INSTITUTE OF THEORETICAL PHYSICS AND ASTRONOMY

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Director - Dr. Habil. *Gražina Tautvaišienė*

59 research fellows and 7 emeritus and affiliated scientists (13 habilitated doctors, 3 doctors with the habilitation procedure, 34 doctors) and 17 doctoral students. Full staff comprises 93 people.

MAIN RESEARCH AREAS OF THE INSTITUTE

Structure and evolution of galaxies, stars, and interstellar matter

Physics of atoms, molecules and condensed matter

New materials, nano-structures and surfaces: synthesis, characterization, technologies

DOCTORAL DISSERTATIONS MAINTAINED IN 2012

Š. Mikolaitis “Evolutionary effects of chemical composition in red giants of open clusters”.

CONFERENCES AND SEMINARS ORGANIZED IN 2012

VISBY International seminar **“On the Theory of Atoms”**, May 21-25, 2012, Vilnius.

Nordic-Baltic research school **“Observational Stellar Astrophysics in the Era of Gaia and Kepler Space Mission”**, July 28 – August 11, 2012, Moletai Astronomical Observatory.

International conference **"Promoting Gender Equality in Science"**, November 20, 2012, Vilnius.

Prof. A. Jucys Readings, September 13, 2012, Vilnius.

ASTRONOMICAL OBSERVATORY

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Head – Habil. Dr. *Gražina Tautvaišienė*

STAFF

Chief Researchers: Dr. Habil. G. Tautvaišienė, Dr. K. Černis, Prof. Emeritus Dr. Habil. V. Straižys, Prof. Dr. Habil. A. Bartkevičius (affiliated), Dr. Habil. K. Zdanavičius (affiliated).

Senior Researchers: Dr. R. Janulis, Dr. A. Kazlauskas, Dr. A. Kučinskas, Dr. E. Pakštienė, Dr. J. Zdanavičius

Researchers: Dr. Y. Chorniy, Dr. V. Laugalys, Dr. E. Puzeras.

Junior Researchers: G. Barisevičius (part time), A. Černiauskas (part time), A. Ivanauskas (part time), M. Maskoliūnas (part time), Dr. Š. Mikolaitis, D. Prakapavičius (part-time), E. Stonkutė (part time), R. Ženovienė (part time).

Doctoral students: G. Barisevičius, V. Čepas, A. Drazdauskas, J. Klevas, M. Macijauskas, M. Maskoliūnas, K. Milašius, D. Prakapavičius, E. Stonkutė, R. Ženovienė.

Lecturers: S. Lovčikas, M. Masaitis.

Engineers: A. Drazdauskas (part time), J. Klevas (part time), M. Macijauskas (part time), Š. Mikolaitis (part-time), G. Valiauga.

Technicians: R. Chmieliauskaitė (part-time).

Administrator: V. Kakarienė.

Manager: 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 2012

Project Supported by University Budget

Characteristics of atmospheric chemical composition and asteroseismic activity of stars and chemical evolution of galaxies. **Dr.** Habil. **G. Tautvaišienė. 2011–2015.**

Main atmospheric parameters, carbon, nitrogen and oxygen abundances, and carbon ratios were determined in a sample of 28 Galactic red clump stars. The mean abundances of C, N and O abundances in the investigated clump stars support our previous estimations that, compared to the Sun and dwarf stars of the Galactic disc, carbon is depleted by about 0.2 dex, nitrogen is enhanced by 0.2 dex and oxygen is close to abundances in dwarfs. The $^{12}C/^{13}C$ and C/N ratios for galactic red clump stars analysed were compared to the evolutionary models of extra-mixing. The steeper drop of $^{12}C/^{13}C$ ratio in the model of thermohaline mixing by Charbonnel & Lagarde better reflects the observational data at low stellar masses than the more shallow model of cool bottom processing by Boothroyd & Sackmann. For stars of about 2 M_{Sun} masses a modelling of rotationally induced mixing should be considered with rotation of about 250 km s^{-1} at the time when a star was at the hydrogen-core-burning stage.

Abundances of ^{12}C, ^{13}C, N, and O in evolved stars of two open clusters Cr 261 and NGC 6253 were determined. The average value of 12C/13C isotope ratios of Cr 261 is equal to 18 ± 2 in four giants and to 12 ± 1 in two clump stars; it is equal to 16 ± 1 in four clump stars of the open cluster NGC 6253. The mean C/N ratios in Cr 261 and NGC 6253 are equal to 1.67 ± 0.06 and 1.37 ± 0.09, respectively. The $^{12}C/^{13}C$ and C/N values in Cr 261 and NGC 6253 within limits of uncertainties agree with the theoretical model of thermohaline-induced mixing as well as with the cool-bottom processing model.

