. Tautvaišienė –**

- vicepresident of Lithuanian Physics Society, since 2007;
- reviewer of the European Science Foundation, 2010-2012;
- member of the International Astronomical Union (IAU), since 1992, National representative, since 2006;
- board member of the IAU Division "Optical & Infrared Techniques", since 2009;
- member of Astrophysics Commission at the International Union of Pure and Applied Physics, since 2005;
- Executive Board member of the Astronet project;
- member of scientific working group “Reference stars” of GAIA Space Observatory (ESA);
- founding member of the European Astronomical Society, since 1994;
- member of the Editorial Board of of the journal Baltic Astronomy, since 2006;
- editor-in-chief of the annual astronomical almanac “Lietuvos dangus”, since 2002.

## DEPARTMENT OF THE THEORY OF ATOM

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**Head** – Dr. *Alicija Kupliauskienė*

### **STAFF**

**Chief Researchers:** Prof. Habil. Dr. P. Bogdanovičius, Prof. Habil. Dr. Z. R. Rudzikas, Prof. Dr. Habil. R. Karazija, Prof. Dr. Habil. G. Gaigalas (part-time).

**Senior Researchers:** Dr. A. Bernotas (part-time), Dr. V. Jonauskas, Dr. R. Karpuškienė, Dr. R. Kisielius, Dr. R. Kivilšienė, Dr. S. Kučas, Dr. A. Kupliauskienė, Dr. G. Merkelis, Dr. A. Tamulis, Dr. J. Tamulienė, Dr. V. Tutlys.

**Researchers:** Doc. Dr. A. Kynienė, Dr. A. Momkauskaitė, Dr. O. Rancova (part-time).

**Junior Researchers:** Dr. R. Juršėnas, Š. Masys (part-time).

**Engineers:** E. Gaidamauskas (part-time).

**Doctoral students:** Š. Masys

### **RESEARCH INTERESTS**

Theoretical atomic spectroscopy

Methods of the theory of complex atomic and ionic spectra

Development of quantum many-body theory

Development and application of algorithms and computer programs for plasma physics, astrophysics and other fields.

Development of quantum mechanics and quantum electrodynamics for characterization of transitions in atoms, molecules and molecular complexes

Investigation of the processes of the interaction of atoms with electrons and radiation

Quantum mechanical modeling of self-assembly of minimal living cells and quantum

processes of photosynthesis in artificial living organisms

History of physics

### **RESEARCH PROJECTS CARRIED OUT IN 2010**

#### **Project Supported by University Budget**

**Cascades in Complex Atoms and Their Influence on X-ray and Auger Spectra: Theory and Interpretation.** Prof. R. Karazija. 2006–2011.

In collaboration with experimenters the investigation of Auger cascades in krypton atoms following the production of vacancies in  $3d_{3/2}$  and  $3d_{5/2}$  subshells has been performed. The initial photoelectron and two Auger electrons were detected in coincidence and analyzed in energy thanks to magnetic bottle electron time of flight spectrometer. The large scale calculations of these complex Auger spectra in the relativistic configuration interaction

approximation were performed, taking into account various possible transitions and correlation effects. The comparison of these calculation results with the experimental coincidence spectra enabled to identify practically all structure of Auger spectrum, including its low-energy part recorded for the first time and thus to explain the complex deexcitation process of strongly perturbed atom.

**Fluorescence and Auger Emission of Polarized Atoms Excited and Ionized by Polarized Electrons.** Dr. A. Kupliauskienė. 2007–2010.

Large scale configuration interaction calculations of energy levels, autoionization probabilities and electron-impact excitation cross sections for the fine structure states of Rb in the autoionizing configurations  $4p^5nl n'l'$  ( $nl=5s, 4d, n'l'=5s, 5p, 6s$ ) were performed by using the basis of radial wave functions obtained in Dirac-Fock-Slater approximation. The results were used for the identification of experimental ejected-electron spectrum.

The technique based on the constituted  $SO(3)$ -irreducible tensor operators has been developed. The key feature of proposed technique is the ability to reduce the  $N$ -electron angular integrals into the sum of single integrals. The method is especially convenient for the calculation of matrix elements of interaction operators on the basis of  $SU(2)$ -irreducible matrix representations.

