INSTITUTE OF THEORETICAL PHYSICS AND ASTRONOMY

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Director - Habil. Dr. *Gražina Tautvaišienė*

STAFF

61 research fellows (9 habilitated doctors, 2 doctors with the habilitation procedure, 34 doctors) and 12 doctoral students. Full staff comprises 74 people. 3 afiliated and 5 project-scientists are involved as well.

MAIN RESEARCH AREAS 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 2011

E. Puzeras “Evolutionary effects in helium core burning star atmospheres”.

Ž. Ežerinskis, “Study and reduction of the matrix effects in analytical ICP mass spectroscopic measurements“

CONFERENCES AND SEMINARS ORGANIZED IN 2011

International Conference “Science, Innovation and Gender”, Dedicated to the 100th anniversary of Marie Sklodovska-Curie's second Nobel prize, November 24-25, 2011.

The Ninth Neon Observing School, July 14-27, 2011.

International Conference "Science, Innovations and Gender", November 24-25, 2011, Vilnius.

ASTRONOMICAL OBSERVATORY

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Head – Habil. Dr. *Gražina Tautvaišienė*

STAFF

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

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

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

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

Doctoral students: G. Barisevičius, V. Čepas, M. Maskoliūnas, Š. Mikolaitis, K. Milašius, D. Prakapavičius, E. Stonkutė, R. Ženovienė.

Lecturers: S. Lovčikas.

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

Technicians: J. Klevas (part-time), R. Chmieliauskaitė (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 2011

Project Supported by University Budget

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

The carbon and nitrogen abundances, C/N and especially the carbon isotope ratios $^{12}C/^{13}C$ are key tools for stellar evolution studies. Investigations of abundances of these chemical elements in atmospheres of clump stars of open clusters may provide a comprehensive information on chemical composition changes. Abundances of ^{12}C, ^{13}C, N, O and up to 26 other chemical elements in two first ascent giants and two core-helium-burning `clump' stars of the open cluster NGC 2506 have been determined. NGC 2506 was found to have a mean [Fe/H]=–0.24 ± 0.05 (standard deviation). Compared with the Sun and other dwarf stars of the Galactic disc, mean abundances in the investigated clump stars suggest that carbon is depleted by about 0.2 dex, nitrogen is overabundant by about 0.3 dex and other chemical elements have abundance ratios close to solar. The C/N and $^{12}C/^{13}C$ ratios are lowered to 1.25±0.27 and 11±3, respectively. The comparison of the observational data with theoretical models of stellar evolution shows that processes of extra-mixing in stars of open clusters with turn-off masses of 2–3 solar masses are larger than predicted.

Detailed analysis of two kinematic groups of F- and G- type stars was in progress. The distinct kinematic properties suggest that they might originate from ancient accretion events in the Milky Way. From high resolution spectra taken with the spectrograph FIES at the Nordic Optical Telescope, La Palma, we determined abundances of oxygen, alpha- and *r*-process elements. 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. This provides the additional evidences that those stellar groups had the common formation and possible origin from disrupted satellites.

We continued the analysis of chromospherically active stars. Photospheric parameters and chemical composition were determined for the single-lined RS CVn-type star 33 Piscium (HD 28). From the high resolution spectra obtained on the Nordic Optical Telescope, abundances of 22 chemical elements, including the key elements such as $^{12}C/^{13}C$, N and O were investigated. The differential line analysis with the MARCS model atmospheres gives Teff=4750 K, logg=2.8, [Fe/H]=–0.09, [C/Fe]=–0.04, [N/Fe]=0.23, [O/Fe]=0.05, C/N=2.14, $^{12}C/^{13}C$ =30, which show the first-dredge-up mixing signatures in this star.

A detailed chemical composition of AY Cet (HD 7672) - a flaring, spotted RS CVn star with a white dwarf companion - atmosphere is determined from its high-resolution spectrum in the optical region. The main atmospheric parameters and abundances of 22 chemical elements, including the key elements such as $^{12}C/^{13}C$, N and O, are determined.The differential line analysis gives Teff=5080 K, log g=3.0, [Fe/H]}=–0.33, [C/Fe]=–0.17, [N/Fe]=0.17, [O/Fe]=0.05, C/N=1.58, $^{12}C/^{13}C$ =21. Despite to the high chromospheric activity, the optical spectrum of AY Cet gives for this star a chemical composition typical for the first ascent giants after the first dredge-up.