Detailed analysis of two kinematic groups of F- and G- type stars was in progress. Our results indicate that the samples of investigated stars are chemically homogeneous and the abundances of oxygen, alpha and *r*-process elements are overabundant in comparison with Galactic disk dwarfs. Pulsations modes of the variable star WD PG2303+243 were identified using periodicity analysis of period spacing of pulsations observed in 2004 and 2005.

An observational mini campaign for observations of the variable WD PG2303+243 was organized in October of 2012. The duration of observations was around one week; length of observed light curves - 55.88 h, total duty cycle is around 32 %. The observed images and light curves were reduced and prepared for spectral analysis of pulsations.

A program for wavelet analysis *Wavefinder* was improved and light curves of eight variable subdwarfs B were analyzed. A paper on one of them (KIC 10139564) was prepared and published (2012MNRAS.424.2686).

In cooperation with astronomer F. Mukadam (USA) observations of three candidates of variable white dwarfs were organized with the VATT telescope (USA) in November of 2012 (observers V. Laugalys and R.P. Boyle). Three light curves of 2.5 h for each of the stars were observed. Light curves were reduced and analyzed. No signs of pulsations were found.

Star formation and dust clouds in the Orion and Perseus arms of the Galaxy Prof. V. Straižys. 2011–2015

Interstellar extinction has been investigated in the direction of two open clusters (NGC 7129 and NGC 7142) in Cepheus and in two areas near the Perseus and Camelopardalis border, containing a bubble of dark clouds discovered in our earlier investigations.

The open cluster IC 1805 in the Cas OB6 association and a young open cluster M29 in Cygnus were investigated. The distance, age and interstellar extinction of the clusters were determined using the results of multicolor photometry and classification of stars. Many new young stellar objects were discovered.

CCD observations in the Vilnius 7-color system were obtained for about 10 new Milky Way areas and open clusters for the future investigations of interstellar extinction and cluster parameters.

Positional Astrometry of Unusual Asteroids and Comets. Dr. K. Černis. 2011–2015.

71 new asteroids have been discovered in 2012 (6 asteroids at the Molėtai Astronomical Observatory). Among them there were 4 unusual objects: Koiper belt asteroid (TNO object) 2012 BX85, two Centaur objects (2012 DS85, 2012 VU85) and NEO Amor type asteroid 2012 XH16. The TNO object 2012 BX85 is 400 km in diameter, it is the largest object discovered in the Solar system in 2012. New Centaurs objects have diameters of about 60-180 km. Up to now more than 470 asteroids are discovered by K. Černis and the collaborators. The main attention now is paid to the refinement and analysis of the orbits and properties of asteroids and comets discovered previously. The asteroids 2004 TL347, 2004 TP16, 2005 TC49, 2006 SP197, 2006 SE368, 2006 SS290, 2008 QY32, 2008 JQ8, 2008 JS8, 2008 JN8, 2008 QX32, 2009 SS148, 2009 SS17, 2009 SR148, 2009 CH2, 2009 SL98 and comets C/2012 S1 (ISON), C/2010 R1 (LINEAR), C/2009 P1 (Garradd), 168P/ Hergenrother, 260P/McNaught, C/2012 J1 (Catalina), C/ 2010 S1 (LINEAR) ir C/2006 S3 (LONEOS) have been observed at the Molėtai Astronomical Observatory and other observatories.

An orbit of the NEO asteroid 2010 BT3 discovered in Moletai Observatory, combined with its apparent brightness, gives the absolute magnitude 21.34 mag and the diameter between 160 m and 360 m, taking albedos of S-type and C-type asteroids, respectively. Photometry of the asteroid 2010 BT3 and a following analysis of the light curves enabled us to determine the period of the asteroid‘s rotation. A probable rotation period of the asteroid seems to be 54 min., with an amplitude 0.108 mag.

Analysis of the orbit of the Centaur group asteroid 2012 DS85 over past 400 years has been carried out. Calculations show that our asteroid has no close approaches with planets. Only some approaches to Saturn are found but they are not closer than 8 AU. Orbital elements of Centaur change only in small ranges. This means that 2012 DS85 moves in a stable orbit. The orbit of the asteroid gives the absolute magnitude 9.43 and the diameter of about 61 km, taking an albedo value of 0.08.

5 asteroids with well defined orbits were named: Maironis (Nr. 252794), Vytautas (321324), Kazlauskas (184096), Bartašiūtė (212587) and Alytus (233661).