A systematic way of inquiry of totally antisymmetric tensors has been brought to a more advanced state. Based on the  $S_1$ -irreducible representations and the conception of tuples, the method to classify the angular reduction schemes of operator string of any length  $l$  has been initiated. Special attention is paid to the case  $l=6$  which characterizes the three-particle operators observed in the applications of effective operator approach to the atomic perturbation theory. As a result, the foundations developed for the irreducible tensor operators associated to distinct angular reduction schemes appear to be well-suited with respect to facility to compute the matrix representations of given operators.

The classification of three-particle operators that act on 2, 3, 4, 5, 6 electron shells of atom has been performed. The irreducible tensor operators associated to their own angular reduction schemes are identified by the classes. The classes are characterized by the number of electron shells the operator acts on and by the number of electrons in a given shell.

The atomic third-order many-body perturbation theory has been considered. To simplify the generation of expansion terms followed by the generalized Bloch equation, the symbolic programming package `NCoperators` written on Mathematica has been produced. The angular reduction of generated terms has been performed making use of `NCoperators` too. The specific technique of reduction has been developed. The algorithm is based on the composed  $SU(2)$ -invariants of the second-order wave operator. Therefore, the irreducible tensor form of terms of the third-order effective Hamiltonian is applicable to other effective operator approaches (such as coupled-cluster) used in MBPT.

**Development of Methods for the Investigation of Spectral Characteristics of Many-electron Atoms and Their Application for Highly Charged Ions in Thermonuclear and Other Plasmas.** Prof. P. Bogdanovich. 2007–2011.

In 2010 great attention was paid to improve the matrix diagonalization codes in use. An attempt to perform the code parallelization planned has revealed that the benefit in the computational time is much smaller than expected. The analysis of the algorithms showed that it is expedient to use the upper triangular of the symmetric matrices instead of the lower one while upgrading the programs for the forming and diagonalizing of matrices. In this way the diagonalization procedure was hasten successfully since in trial calculations the matrix

diagonalization time was reduced more than twice. The code parallelization procedure applied to the last algorithm allowed to hasten the diagonalization even more but the effect is not essential.

While implementing the theoretical investigation of the spectral characteristics of tungsten ions, the calculations of the energy spectra, wavelengths, characteristics of electric dipole, electric quadrupole and magnetic dipole transitions as well as radiative lifetimes of tungsten ions  $W^{37+}$ ,  $W^{36+}$  and  $W^{35+}$  in configurations  $4p^6 4d^N$ ,  $4p^5 4d^{N+1}$  and  $4p^6 4d^{N-1} 4f$  ( $N = 1, 2$  and  $3$ ) were performed within the *ab initio* quasirelativistic approximation. The correlation effects and influence of the admixed configurations was explored for the  $W^{37+}$  ion as an example. It is shown that the magnetic dipole transitions can influence the radiative lifetimes of some excited levels even in the cases when the electric dipole transitions are allowed from these levels to the lower ones of the ground configuration.

The investigations of the energy spectra of the highly-charged ions with filling 2p-shell and the tungsten ions mentioned have revealed that it is necessary to take into account the quantum electrodynamics effects seeking for further improvement of the accuracy of the spectral characteristics under research.

### **Theoretical Investigation of Plasmas Spectra by Using Collisional-Radiative Model.** Dr. V. Jonauskas. 2008–2013.

Theoretical study of radiative spectra for  $W^{12+}$  and  $W^{13+}$  ions has been performed in the range 33,5 – 39,5 nm. Atomic data for the energy levels, radiative transition probabilities and electron impact excitation cross sections were obtained for the ground configurations and several excited configurations. Modelling of the emission spectra was accomplished by making an assumption that the ground and the first metastable levels are mostly populated in the EBIT plasma. To find the populations of the excited levels, the data of electron impact excitation rates have been obtained for the various electron beam energies. Additionally, the influence of the population from the higher levels was determined by iterative procedure. Further analysis of spectra was considered by including the process of radiative cascades.