PG 2303+243 is a cool DA variable (also called ZZ Ceti) star with a rich pulsation spectrum and variable amplitudes. A mini-campaign involving six observatories yielded time-resolved photometric measurements of PG 2303+243 during the period 2004 September 5-20. A duty cycle of 35 per cent was achieved. We detected 24 possible independent frequencies, their amplitudes and phases for future mode identification. We confirm the occurrence of short-term amplitude and frequency variations. Our analysis suggests an l= 1 rotational splitting around 8.4 μHz, implying a rotation period of 16.5 h.

KPD 1930+2752 is a short-period pulsating subdwarf B (sdB) star. It is also an ellipsoidal variable with a known binary period of 2.3 h. The companion is most likely a white dwarf and the total mass of the system is close to the Chandresekhar limit. This year we reported the results of Whole Earth Telescope (WET) photometric observations during 2003 and a smaller multisite campaign of 2002. From 355 h of WET data, we detected 68 pulsation frequencies and suggest an additional 13 frequencies within a crowded and complex temporal spectrum between 3065 and 6343 μHz (periods between 326 and 157 s). We examined pulsation properties including phase and amplitude stability in an attempt to understand the nature of the pulsation mechanism. We examined a stochastic mechanism by comparing amplitude variations with simulated stochastic data. Our results indicated a complicated pulsation structure that includes short-period (≈16 h) amplitude variability, rotationally split modes, tidally induced modes and some pulsations which are geometrically limited on the sdB star.

PG 1351+489 is one of the 20 DBVs - pulsating helium-atmosphere white dwarf stars - known and has the simplest power spectrum for this class of star, making it a good candidate to study cooling rates. We reported accurate period determinations for the main peak at 489.334 48 s and two other normal modes using data from the Whole Earth Telescope (WET) observations of 1995 and 2009. In 2009, we detected a new pulsation mode and the main pulsation mode exhibited substantial change in its amplitude compared to all previous observations. We were able to estimate the star's rotation period, of 8.9 h, and discuss a possible determination of the rate of period change of (2.0 ± 0.9) × 10-13 s s -1, the first such estimate for a DBV.

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 region of the Cepheus Flare in the direction of the dark cloud TGU 619. The study is based on photometric classification of 658 stars down to V=16 mag using photometry in the Vilnius System. The distance of the cloud (286 pc) is determined. The interstellar extinction in the 1.5 square degree area is found to be very uneven, ranging from 0.3 to 2.6 mag. (K. Zdanavičius, M. Maskoliūnas, J. Zdanavičius, V. Straižys, A. Kazlauskas).

Interstellar extinction has been investigated on the basis of the photometry and spectral classification of 120 stars in the direction of emission nebula Sh2-231 in the Aur OB1 association. The distance of the interstellar dust cloud is determined (1.3 kpc). The conclusion has been made that the emission nebula Sh2-231 is farther than 2 kpc and belongs to the Perseus Arm (V. Straižys, V. Laugalys).

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

30 new asteroids have been discovered in 2011 (24 asteroids at Molėtai Astronomical Observatory). Among them was the unusual Jupiter Trojan asteroid 2011 QA50. Up to now more than 400 asteroids are discovered by K. Černis and the collaborators. The main attention now is paid to refinement and analysis of the orbits and properties of asteroids and comets discovered previuosly. The asteroids 2002 FD14, 2004 TJ16, 2004 TW17, 2004 TG115, 2004 TM367, 2006 SD368, 2007 GV51, 2007 GR75, 2007 HN97, 2008 RJ98, 2009 CO2, 2009 CL2, 2010 BN5, 2010 EQ30, 2010 ES30 and comets C/2009 P1 (Garradd), 45P/ Honda - Mrkos- Pajdušakova, 29P/Schwassmann-Wachmann, 103P/Hartley, 213P/ Van Ness, C/ 2006