The asteroid project together with the Vatican Observatory has been carried out. During the search for new asteroids with the 1.8 m reflector at Mount Graham Observatory 64 asteroids have been discovered.

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) one new asteroid 2012 GA2 was discovered. Astronomical observations were performed with the Schmidt telescope (0.80/1.20 m, f/3.5) of the Baldone Observatory.

Projects Supported by Research Council of Lithuania

Galactic globular clusters – indicators of chemical evolution of the early Universe

Dr. A. Kučinskas. 2011–2012.

Postdoctoral research **“Investigation of brightness variations of YSOs (Young Stellar Objects)”** (Dr. V. Laugalys), scientific supervisor Dr. R. Janulis. 2011–2012.

Projects Supported by FP7

Nordic-Baltic research school **“Observational Stellar Astrophysics in the Era of Gaia and Kepler Space Missions”,** Dr. Habil. G. Tautvaišienė. 2012.

Researchers’ Night in Lithuania 2012 (Night2012**).** Dr. A. Kazlauskas. 2012.

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, Dr. Š. Mikolaitis.

International project **Gaia-ESO Spectroscopic Survey** (2011 – 2016)**.** Dr. Habil. G. Tautvaišienė, Dr. Š. Mikolaitis, Dr. E. Puzeras, Dr. Y. Chorniy, G. Barisevičius, A. Drazdauskas.

Kepler Asteroseismic Science Consorcium. Dr. R. Janulis, Dr. E. Pakštienė.

EVENTS

The Nordic Baltic research school **“Observational Stellar Astrophysics in the Era of Gaia and Kepler Space Missions”** took place on July 28 – August 11, 2012 at the Molėtai Astronomical Observatory. 25 PhD students from 15 European countries attended the school. They have studied methods of observations of stellar and galactic spectra, learned to use modern techni**ques and interpreted the results of observations. The observations were carried out with two telescopes at Molėtai Observatory (165 cm and 35/51 cm Maksutov) and with the 2.5 m Nordic Optical Telescope at La Palma, Canary Islands. The later one was remotely controlled from MAO. The coordinator of the school G. Tautvaišienė (Vilnius University, Lithuania) headed the international team of tutors: T. Bedding (Australia),** L. Buchhave (Denmark), F. Grundahl (Denmark), U. Heiter (Sweden), Ch. Karoff (Denmark), H. Kjeldsen (Denmark), A. Korn (Sweden), R. Ostensen (Belgium), K. Smith (Germany), E. Stempels (Sweden), R. Janulis, **E. Pakštienė (all VU). They gave the lectures and guided the students in real research projects, which results will be published in scientific journals.**

The big event for wide public was organized at the Molėtai Astronomical Observatory (MAO) on September 28. It was held within the framework of the FP7 project **Researchers’ night 2012**. All staff of the AO was involved in the preparation and performance of this event. More than 800 people from all regions of Lithuania listened to the lectures of astronomers and physicists, attended professional telescopes.

Among other events at MAO two nights of equinox-music *etc*. should be mentioned.

Altogether 341 groups (about 7000 people) visited the Observatory during the year.

MAIN PUBLICATIONS

COOPERATION

Astrophysical Institute Potsdam (Germany)

Bologna Observatory (Italy)

Copenhagen University (Denmark)

Kiepenheuer Institut fur 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 the Board of Directors of the international journal *Astronomy & Astrophysics*.

Prof. V. Straižys –

- 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);
- member of the European Astronomical Society.

Dr. *Habil. G. Tautvaišienė* –

- vicepresident of Lithuanian Physics Society;
- reviewer of the European Science Foundation, 2010-2012;
- member and national representative at the International Astronomical Union (IAU);
- board member of the IAU Division *Optical & Infrared Techniques*;
- secretary of Astrophysics Commission at the International Union of Pure and Applied Physics;
- executive board member of the international *Astronet* project;
- member of scientific working group *Reference Stars* of GAIA Space Observatory (ESA);
- founding member of the European Astronomical Society;
- editorial board member of the journal *Baltic Astronomy*;
- editor-in-chief of the annual astronomical almanac *Lietuvos dangus* (*Sky of Lithuania*).

DEPARTMENT OF THE THEORY OF ATOM

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Chief Researchers: Prof. Dr. Habil. P. Bogdanovičius, Prof. Dr . Habil. R. Karazija (affiliated), Dr. A. Kupliauskienė, Prof. Dr. Habil. G. Gaigalas (part-time)
Senior Researchers: Dr. V. Jonauskas, Dr. R. Karpuškienė, Dr. R. Kisielius, Dr. R. Kivilšienė, Dr. S. Kučas, Dr. G. Merkelis, Dr. A. Tamulis, Dr. J. Tamulienė.
Researchers: Dr. R. Juršėnas, Doc. Dr. A. Kynienė, Dr. A. Momkauskaitė.
Junior Researchers: Š. Masys (part-time).
Technician: G. Kerevičius.
Doctoral students: Š. Masys, A. Šliogeris, L.Radžiūtė.