The configuration interaction method based on the Slater-type radial orbitals was used to determine the energy levels, electric-dipole transition wavelengths, absorption oscillator strengths and radiative transition probabilities for the inner-shell excitation of transitions in Fe XIV, Fe XV and Fe XVI ions. The transitions of types  $2s - 3l$ ,  $4l$  and  $2p - 3l$ ,  $4l$  have been considered. Obtained atomic data, after assessment of their accuracy, are being employed in modeling the Unresolved Transition Array (UTA) spectra of various astrophysical objects for the X-ray wavelength range from 12 Å to 18 Å.

### **Development and applications of relativistic theory for many-electron atoms.** Prof. G. Gaigalas. 2009–2014.

Multiconfiguration expansions frequently target valence correlation and the correlation between valence electrons and the outermost core electrons. Correlation within the core is often neglected. A large orbital basis is needed to saturate both the valence and core–valence correlation effects. This in turn leads to huge numbers of configuration state functions (CSFs), many of which are unimportant. To avoid the problems inherent to the use of a single common orthonormal orbital basis for all correlation effects in the multiconfiguration Hartree–Fock (MCHF) method, was proposed to optimize independent MCHF pair-correlation functions (PCFs), bringing their own orthonormal one-electron basis. Each PCF is generated by allowing single- and double-excitations from a multireference (MR) function. This computational scheme has the advantage of using targeted and optimally localized orbital sets

for each PCF. These pair-correlation functions are coupled together and with each component of the MR space through a low dimension generalized eigenvalue problem. Nonorthogonal orbital sets being involved, the interaction and overlap matrices are built using biorthonormal transformation of the coupled basis sets followed by a counter-transformation of the PCF expansions. Applied to the ground state of beryllium, the new method gives total energies that are lower than the ones from traditional complete active space (CAS)-MCHF calculations using large orbital active sets. It is fair to say that we now have the possibility to account for, in a balanced way, correlation deep down in the atomic core in variational calculations.

Large-scale multiconfiguration Dirac-Fock calculations have been performed for the superheavy element eka-thorium,  $Z = 122$ . The resulting atomic structure is compared with that obtained by various computational approaches involving different degrees of approximation in order to elucidate the role that correlation, relativistic, Breit, and quantum electrodynamics corrections play in determining the low-energy atomic spectrum. The accuracy of the calculations is assessed by comparing theoretical results obtained for thorium with the available experimental data.

Tungsten (W) is planned to be used as a plasma wall material in future tokamaks, such as ITER and DEMO. Therefore, a detailed analysis of its thermonuclear plasma spectra, the impurities within it, and knowledge of the large number of its free-ion spectroscopic parameters are needed. For this purpose it is important to perform a comprehensive theoretical modeling of the atomic structure of various tungsten ions. Such ions, having simple electronic configurations of open shells (up to highly ionized atoms), have been studied both experimentally and theoretically fairly completely, but this is not the case for ions, having an open f shell. It has been extremely difficult or even impossible to perform such calculations for tungsten ions with its open f shell owing to the large number of atomic states. In this project we got the results of the large-scale multiconfiguration calculations of the energetically lowest  $W^{24+}$  configurations, demonstrating the feasibility of such studies.

### **Projects Supported by Research Council of Lithuania**

Project: Experimental and Theoretical Investigation of Electron-Impact Excited Complex Atoms and Ions. Dr. A. Kupliauskienė. 2009 04 01 - 2010 12 31.

Project: Theoretical Investigation of the Cascades of Elementary Processes in Complex Atoms. Prof. R. Karazija. 2010 07 01 - 2011 12 31.

Project: Support for the International Conference on Atomic and Molecular Data and Their Applications. Dr. A. Kupliauskienė. 2010.

Project: COST MP0802. Self-assembled guanosine structures for molecular electronic device. Dr. J. Tamulienė. 2010.

Project: COST D35. Action D35: From Molecules to Molecular Devices: Control of Electronic, Photonic, Magnetic and Spintronic Behaviour. Dr. A. Tamulis. 2009-2011.

Project: COST CM0703. Systems Chemistry. Dr. A. Tamulis. 2010.