S3 (LONEOS), C/2010 G2 (Hill), C/2010 X1 (Elenin), C/2011 L3 (McNaught) ir C/2011 S1 (Gibbs) have been observed at Molėtai Astronomical Observatory and at other observatories during 2011 (K. Černis, J. Zdanavičius, K. Zdanavičius).
Analysis of the orbit of the Centaur group asteroid 2009 HW77 over past 100 mln. years has been carried out. The photometry and astrometry of the asteroid 2010 BT3 and a following analysis of the light curves enabled to determine the period of the asteroid‘s rotation and to calculate an evolution of the orbit (K. Černis).
4 asteroids with well defined orbits were named: Sūdžius (Nr. 175548), Meištas (187276), Palanga (166229) and Neris (237845).

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 three asteroids have been discovered: 2011 SK248, 2011 SL248 ir 2011 SM248 (K. Černis, V. Laugalys).

According to 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: 2011 HO28, 2011 QA50 ir 2011 QE80. Astronomical observations have been performed with the Schmidt telescope (0.80/1.20 m, f/3.5) of Baldone Observatory (K. Černis)..

Together with Prof. A. Dubietis (VU Faculty of Physics) K. Černis carried on an analysis of systematic visual and photographic observations of noctilucent clouds seen from Lithuania during the years 2010-2011.

Projects Supported by Research Council of Lithuania

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

A. Kučinskas. 2011–2012.

Problems of Modern Astrophysics, A. Kučinskas. 2011

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

The ninth Neon Observing school. Habil. Dr. G.. Tautvaišienė. 2011.

Researchers’ Night in Lithuania 2011 (Night2011). Dr. A. Kazlauskas. 2011.

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, Habil. Dr. G. Tautvaišienė, Habil. Dr. K. Zdanavičius, Dr. A. Kazlauskas, Š. Mikolaitis.

EVENTS

The big event for wide public was organized at the Molėtai Astronomical Observatory (MAO) on September 23. It was held in a framework of the FP7 project *Researchers' night 2011*. All the 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 the professional telescopes.

Another important event at the Molėtai Astronomical Observatory took place on July 14-27. It was the Ninth Neon Observing School, supported by FP7 project OPTICON (Optical Infrared Coordination Network). 20 Phd students from 15 European countries attended the school. They have studied methods of observations of stellar and galactic spectra, learned to use modern techniques and interpreted results of observations. The observations were carried out with two telescopes at Moletai 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 coordinators of the school J. Dennefield (France) and G. Tautvaišienė (Vilnius University, Lithuania) headed the international team of tutors: T. Augusteijn (Spain), H. Korhonen (Denmark), L. Morelli (Italy), S. Ramsay (Germany), R. Janulis, V. Laugalys, E. Pakštienė, J. Sūdžius, J. Zdanavičius (all VU). They gave the lectures and guided the students in real research projects, which results will be published in scientific journals.

Among other events at MAO two nights of equinox-music *etc*. should be mentioned.
Altogether more than 400 groups and about 10000 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 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. 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.

Habil. Dr. G. Tautvaišienė –

- vicepresident of Lithuanian Physics Society;
- reviewer of the European Science Foundation, 2010-2012;
- secretary of the International Astronomical Union (IAU), National representative;
- board member of the IAU Division *Optical & Infrared Techniques*;
- member of Astrophysics Commission at the International Union of Pure and Applied Physics;

- 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;
- editorial board member of the journal *Baltic Astronomy*;
- editor-in-chief of the annual astronomical almanac *Lietuvos dangus* (*Lithuania's Sky*).

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. R. Karazija, Dr. A. Kupliauskienė, Prof. Habil. Dr. G. Gaigalas (part-time), Prof. Habil. Dr. Z. Rudzikas (till June 08).
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, Dr. V. Tutlys.
Researchers: Dr. O. R. Juršėnas, Doc. Dr. A. Kynienė, Dr. A. Momkauskaitė, Dr. O. Rancova (till September 31).
Junior Researchers: Š. Masys (part-time).
Engineers: E. Gaidamauskas (part time, till October), G. Kerevičius (part-time, since October 01).
Doctoral students: Š. Masys, A. Šliogeris.