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 modelling of self-assembly of minimal living cells and quantum processes of photosynthesis in artificial living organisms

History of physics

RESEARCH PROJECTS CARRIED OUT IN 2012

Project Supported by University Budget

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

Theoretical study of energy levels, radiative transition probabilities, and electron impact excitation rates in the distorted wave approximation has been performed using Dirac-Fock-Slater method for W^{25+} ion. Spectra corresponding to coronal approximation, collisional radiative model, and radiative cascade have been investigated. It was suggested that collisional radiative model has to be supplemented by radiative cascade having an aim to heighten some lines which can be identified in electron beam ion trap (EBIT) spectra. Radiative cascade has to be taken into account because ions interact with electrons only in electron beam but not outside it. Trajectory of ions in the trap is determined by Coulomb force and impact with electrons. Coulomb force directed towards electrons attracts ions to the beam while impact with electrons pushes them from the electron beam. Trapped ions interact with electrons in the beam region but due to cycloidal orbits the ions can spend part of their time outside the electron beam. Radiative cascade has to start when interaction with electrons ends. This effect is more important for ions in the lower or medium charge states.

$4f^{13}\ 5s\ 5p - 4f^{13}\ 5s^2$ transitions have been investigated in W^{13+} ion using Dirac-Fock method with extended basis of interacting configurations. Identification of spectral lines observed in EBIT plasma is proposed.

Geometry optimization for various crystalline structures and elastic properties of $SrRuO_3$ crystal have been investigated using ordinary and modified methods of density functional theory (DFT) implemented in quantum chemistry package CRYSTAL09. The obtained results extend our knowledge about elastic properties of $SrRuO_3$ crystal and features used in DFT methods.

Development and Applications of Relativistic Theory for Many-electron Atoms. Prof. G. Gaigalas. 2009–2014.

Energies, lifetimes, and wave-function compositions have been computed for all levels of $4p^64d$, $4p^64f$, and $4p^54d^2$ using single and double excitations from a multireference set (SD-MR) to generate expansions for the multiconfiguration Dirac-Hartree-Fock (MCDHF) approximation. An extended version of the general relativistic atomic structure package, GRASP2K, was used to deal with configuration state functions with as many as six open shells and with configurations containing as many as three f electrons. E1, E2, M1 transition probabilities are reported for transitions between the levels as supplemental material. Results are compared with other theory and with experiment, when available.

It was recently shown that dielectronic recombination measurements can be used for accurately inferring changes in the nuclear mean-square charge radii of highly charged lithium like neodymium [Brandau *et al.*, Phys. Rev. Lett. 100, 073201 (2008)]. To make use of this method to derive information about the nuclear charge distribution for other elements and

isotopes, accurate electronic isotope shift parameters are required. We calculated and discussed the relativistic mass- and field-shift factors for the two $2s\,^2S_{1/2}$ - $2p\,^2P^o_{1/2,3/2}$ transitions along the lithium isoelectronic sequence. Based on the multiconfiguration Dirac-Hartree-Fock method, the electron correlation and the Breit interaction are taken into account systematically. The analysis of the isotope shifts for these two transitions along the isoelectronic sequence demonstrates the importance and competition between the mass shifts and the field shifts.

Energy structure calculations for W^{+8} in Dirac-Fock and Dirac-Fock-Sleter approximations using extended interacting configuration basis were performed.

Investigation of the spectroscopic characteristics of complex toms and their derivatives. Dr. A. Kupliauskienė. 2012–2017.

The spectral parameters of S II ion were studied in a collaborative research with astrophysicists from USA. The electron-impact excitation of the 2s - 2p transition in Fe^{21+} ions was investigated. The influence of the magnetic quadrupole M2 and electric octupole E3 transitions from the excited $4p^54d^{N+1}$ + $4p^64d^{N-1}4f$ configurations on the ground configuration $4p^64d^N$ was explored along the extended isoelectronic sequences for the ions with different number of electrons in 4d shell. It was demonstrated that an inclusion of such „unusual“ transitions could lead to a substantial decrease of the radiative lifetimes for the levels which have no electric dipole E1 transitions to the ground configuration but have the E2 and M1 transitions within the levels of excited configurations. Our determined electron-impact excitation cross-sections for light atoms agree very well with those from the NIST database.