Students Summer Practice (supported by the EU structural funds): G. Medzevičius, supervisor – Dr. A. Tamulis, 2010; A. Šliogeris, supervisor – Dr. J. Tamulienė.

## **Projects Supported by Agency for International Science and Technology Development Programmes**

Project: *Contract of Association EURATOM – Lithuania for ITER*. Dr. A. Kupliauskienė. 2010.

## **International Science Programmes and Projects**

EU FP7 project: *Contract of Association EURATOM - Lithuania*. Dr. A. Kupliauskienė. 2008–2013.

EU FP7 project: ADAS for Fusion in Europe (ADAS-EU). Dr. A. Kupliauskienė. 2010–2012.

## **Other Projects**

Erasmus/Mundus project (Malmö university (Sweden)) Habil. Dr. G. Gaigalas. 2006-2010

VISBI project „Computational atomic structure with applications to astronomy and plasma physics (Sweden, Lithuania and Poland) “Habil. Dr. G. Gaigalas. 2010-2013.

## **COOPERATION**

University of Strathclyde, Glasgow (UK)

Lund University (Sweden)

Universite Pierre et Marie Curie (Paris, France)

Joint European Torus, Culham (UK)

Institute of Electron Physics of Ukraine Academy of Sciences, Uzhgorod (Ukraine)

University of Kentucky, Lexington (USA)

Queen's University, Belfast (UK)

University College London, London (UK)

Royal Observatory of Belgium, Brussels (Belgium)

Nature Environment Society, Malmö University, Malmö (Sweden)

Chimie Quantique et Photophysique, Université Libre de Bruxelles (Belgium)

National Institute of Standards and Technology (USA)

Instytut Fizyki imienia Mariana Smoluchowskiego, Uniwersytet Jagielloński (Poland)

College of Physics and Electronic Engineering, Northwest Normal University, Lanzhou (People's Republic of China)

## **OTHER SCIENTIFIC ACTIVITIES**

**Prof. P. Bogdanovičius** –

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”;
- Head of Lithuanian Physics Olympiad Team.

**Prof. G. Gaigalas** –

- chief of the Department of General Physics of the Vilnius Pedagogical University;

- member of the group of expert evaluation of curriculum in physics at Lithuanian center for quality assessment in higher education;
- chairman of the joint committee of doctoral studies between the Vilnius University; Institute of Theoretical Physics and Astronomy and the Vilnius Pedagogical University;
- secretary of the Senate of Vilnius pedagogical University;
- editorial board member of the Lithuanian Journal of Physics.

**Prof. R. Karazija –**

- editorial board member of the journal “Lithuanian Journal of Physics”;
- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”;
- Member of the Lithuanian Academy of Sciences.

**Prof. Z. R. Rudzikas –**

- chair of International Program Committee of Seventh International Conference “Atomic Molecular Data and Their Applications”;
- member of the European Economic and Social Committee;
- member of the European Research Council PE2 Panel;
- member of the Academia Europae;
- member of the Lithuanian Academy of sciences.

**Dr. A. Bernotas –**

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”

**Dr. V. Jonauskas –**

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”;
- secretary of the board of the Institute of Theoretical Physics and Astronomy, Vilnius University.

**Dr. R. Kisielius –**

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”.

**Dr. A. Kynienė –**

- President of the Vilnius city board's of the Physics Teachers' Association;
- member of Vilnius city Physics methodical board.

**Dr. R. Kivilšienė –**

- Board member of Group History of Physics (HoP) of the European Physical Society (EPS).

**Dr. A. Kupliauskienė –**

- expert of Europe Commission FP6, FP7 RTN (Research Training Networks) and Human Resources and Mobility;
- chair of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”;
- head of the board of Association “BASNET Forumas”.

**Dr. O. Rancova** –

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”.

**Dr. J. Tamulienė** –

- member of LOC of Seventh International Conference “Atomic and Molecular Data and Their Applications”;
- member of Management committee of Lithuanian Physics Society.