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 2011

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.

Theoretical study of Auger cascades during decay of and vacancies in krypton has been performed by level-by-level calculations using a wide configuration interaction basis. Auger spectra for all steps of cascade are presented and compared with the existing experimental data. The fairly good correspondence to the known experimental data for the ion distribution in different ionization stages and for Auger spectra corresponding to the first step of cascade is obtained. The largest influence on the branching ratios of $3p_{1/2}$ and $3p_{3/2}$ cascades has the strong interaction of configurations $4s4p^{N+1}$ and $4s^24p^{N+1}4d$ at the presence or absence of 3d vacancy. The Auger spectra generated during all steps of 3p cascades has been calculated, these results will be used for the provided investigations by the multielectron spectroscopy method.

The investigation of cascades is also actual for modelation of processes in the vicinity of cosmic x-ray sources: production of highly charged ions and their x-ray emission. The cascades in the light astrophysically important elements Ne, Mg, Si, S ir Ar after production of a vacancy in the K-shell were considered theoretically. The populations were presented not only for the levels of final configurations, but also for ones of the excited configurations after closing Auger transitions; from such levels an intense characteristic emission can be observed. All isonuclear sequence of ions for a given element is considered. For the first time dependence of cascade on the initial vacancy state was investigated. It is shown that the significant redistribution of ion yields can take place in the isoelectronic sequence of initial ions.

The ions in various ionization stages are produced during the cascades, thus it is an actual task to investigate the many-electron effects in such ions. In our work the strong mixing of $3s3p^{N+1}$ and $3s^23p^{N-1}3d$ configurations and its influence on the electric dipole transitions from/to the ground configuration $3s^23p^N$ have been considered in the isoelectronic sequences at the ionization degrees $5 \leq q \leq 35$ and various numbers of electrons in the $3p^N$ shell. The main results of this and the previous articles of our group as well as of other groups on the mixing of configurations with symmetric exchange of symmetry was summarised in the review article. The conditions of manifestation of such effect were established and the main regularities were formulated: its dependence on the mutual position of the energy level spectra of both excited configuration, ionization degree and atomic number. These conclusions can be useful for the elaboration of vacuum ultraviolet and x-ray sources. The other reason of the essential narrowing of spectrum – formation of two groups of levels by Coulomb exchange

interaction - was also analysed and the similar features of both manifestations of considered effect indicated.

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.

The research was performed within several tasks while implementing the work on this Project. Two different methods were applied to explore the inclusion of quantum electrodynamics corrections within a quasirelativistic approximation. The first of them was to interpolate Lande-factors of the hydrogen-like ions for the case of many electron atoms and ions by applying the values of the electron density near a nucleus. This method implies the averaging of relativistic electrons and their corresponding electrodynamics corrections over the complete electron momenta and allows to further extrapolate Lande-factors for quasirelativistic functions. Some additional uncertainties are introduced by using this method. Within the second method, these corrections are determined by integrating the specifically-designed potential, although the potential itself is an approximate one. The computer code implementing these two methods is created. The further studies of their applicability are in progress.

Two computer codes for the calculation of electron-impact excitation cross-sections and other parameters in Born approximation within both non-relativistic Hartree-Fock method and quasirelativistic method developed in Department of Atom Theory. These two methods allow the inclusion of numerous correlation effects. The first trial calculations have demonstrates that determined data agree very well with the existing experimental data and the most sophisticated theoretical calculation results.

The further study of theoretical spectral parameters of multicharged tungsten ions was performed. The correlation effects on the spectra from the $4p^6 4d$, $4p^5 4d^2$ and $4p^6 4f$ configurations of the W^{+37} ion were analyzed. A noticeably good agreement of the energy level values obtained in the quasirelativistic approach with the experimental data was accomplished, and the accuracy of our calculations was higher comparing to other theoretical results. Similar calculations were performed for the $4p^6 4d^2$, $4p^5 4d^3$ and $4p^6 4d4f$ configurations of the W^{+36} ion. Following the exploration of the spectral parameters of this ion, it was demonstrated for the first time that in the absence of electric dipole transitions from the excited configuration to the ground one, the radiative lifetime of the level can depend not only on electric quadrupole and magnetic dipole transitions inside excited configuration but also on the electric octupole transitions into the ground configuration.