The results of detailed level-by-level calculations of cascades after K vacancy production are presented for the astrophysically important elements Ne, Mg, Si, S and Ar. The populations of excited levels after Auger transitions as well as the distribution of ions in the final configurations and levels after cascade are presented. These results enable us to take into account such process for the modeling of highly charged ions production in the vicinity of cosmic x-ray sources. The dependence of cascade on the many-electron quantum numbers for ions with an open shell is investigated for the first time.

The identification of the measured ejected-electron spectra from the autoionizing states $4p^5nln'l'$ LSJ of Rb excited by 30 eV and 400 eV electrons was performed for the first time by using excitation energies, excitation cross sections and autoionization probabilities calculated in relativistic Dirack-Fock-Slater approximation.

The self-assembly and emergence of protocells complex systems consisting up to 650 atoms were modelled by time dependent density functional theory (TD-DFT) quantum mechanical methods including electron correlations. Phenomenon of quantum entanglement in a system composed of two minimal protocells was discovered using these TD-DFT methods. The quantum entanglement molecular logic gates and devices controlling the photosynthesis were modelled in separate artificial cells and in the system composed of two minimal protocells. Neutral radical molecules were used for modelling of safe artificial cells living forms performing photosynthesis only in one direction external magnetic fields.

Results of quantum mechanical investigations performed allowed us to obtain new stable nano-diamonds that are not mentioned in scientific literature. We showed that L, DL and D-alanine fragmentation due to low-energy-electron impact is different. Additionally new alanine fragmentation reactions are suggested and confirmed.

In the open-shell Rayleigh-Schrodinger PT approach, the SU(2)-invariant terms of the 2nd order wave operator have been established with the help of NCoperators, the symbolic programming package written on Mathematica. Obtained symbolic preparation of terms is convenient to implement it in the computer codes. Also, the three-body Schrodinger operator

in the space of L^2-functions has been considered. It was shown that the operator is a certain extension of operators which generate the exponential unitary group containing a subgroup with nilpotent Lie algebra. As a result, the solutions to the three-body Schrodinger equation with decaying potentials were shown to exist in the associated commutator subalgebras. For a particular Coulomb three-body system, the task is to solve – in these subalgebras – the radial Schrodinger equation in three dimensions. The obtained analytic results were applied to the helium atom and to the positronium negative ion.

Projects Supported by Research Council of Lithuania

European Social Fund under the Global Grant measure **"Establishing and development of atomic data base for astrophysical, technological and laboratory plasma modeling"**. Dr. Habil. P. Bogdanovičius. 2012–2015.

European Social Fund under the Global Grant measure **"Investigation of plasma spectra of tungsten ions"**. Dr. V. Jonauskas. 2012–2015.

International Science Programmes and Projects

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

EU FP7 project: **ADAS for Fusion in Europe** (ADAS-EU). Dr. Habil. P. Bogdanovičius. 2012.

Other Projects

Erasmus/Mundus project (Malmö university, Sweden) Dr. Habil. G. Gaigalas. 2006–2012.

VISBY project: **Computational Atomic Structure with Applications to Astronomy and Plasma Physics** (Sweden, Lithuania and Poland) Dr. Habil. G. Gaigalas. 2010–2013.

NSF (USA) project: **Collaborative Research: Spectral Diagnostics of Heavy Elements at High Redshift** (USA, Lithuania) Dr. R. Kisielius. 2012 – 2015.

MAIN PUBLICATIONS

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)

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 –

- Head of Lithuanian Physics' Olympiad Team.

Prof. G. Gaigalas –

- member of the Senat of Vilnius pedagogical University;
- member of the committee for research at Vilnius pedagogical University.
- member of the group of expert evaluation of curriculum in physics at Lithuanian Centre 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;

Prof. R. Karazija –

- editorial board member of the *Lithuanian Journal of Physics*;
- member of the Lithuanian Academy of Sciences.

Dr. V. Jonauskas –

- secretary of the board of the Institute of Theoretical Physics and Astronomy, Vilnius University.

Dr. A. Kynienė –

- President of the Vilnius City Board 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.

Dr. A. Kupliauskienė –

- expert of Europe Commission FP6, FP7 RTN (Research Training Networks) and Human Resources and Mobility;
- head of the board of Association "BASNET Forumas".

Dr. A. Tamulis –

- expert of the European Commission programme "Future and Emerging Technologies".

Dr. J. Tamulienė –

- management committee member of Lithuanian Physics Society.

DEPARTMENT OF THE THEORY OF NUCLEUS

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Chief Researchers: Dr. Habil. S. Ališauskas (affiliated).