## DEPARTMENT OF THE THEORY OF NUCLEUS

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**Head** – Prof. Dr. (HP) *Egidijus Norvaišas*

### **STAFF**

**Senior Researchers:** Dr. A. Juodagalvis, Prof. Dr. (HP) E. Norvaišas.

**Researchers:** Doc. Dr. A. Acus, Dr. D. Jurčiukonis, Dr. V. Šimonis, Dr. K. Tamošiūnas.

**Doctoral students:** V. Regelskis, T. Sabonis.

### **RESEARCH INTERESTS**

Development of algebraic techniques for nuclear and particle physics.

Investigation of symmetries in nuclear and particle physics.

Development of topological soliton model.

Investigation of electroweak vector bosons in  $pp$  collisions.

Investigation of lepton-nucleus interactions in the supernova matter.

### **RESEARCH PROJECTS CARRIED OUT IN 2010**

#### **Project Supported by University Budget**

**Investigation of Subatomic Systems and Their Dynamics by the Methods of Group Theory and Topology.** Prof. Dr. E. Norvaišas. 2006-2010.

The classical two dimensional Skyrme model solutions are not stable without a symmetry breaking term. The canonical quantization procedure stabilized the baby skyrmions (solutions

of the two dimensional model) due to the appearance of a negative quantum mass correction. The skyrmions with a non zero angular momenta were studied. In particular, heavy baryons were studied as skyrmions in the Callan – Klebanov approach. The pionic degrees of freedom were canonically quantized and the degree of freedom connected to the  $K$  or charmed mesons were quantized semiclassically. The  $SU(2)$  Skyrme model was modified for the  $SU(2) \times SU(2)$  group, and a skyrmion with a different spin and isospin was established.

Work on nuclear input for supernova simulations was continued. Electron capture rates on nuclei in the hot medium of exploding stars have been calculated and published. A hybrid approach has been employed as there is no nuclear model that would be both feasible and reliably predict the nuclear spectra. The improved estimates of the electron capture rates on around 3000 nuclei were calculated and averaged over the relevant matter conditions. This data would improve the estimation of the matter deleptonization and the spectra of the emitted neutrinos in the modeling of the core-collapse supernovae. A similar rate table for the inelastic neutrino scattering by nuclei is foreseen.

### **Projects Supported from EU Structural Funds**

Science for Business and Society. V. Daniūnas. 2009–2011.

### **Other Projects**

**Collaboration agreement between CERN and Lithuanian Academy of Science.** Dr. A. Juodagalvis, Dr. K. Tamošiūnas, T. Sabonis, since 2006.

Collaboration with CERN was continued, although due to the lack of funding a reduction in activities is observed. A major part of contribution to the CMS data analysis was related to the work of the CMS Electroweak analysis group. The Drell-Yan analysis subgroup has been joined at the end of the year. The process of the quark-antiquark pair annihilation into a pair of an electron and a positron constitutes an identifiable background for other reactions. The main effort at the institute over the year was to increase the manpower by educating prospect scientists. Several students have defended their theses and/or course works on the CMS topics, related to the analysis of data from proton-proton collisions. Funding for a postdoctoral position was obtained. The collaboration with the CMS Heavy ion group was also pursued.

### **COOPERATION**

Helsinki Institute of Physics (Finland)

School of Theoretical Physics, Trinity College Dublin (Ireland)

GSI Helmholtzzentrum (Darmstadt, Germany)

Oak Ridge National Laboratory (Tennessee, USA)

Department of Mathematics, University of York (UK)

## ***OTHER SCIENTIFIC ACTIVITIES***

### **Prof. E. Norvaišas –**

- Referee of the European Research Council PE2 Panel
- Member of the Institute of Physics (UK)

### **Dr. K. Tamošiūnas –**

- Referee of the European Research Council PE2 Panel

## **DEPARTMENT OF THE THEORY OF PROCESSES AND STRUCTURES**

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**Head** - Prof. Habil. Dr. *Bronislovas Kaulakys*

### ***STAFF***

**Chief Researchers:** Prof. Dr. Habil. B. Kaulakys, Prof. Dr. Habil. P. Serapinas, Dr. Habil. G. Juzeliūnas, Dr. Habil. V. Gineitytė, Dr. (HP) V. Gontis.