One of the main goals of effective operator approach is to calculate transition probabilities. Two alternatives can be associated with the task. The first one refers to the transition operator that has been considered by using the Rayleigh—Schrodinger perturbation theory. The wave function is represented by the series of wave operator up to the second order. The symbolic programming package *NCoperators* running over *Mathematica* has been developed to generate the terms of wave operator. The second alternative has been chosen to find out transition probabilities in a completely different way. It is the method based on the analytical approach for solving the three-body Schrodinger equation. The approach refers to the group-theoretic methods combined with the constructed similarity conditions for the bounded operators on Hilbert spaces. In the present case, the Hamiltonian operator involves the translation invariant decaying potential whose commutative properties in certain Lie

subalgebras appear to be the key feature for the calculation of eigenstates. Eventually, the transition probability is represented in terms of inner products of eigenfunctions.

In collaboration with experimenters the excitation functions of lines in ejected-electron spectra of cesium atoms were investigated in a broad electron impact energy range. The data obtained together with other available experimental and theoretical data were used for the accurate spectroscopic assignment of spectral lines and for the analysis of excitation dynamics of levels in the $6s^2$, 5d6s, 5d6p and 6s6p configurations of Cs. The new spin-orbital splitting for the $(5p^5 6s^2)^2P_{3/2,1/2}$ levels was established at 1.900±0.005 eV. The latter work was exposed in LabTalk section of the Journal of Physics B as one of three best papers of the issue.

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

Investigation of energy levels and electric dipole transitions were performed for $4f^8$, $4f^7 5l$ ($l \leq 4$), $4d^9 4f^9$, $4d^9 4f^8 5s$, $4f^6 5s^2$, $4f^6 5p^2$, $4f^6 5s5p$ and $4f^6 5s5d$ configurations of W^{20+} in Dirac-Fock-Slater approximation. Electric quadrupole and magnetic dipole transitions are obtained for transitions among levels of 5 lowest configurations: $4f^8$, $4f^7 5s$, $4f^7 5p$, $4f^6 5s^2$ and $4f^6 5s5p$. Electron impact excitation data are investigated for these configurations in the distorted wave approximation. Basis of interacting configurations consists of 35779 levels. Very large mixing of configurations is obtained for configurations with symmetric exchange of symmetry. There are 3067 levels which main percentage composition for intermediate wave functions are smaller than 50 % and the first two configuration state functions with the largest expansion coefficients belong to the different configurations. Spectrum of W^{20+} ion was obtained in coronal approximation finding population of levels after excitation from the ground level. Process of radiative cascade after electron impact excitation from the ground level was investigated. It was found that many lines from various transitions coalesce in the range Å where experimental measurements are available. $4f^7 5d \rightarrow 4f^7 5p$, $4f^7 5f \rightarrow 4f^7 5d$ and $4f^6 5s5p \rightarrow 4f^6 5s^2$ transitions give the main contribution to the formation of spectra in the considered region of wavelengths. Furthermore, there are no strong transitions back to the ground level. Main transitions to the ground level have shorter wavelengths and take place from levels of $4f^7 5d$, $4d^9 4f^9$ and $4f^7 5g$ configurations.

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

Within the lowest-order relativistic approximation ($\sim v^2/c^2$) and to first order in me/M, the tensorial form of the relativistic corrections of the nuclear recoil Hamiltonian is derived, opening interesting perspectives for calculating isotope shifts in the multiconfiguration Dirac–Hartree–Fock framework. Their calculation is illustrated for selected Li-, B- and C-like ions. This work underlines the fact that the relativistic corrections to the nuclear recoil are definitively necessary for obtaining reliable isotope shift values.

Hyperfine induced $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$ transition rates in an external magnetic field for Be-like ^{47}Ti were calculated based on the multiconfiguration Dirac–Fock method. It was found that the transition probability is dependent on the magnetic quantum number M_F of the excited state, even in the weak field. The present investigation clarifies that the difference of the hyperfine induced transition rate of Be-like Ti ions between experiment [Schippers, et al.,

Phys. Rev. Lett. 98 (2007) 033001(4)] and theory does not result from the influence of external magnetic field.