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

Researchers: Dr. D. Jurčiukonis (part-time), Dr. V. Šimonis, Dr. K. Tamošiūnas.

Post-doctoral fellows: Dr. D. Jurčiukonis.

Junior research fellow: T. Sabonis (part-time).

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

The neutrino sector parametrization in the Standard model of the elementary particles

Investigation of lepton-nucleus interactions in the supernova matter

Structure of $N=Z$ nuclei

RESEARCH PROJECTS CARRIED OUT IN 2012

Project Supported by University Budget

Research of Subatomic Systems and Their Dynamics Applying Algebraic and Topology Methods. Prof. E. Norvaišas. 2011–2015.

The Faddeev-Skyrme mode**l was investigated.** Similarity between the Lagrangians of Faddeev-Skyrme and Skyrme models suggests that the rotational collective degrees of freedom of the Hopfions should be taken into account in quantization. The excitations of Hopfions with charges Q = 1 and 2 contribute to the kinetic energy of the configuration and strongly affect other properties of spinning Hopfions. A relationship between the nucleon-nucleon interaction and two topological SU(2) solitons was discovered in collaboration with dr. A. Deltuva (Lisbon university). The canonical quantization of the solitons allows **us to extract the long-range and spin-orbit components of the interaction, which originate from the orbital and rotational motion of the solitons. An expression for the spin-orbit and quadratic spin-orbit interaction components was derived. This approach treats baryons as topological solitons. If the semi-classical quantization is applied to the SU(3) topological soliton model, the calculated mass spectra differ from experimental data. The canonical quantization procedure changes the mass spectra of hyperons and ensures the stability of the quantum soliton. Different roles of symmetry** breaking and quantum correction terms at **the origin was elucidated. Physical parameters are evaluated for baryons using specific profile functions. These functions are calculated with respect to the energy functional of the quantum soliton with fixed quantum numbers.** One dimensional two component system with a self-focusing cubic nonlinearity of Bose-Einstein condensate was investigated. Evolution of the spontaneous symmetry scenarios in the system was studied, and symmetry types of solutions were classified.

The neutrino sector with the seesaw mechanism of type I was analyzed. The analysis was performed for two cases of a minimal extension of the Standard Model when one or two right-handed fields were added to three left-handed fields. Analytical expressions for three level and for one loop corrections were derived. Light neutrino masses were numerically evaluated as functions of the heavy neutrino masses. Parameters of the model were varied to find such light neutrino masses that are compatible with the experimental data of solar and atmospheric neutrino oscillations for normal and inverted hierarchy. The work on nuclear input for supernova simulations was continued. The rates of an electron capture by nuclei in the thermal environment of a collapsing massive star are of interest to researchers who model last stages of star evolution. The calculated tables of electron capture and the resulting neutrino emission rates were provided to several groups abroad. The properties of N=Z nuclei below Sn100 have been studied in collaboration with the researchers from Lund Institute of Technology (Sweden). The focus was on the differences in the properties of odd-odd, odd-even and even-even N=Z nuclei.

Collaboration with CERN was continued, mainly in connection to the Drell-Yan analysis (this subgroup has been joined at the end of the year 2010). The process of the quark-antiquark pair annihilation into a pair of an electron and a positron constitutes an identifiable background for other reactions. It is also a precision measurement, able to differentiate various

theoretical parton distribution functions in proton. The analysis was performed on 2011 data collected at the proton-proton collision energy of 7 GeV.

Dynamics of the heavy ion reactions at the energies of LHC were studied using relativistic hydrodynamic models. Azimuthal distribution of the particles before the collision was estimated using the CMS experiment data. Several dependencies of this distribution were studied, for example, the dependency of the second harmonics on the centrality of the ion-ion collision, and the dependency on the rapidity. Glauber Monte-Carlo approach was used to model the initial conditions of the collisions as well as the influence of fluctuations on the azimuthal distribution of particles.

Internet stream from CERN CMS experiment (CMS TV) was adapted to Lithuanian audience by translating presented information and providing additional explanations in Lithuanian. The page is accessible at www.mif.vu.lt/cern

International Science Programmes and Projects

Collaboration Agreement between CERN and Lithuanian Academy of Sciences. Dr. A. Juodagalvis, **Dr. D. Jurčiukonis, Dr. K. Tamošiūnas, T. Sabonis, since 2006.**

COST Action: **MP 1006 Fundamental Problems in Quantum Physics.** Coordinator Prof. E. Norvaišas. 2011–2014.