**Senior researchers:** Dr. G. Vektaris, Dr. J. Ruseckas (part-time).

**Post-doctoral fellows:** Dr. V. Kudriašov, Dr. A. Mekys, Dr. J. Ruseckas.

**Research fellows:** Dr. M. Alaburda, Dr. A. Vektarienė, Dr. V. Pyragas (part-time).

**Junior research fellow:** Ž. Ežerinskis (part-time).

**Engineers:** A. Kononovičius (part-time).

**Technician:** S. Grubinskas (part-time).

**Doctoral students:** Ž. Ežerinskis

### ***RESEARCH INTERESTS***

Quantum Chemistry

Quantum Optics

Bose-Einstein Condensates

Spectroscopy, Phase Transitions

Condensed Molecular Structures

Econophysics and Physics of Finance

Fluctuations and Noise, Theory of 1/f noise

Optical and Kinetic Properties of Cold Atoms

## **RESEARCH PROJECTS CARRIED OUT IN 2010**

### **Projects Supported by University Budget**

#### **Optical Properties of Cold Atoms and Condensed Structures: Development of the Theory**, Habil. Dr. G. Juzeliūnas, 1995-2010.

A theory was developed describing the slow polaritons containing the orbital angular momentum. A method was proposed and considered enabling to produce for cold atoms the spin-orbit coupling for the spin 1 case.

An analytical description of  $\pi$  electrons of a finite-size bilayer graphene was developed within a framework of the tight-binding model. The formalism was applied to analyze the dispersion relations, the density of states and the conductance quantization. Theory of relative stabilities of conjugated hydrocarbons was investigated in terms of topological matrices of direct and indirect interorbital interactions. The harmonic vibrational frequencies of benzofused thieno[3,2-b]furans were calculated using the density functional theory methods. The calculated harmonic vibrational frequencies are consistent with the experimental IR spectra. Investigation of the methylsulfenyl chloride addition to propene was performed employing ab-initio calculations. The most probable stepwise reaction mechanism was proposed for this reaction. NMR spectra of the modeled non-canonical basis pairs were obtained. Quantum mechanical investigations of self-assembly of minimal artificial cells based on electron correlation effects and processes of photosynthesis were performed. Electron charge and spin density transfer in the molecular logical devices controlling artificial living cells were investigated.

#### **Power-laws and $1/f$ Fluctuations in Dynamical Chaotic and Stochastic Systems**. Prof. B. Kaulakys. 1995-2010.

A class of the nonlinear stochastic differential equations, giving the power-law behavior of the power spectral density in any desirably wide range of frequency is considered. Such equations were obtained starting from the point process models of  $1/f^\beta$  noise. The power-law behavior of spectrum is derived directly from the stochastic differential equations, without using the point process models. The analysis reveals that the power spectrum may be represented as a sum of the Lorentzian spectra. Such a derivation provides additional justification of equations, expands the class of equations generating  $1/f^\beta$  noise, and provides further insights into the origin of  $1/f^\beta$  noise.

A nonlinear stochastic differential equation which mimics the probability density function of the return and the power spectrum of the absolute return in financial markets is presented. Absolute return as a measure of market volatility is considered in the proposed model as a long-range memory stochastic variable. The nonlinear stochastic differential equation is obtained from the analogy with an earlier proposed model of trading activity in the financial markets and generalized within the nonextensive (Tsallis) statistical mechanics framework. The proposed stochastic model generates time series of the return with two power law statistics, i.e., the probability density function and the power spectral density, reproducing the empirical data for the one-minute trading return in the NYSE.

## **Projects, Programmes, Issues Supported by the Research Council of Lithuania (LMT)**

Light-induced gauge potentials in ultra-cold atoms, Gilibert / LMT grant no. TAP-44/2010-LMT and TAP-17/2010-LMT. Habil. Dr. G. Juzeliūnas. 2009 – 2010.

Electronic, Transport and Electromagnetic Properties of Graphene Layers and Nanoribbons. Visby / LMT research group grant no. MIP-123/2010-LMT. Habil. Dr. G. Juzeliūnas. 2010-2011.

Propagation and storing of light in atomic gases. LMT postoc grant for A. Mekys, grant no. MOS-2/2010-LMT. Habil. Dr. G. Juzeliūnas. 2008-2010.