Energies, electric dipole, magnetic dipole, and electric quadrupole transition rates, hyperfine structures, and Landé gJ factors from relativistic configuration interaction calculations are calculated for the states of the $(1s^2)2s^22p^2$, $2s2p^3$, and $2p^4$ configurations in all carbon-like ions between F IV and Ni XXIII. Valence, core–valence, and core–core correlation effects were accounted for through single/double-excitation multireference expansions to increasing sets of active orbitals. The calculated energy levels generally agree within a few hundred cm^{-1} with the experimentally compiled results, and the Babushkin (length), and Coulomb (velocity) forms of transition rates agree within less than 1% for a majority of the allowed transitions. Usually it is accepted that the probabilities of the electric-multipole electron transitions are rapidly decreasing functions of their multipolarity. Therefore while calculating the probabilities of electronic transitions between the configurations of certain chosen parities, it seems sufficient to take into account the first nonzero term, i.e., to consider the electron transitions of lowest multipolarity permitted by the exact selection rules. This work aims at verifying this assumption on the example of electric-octupole transitions in W^{24+} ion. For this purpose the large-scale multiconfiguration Hartree-Fock and Dirac-Fock calculations have been performed for the configurations $[Kr]4d^{10}4f^4$ and $[Kr]4d^{10}4f^35s$ energy levels of W^{24+} ion. The relativistic corrections were taken into account in the quasirelativistic Breit-Pauli and fully relativistic Breit (taking into account QED effects) approximations. The role of correlation, relativistic, and QED corrections is discussed. Line strengths, oscillator strengths, and transition probabilities in Coulomb and Babushkin gauges are presented for E1 and E3 transitions among these levels.

Projects Supported by Research Council of Lithuania

Project: **Theoretical Investigation of the Cascades of Elementary Processes in Complex Atoms.** Prof. R. Karazija. August 01, 2010–December 31, 2011.

Project: COST MP0802. **Self-assembled Quanosine Structures for Molecular Electronic Device.** Dr. J. Tamulienė. 2011.

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. 2011.

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. 2006–2012.

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

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.

Prof. Z. R. Rudzikas –

Chair of International Program Committee of the 7th international conference *Atomic and 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. 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 (EPS).

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. J. Tamulienė –

- management committee member of Lithuanian Physics Society.

DEPARTMENT OF THE THEORY OF NUCLEUS

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Head – Prof. Dr. *Egidijus Norvaišas*

STAFF

Senior Researchers: Doc. Dr. A. Acus, Dr. A. Juodagalvis, Prof. Dr. 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

Investigation of lepton-nucleus interactions in the supernova matter

Structure of N=Z nuclei

RESEARCH PROJECTS CARRIED OUT IN 2011

Project Supported by University Budget

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

The phenomenology of nucleon-nucleon interaction is developed for many decades. The approach of physical system with two topological SU(2) solitons emulate the nucleon-nucleon interaction was discovered. The attractive long range and spin-orbit components of

interaction are due to the orbital and rotational motion of the soliton. They are obtained from the time derivatives in the model Lagrangian density of two solitons system. The canonical quantization of the solitons provide the rich geometrical structure for them. The expression for the spin-orbit and quadratic spin-orbit interaction components was estimated. The elementary particles - baryons can be considered as topological solitons. The mass spectra evaluated by semiclassical quantization applied to SU(3) topological soliton model differ from experimental data. The quantum mass correction which appears in the canonical quantization procedure improves the mass spectra for the strange baryon octet and decuplet. With including Wess-Zumino-Witten and symmetry breaking terms the deviation from experimental masses are only a few percents. The masses are evaluated by variation of energy functional what maintain the stability of the quantum soliton.
The one dimensional square double quantum well (DQW) was investigated and demonstrated that closed form analytical expression for normalized wave function, which satisfy general BenDaniel-Duke boundary conditions can be obtained with the help of Gröbner basis techique. We notice, that the closed form can be obtained without knowing explicit values of eigenergy, which is known cannot be exactly solved due to transcendentality of the equation. Cylindrical double quantum well problem was also explored in different work. We obtained, that in this case normalized wave function can be explicitly written in terms of Bessel functions only. Both cases in fact reduces problem of solution of corresponding differential equation to purely algebraic problem of finding roots of transcendental eigenenergy equation.