MAIN PUBLICATIONS

COOPERATION

Helsinki Institute of Physics (Finland)

GSI Helmholtzzentrum, Darmstadt (Germany)

Oak Ridge National Laboratory, Tennessee (USA)

Department of Mathematics, University of York (UK)

Lund Institute of Technology at Lund University, Lund (Sweden)

Nuclear Physics Center at Lisbon University (Portugal)

Technical Institute of Lisbon, Lisbon, (Portugal)

Federico Santa María Technical University, Valparaiso, (Chile)

Purdue University, West Lafayette, Indiana (USA)

University of Nebraska-Lincoln, Lincoln, Nebraska (USA)

European Organization for Nuclear Research CERN (Switzerland)

OTHER SCIENTIFIC ACTIVITIES

Prof. E. Norvaišas –

- member of the International Advisory Committee of Second European Nuclear Physics Conference
- member of the Institute of Physics (UK);

Dr. A. Juodagalvis –

- coordinator of the Standard Model Physics Data and Monte Carlo validation (SMP PdmV) effort at the CMS experiment at CERN
- referee in institutional review process of CMS publications

DEPARTMENT OF THE THEORY OF PROCESSES AND STRUCTURES

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Chief researchers: Prof. Dr. Habil. B. Kaulakys, Dr. Habil. G. Juzeliūnas, Dr. (HP) V. Gontis, Prof. Dr. (HP) E. Anisimovas (part-time), Prof. Dr. Habil. A. Matulis (part-time), Prof. Dr. Habil. P. Serapinas (affiliated).
Senior researchers: Dr. Habil. V. Gineitytė, Dr. G. Vektaris, Dr. J. Ruseckas, Doc. Dr. D. Šatkovskienė (affiliated).
Researchers: Dr. M. Alaburda, Dr. A. Vektarienė, Dr. A. Mekys (part-time), Dr. V. Kudriašovas (part-time).
Postdoctoral researchers: Dr. R. Juršėnas.-
Junior researchers: A. Kononovičius (part-time).
Engineers: R. Kazakevičius (part-time), T. Andrijauskas (part-time).
Doctoral students: A. Kononovičius, V. Juknevičius.

RESEARCH INTERESTS

Quantum optics and ultra-cold atoms
Bose-Einstein condensates

Quantum chemistry
Spectroscopy, phase transitions

Condensed molecular structures
Econophysics and physics of finance

Fluctuations and noise, theory of 1/f noise

RESEARCH PROJECTS CARRIED OUT IN 2012

Projects Supported by University Budget

Optical and Kinetic Properties of Cold Atoms and Condensed Molecular Structures. Habil. Dr. G. Juzeliūnas, 2011–2015.

A method has been described for creating a three-dimensional analogue to the Rashba spin-orbit coupling for ultra-cold atoms. This laser induced coupling makes use of the Raman transitions to link four internal atomic states with a tetrahedral geometry. The resulting atomic spectrum contains a Dirac point that is robust against environmental perturbations. For fermionic atoms such a spin-orbit coupling always gives rise to a molecular bound state. A method has been proposed and explored to produce a square optical lattice affected by a non-staggered magnetic flux. It is shown that such a lattice can be created using the Raman transitions induced by a set of properly chosen polarization-dependent standing waves propagating at a right angle and containing a time-phase difference. Regions have been identified where the non-zero magnetic flux produces a topologically non-trivial band structure for this lattice. A perturbative approach has been developed and applied to evaluate relative stabilities of separate Kekule valence structures of benzenoid hydrocarbons. Structural features favouring the formation of quinazolino[3,2-a][1,5]benzodiazepine derivatives have been investigated by means of the quantum chemical methods. A possible mechanism of this process was proposed and it was suggested that initiation of the heterocyclization reaction becomes possible after hydroxylamine intermediate is formed. It was demonstrated that the heterocyclization reaction is an internal molecular rearrangement strongly controlled by the frontier molecular orbitals, whereas the charges do not play a significant role for the reaction.

Theory and Applications of Processes in Complex Systems. Prof. B. Kaulakys. 2011–2015.

The nonlinear stochastic differential equations, generating processes with the q-exponential and q-Gaussian distributions of the observables, i.e. with the long-range power-law autocorrelations and $1/f^{\beta}$ power spectral density are presented. Similarly, the Tsallis q-distributions have been obtained in the superstatistical framework as a superposition of different local dynamics at different time intervals. In such approach, the average of the stochastic variable is generated by the nonlinear stochastic process, while the local distribution of the signal is exponential or Gaussian one, conditioned by the slow average. Further, the relevance of the generalized and adapted equations for modeling the financial processes is analyzed. The inter-trade durations, the trading activity and the normalized return using the superstatistical approaches with the exponential and normal distributions of the local signals driven by the nonlinear stochastic process are modeled.