Dynamics and control of slow and stationary polaritons. LMT postoc grant for V. Kudriašovas, grant no. MOS-13/2010-LMT. Habil. Dr. G. Juzeliūnas. 2009-2011.

Multicomponent slow polaritons in cold atomic gases. LMT postoc grant for J. Ruseckas, grant no. VP1-3.1- ŠMM-01-V-01-001. Habil. Dr. G. Juzeliūnas. 2009-2011.

## **International Science Programmes and Projects**

EU FP7 Project: Nanodesigning of atomic and molecular quantum matter - enlarged European Union. Habil. Dr. G. Juzeliūnas. 2010-2012.

COST Action: D37 Grid Computing in Chemistry: GRIDCHEM. Dr. A. Vektarienė and G. Vektaris. 2006-2010.

COST Action: MP 0801 Physics of Competition and Conflicts. Prof. B. Kaulakys and Habil. Dr. V. Gontis. 2009-2012.

## **Projects Supported from EU Structural Funds**

Science for Business and Society. V. Daniūnas. 2009–2011.

## **COOPERATION**

Technische Universität Kaiserslautern and Leibniz Universität Hannover (Germany),  
ICREA and ICFO (Spain),  
San Diego University (USA)  
National Institute of Standards and Technology (USA)  
Heriot-Watt University (UK)  
University of Strathclyde, Glasgow (UK)  
Linköping University (Sweden)  
CNRS Paris (France).

## **OTHER SCIENTIFIC ACTIVITIES**

**Prof. B. Kaulakys**, <http://www.itpa.lt/kaulakys/> –

- member of the Institute of Physics (UK);
- editorial board member of the Lithuanian Journal of Physics;
- editorial board member of the Journal Nonlinear Analysis. Modeling and Control;

- vice-president of the Lithuanian Association of Nonlinear Analysts;
- member of the council of the Lithuanian Scientific Society;
- member of the organization and program committee of the Humboldt Forum on Science and Society in Modern Europe, Vilnius, 23-26 September 2010.

**Habil. Dr. G. Juzeliūnas**, <http://www.itpa.lt/~gj> –

- Vilnius University Rector's science award (2010);
- Member of the Institute of Physics (UK);
- chairman of the Organization and program committee of the Humboldt Forum on Science and Society in Modern Europe, Vilnius, 23-26 September 2010;
- member of the Program committee of the 12-th International Conference-School on Advanced Materials and Technologies, Palanga, 27-31 August 2010.

**Prof. P. Serapinas** –

- chairman of the National Committee on Accreditation of Chemical Laboratories;
- member of the Technical Committee on Standardization in Chemical Analysis;
- expert of ISO REMCO.

**Habil. Dr. V. Gontis**, <http://gontis.eu> –

- vice-president of the Lithuanian Scientific Society;
- director of the Institute of Lithuanian Scientific Society;
- member of the association Euroscience <http://www.euroscience.org/>

**Dr. J. Ruseckas**, <http://www.itpa.lt/~ruseckas> –

- Vilnius University Rector's science award for young researchers (2010);
- member of the Organization and program committee of the Humboldt Forum on Science and Society in Modern Europe, Vilnius, 23-26 September 2010.

## PLANETARIUM

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**Director** – *Danutė Sperauskienė*

### STAFF

**Lecturers:** N. Kochanskas, D. Matulytė, D. Sperauskienė

**Engineer:** D. Meshalkin

**Booking-clerk:** A. Kvaraciejienė

**Photographer:** D. Janavičius (part-time).

## **Projects Supported by FP7**

Researchers' Night 2010 V. Lapinskaitė, 2010.

### *EVENTS*

The largest event was a part of the „Researchers' Night 2010“ project supported by FP7. It included the introductory ceremony on September 21-st and the event itself on September 24-th. The event attracted more than 300 visitors.

Among other events organized for the wide public it should be mentioned „The Earth Day“ (March 20), the 20-th anniversary of the Hubble telescope (April 22), exhibition of paintings by the artist I. Ercmonaitė (August-December).

Altogether 600 lectures were offered to the visitors of the Planetarium. More than 26 000 people attended Planetarium during 2010.