Work on nuclear input for supernova simulations was continued. Following the presentation of the obtained results last year, the electron capture and the resulting emitted neutrino rate tables were produced for relevant matter conditions. This data would improve estimation of the matter deleptonization and the spectra of the emitted neutrinos in the modeling of the core-collapse supernovae. The results were shared with the collaborators. Computation took about 1.6 years and would not be feasible without the computer grid infrastructure, supported by the EGI project. The properties of N=Z nuclei below Sn100 have been studied in collaboration with the researchers from Lund Institute of Technology (Sweden). Recently, the spin-aligned proton-neutron pairing has been discussed in the nucleus Pd92. The experimentally determined equidistant excitation spectrum suggested special structure features for the yrast states with the total angular momentum up to 6^+ (which is the highest experimentally measured state). The performed shell model studies using interactions in different model spaces put doubt on the claims of other researchers about the special kind of pairing in this nucleus.

The Landau hydrodynamic solution for multiparticle production applied to non-central relativistic heavy-ion collisions was generalized. The obtained results show the longitudinal scaling of elliptic flow, v_2, as a function of rapidity shifted by beam rapidity ($y - y_{beam}$) for different energies ($\sqrt{}$sNN=62.4GeV and 200 GeV) and for different systems (Au-Au and Cu-Cu). It is argued that the elliptic flow and its longitudinal scaling are due to the initial transverse energy density distribution and initial longitudinal thickness effect.

Projects Supported from EU Structural Funds

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

As a final result of this project book A. Dargys and A. Acus “Two and three level atoms and systems in quantum mechanics” , 340 p., 68 fig. was published (http://mokslasplius.lt/files/2L3L_web.pdf) The corresponding supplement material (http://mokslasplius.lt/files/2L3LCD.tgz) was added to web portal MokslasPlius.lt (http://mokslasplius.lt/eksperimentai/2l-ir-3l-sistemos). The book and web material is primary devoted to the reader being interested in applied quantum optics and electronics.

Other Projects

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

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 between different theoretical parton distribution functions in proton. The analysis of 2010 data focused on the one-dimensional differential reaction cross-section $d\sigma/dM_{ee}$, resulted in one co-authored CMS publication. A similar study of 2011 data resulted in CERN CMS Physics analysis summary (PAS). Owing to the significantly increased amount of experimental data in 2011, work on the two- and three-dimensional differential reaction cross-sections ($d^2\sigma/dM_{ee}dP_T$, $d^2\sigma/dM_{ee}dY$ and $d^3\sigma/dM_{ee}dP_TdY$) has started. A theoretical study of the right-handed neutrinos was also pursued. The focus was on the parameterization of the neutrino sector in the Standard Model. The available results as well as future plans were presented by a collaborator T.Gajdosik (VU Physics Department) at the international conference “Matter to the Deepest” (Ustron, Poland) and the Lithuanian National Physics Conference. Dr.D.Jurčiukonis has joined the CERN CMS collaboration team as a postdoc. The collaboration with the CMS Higgs group ($H\rightarrow ZZ\rightarrow ll\mathit{bb}$ subgroup) as well as Heavy ion group was also pursued.

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

MAIN PUBLICATIONS

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)

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

OTHER SCIENTIFIC ACTIVITIES

Prof. E. Norvaišas –

- member of the International Advisory Committee of Second European Nuclear Physics Conference
- 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. Habil. Dr. B. Kaulakys, Prof. Habil. Dr. P. Serapinas, Habil.Dr. G. Juzeliūnas, Dr. V. Gontis.
Senior researchers: Habil. Dr. V. Gineitytė, Dr. G. Vektaris, Dr. J. Ruseckas.
Research fellows: Dr. M. Alaburda, Dr. A. Vektarienė, Dr. V. Pyragas (part-time), Dr. A. Mekys (part-time), Dr. V. Kudriašovas (part-time).
Postdoctoral research fellows: Dr. J. Ruseckas, Dr. V. Kudriašovas
Junior research fellow: Ž. Ežerinskis (part-time).
Engineer: T. Andrijauskas, A. Kononovičius (part-time).
Technician: S. Grubinskas
Doctoral student: Ž. Ežerinskis, A. Kononovičius.