Examples of agent-based and stochastic models of competition and business processes in economics and finance are presented. Start from simple models which have microscopic, agent-based versions and macroscopic treatment of behavio**ur the microscopic and macroscopic versions of the herding model proposed by Kirman and Bass for the new product diffusion are considered as two basic ideas. It is demonstrated that general herding behaviour can be considered as a background of the nonlinear stochastic model of the financial fluctuations.**

Projects, Programmes, Issues Supported by the Research Council of Lithuania

European Social Fund under the Global Grant measure **"Topological phenomena in cold-atom and condensed matter systems"**. Dr. Prof. E. Anisimovas. 2012–2015.

"**Engineering and control of artificial magnetic field and spin-orbit coupling for ultracold atoms**"**.** Collaboration with the USA / research group grant no. MIP-82/2012-LMT. Dr. Habil. G. Juzeliūnas. 2012**–**2014.

"**Coherent manipulation of matter by light and light by matter**" (2012-2014), collaboration with Latvia and Taiwan project no. TAP-LLT-**01/2012.** Dr. Habil. G. Juzeliūnas. 2012**–**2014.

Spin-orbit coupling in ultracold atomic gases. LMT postoc grant for R. Juršėnas, grant no. 004/15/MTDS-550000-398. Dr. Habil. G. Juzeliūnas. 2002**–**2014.

International Science Programmes and Projects

EU FP7 Project: **NAMEQUAM - Nanodesigning of Atomic and Molecular Quantum Matter-enlarged European Union.** Dr. Habil. G. Juzeliūnas. 2010**–**2012.

EU FP7 IRSES project: **COLIMA - Coherent Manipulation of Light and Matter via Interferences of Laser-dressed States**. Dr. Habil. G. Juzeliūnas. 2011**–**2015.

COST Action: **MP 0801 Physics of Competition and Conflicts.** Prof. B. Kaulakys and Dr. (HP) V. Gontis. 2009**–**2012.

MAIN PUBLICATIONS

COOPERATION

National Institute of Standards and Technology (USA)

National Tsing Hua University (Taiwan)

University of Latvia (Latvia)

Technische Universität Kaiserslautern and Leibniz Universität, Hannover (Germany)

ICREA and ICFO (Spain)

Heriot-Watt University (UK)

Linköping University (Sweden)

Université Libre de Bruxelles (Belgium)

St. Petersburg State University (Russia)

Institute of Semiconductor Physics (Novosibirsk, Russia)

OTHER SCIENTIFIC ACTIVITIES

Prof. B. Kaulakys –

- member of the Institute of Physics (UK);
- member of AAAS, American Association for the Advancement of Science, www.aaas.org ;
- editorial board member of the *Lithuanian Journal of Physics*;
- editorial board member of the journal *Nonlinear Analysis. Modelling and Control*;
- vice-president of the Lithuanian Association of *Nonlinear Analysts;*
- council member of the Lithuanian Scientific Society;

Dr. Habil. G. Juzeliūnas –

- Deputy Director of the Institute of Theoretical Physics and Astronomy, Vilnius University
- member of the Institute of Physics (UK);
- member of the Program committee of the 12th international Conference-School on Advanced Materials and Technologies (Palanga, 27–31 August, 2012).
- Invited talk at the Conference “Photonics West” (San Francisco, USA, 21-26 January 2012)
- Invited talk at the 2012 Taiwan International Workshop on Ultracold atoms and molecules (Sun Moon Lake, Taiwan, 18 - 20 May 2012).

Dr. (HP) V. Gontis –

- President of the Lithuanian Scientific Society*;*
- Director of the Institute of Lithuanian Scientific Society*;*
- member of the association Euroscience,http://www.euroscience.org/.

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Engineer: D. Mešalkin

Booking-clerk: A. Kvaraciejienė

Photographer: D. Janavičius (part-time).

Projects Supported by FP7

Researchers' Night 2012. VU Coordinator V. Lapinskaitė, 2012.

EVENTS

The largest event was a part of the **Researchers' Night 2012** project supported by FP7. It took place on September 28th **and attracted 425 visitors.** Another big event, organised together with the Vilnius municipality department of culture and education, took place on June 16 and was attended by 375 people.

A g**reat attention of wide public was attracted by the cycle of 8 concerts and Planetarium shows "The bards among stars"** held from February till December and attended by roughly 1500 visitors.

Altogether 590 lectures were offered to the visitors of the Planetarium. More than 27 000 people attended Planetarium during 2012.