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 and kinetic properties of cold atoms and condensed molecular structures. Habil. Dr. G. Juzeliūnas, **2011-2015**

The stability analysis was presented of the dark states in the adiabatic passage for the linear and nonlinear lambda and tripod systems. A new class of atom-laser coupling schemes was proposed which provides the spin-orbit-coupling acting on ultracold neutral atoms in the ground state manifold. An exact analytical description was developed of the electronic state function at the graphene and bilayer graphene interface based on tight-binding model. It was shown that the topological factors play an important role in the formation of signs and absolute values of indirect interactions of external subsystems through an alternant hydrocarbon. Electron-impact-induced methionine and glycine molecules fragmentation was investigated and the UV properties of the PPI dendrimers were obtained. Change of Mulliken charge was investigated along Intrinsic Reaction Coordinate in sulfenyl chloride addition reaction to propene. Theoretical investigation has been carried out of heterocyclization process on annulated two-nuclear heterocycles in the presence of electrophiles. Quantum mechanical origin and evolution of living systems containing nucleotides and vitamin D was discovered and quantum entanglement photosynthesis in minimal artificial cells was found.

Theory and applications of processes in complex systems. Prof. B. Kaulakys. 2011–2015

Probability distributions which emerge from the formalism of nonextensive statistical mechanics have been applied to a variety of problems. We unite modeling of such distributions with the model of widespread 1/f noise. We propose a class of nonlinear stochastic differential equations giving both the q-exponential or q-Gaussian distributions of signal intensity, revealing long-range correlations and $1/f^{\beta}$ behavior of the power spectral density. The superstatistical framework to get $1/f^{\beta}$ noise with q-exponential and q-Gaussian distributions of the signal intensity in is proposed, as well.

The special nonlinear stochastic differential equations generating power-law distributed signals and 1/f noise are considered. The models involve the generalized Constant Elasticity of Variance (CEV) process, the Bessel process, the Squared Bessel process and the Cox-Ingersoll-Ross (CIR) process, which are applied for modeling the financial markets, as well. $1/f^{\beta}$ behavior of the power spectral density is derived directly from the nonlinear stochastic differential equations and the exact solutions for the particular CEV process are presented. One of stylized facts emerging from statistical analysis of financial markets is the inverse cubic law for the cumulative distribution of a number of events of trades and of the logarithmic price change. A simple model, based on the point process model of 1/f noise,

generating the long-range processes with the inverse cubic cumulative distribution is proposed and analyzed.

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

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.

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

EU FP7 IRSES project **COLIMA - Coherent manipulation of light and matter via interferences of laser-dressed states**. Habil. Dr. G. Juzeliūnas. 2011–2015.

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.

MAIN PUBLICATIONS

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);
- 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;

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

- 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, 2010).
- Invited talk at the Conference 'Newspin2' (College Station, TX, USA, 12 – 18 December 2011).
- Plenary talk at the Quantum Technologies Conference II: Manipulating photons, atoms, and molecules (Krakow, Poland, 30 August – 4 September 2011).
- Invited talk at the 42nd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics (DAMOP 2011) (Atlanta, USA, 13-17 June 2011).

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/.

PLANETARIUM

12a Konstitucijos pr., LT-09308 Vilnius
Tel. 272 4177, fax 272 4177
E-mail: planet@tfai.vu.lt

Director – *Danutė Sperauskienė*

STAFF

Lecturers: N. Kochanskas, E. Dačinskaitė (from September 1, part-time), D. Matulytė (untill November 1), D. Sperauskienė

Engineer: D. Mešalkin

Booking-clerk: A. Kvaraciejienė

Photographer: D. Janavičius (part-time).

Projects Supported by FP7

Researchers' Night 2011. V. Lapinskaitė, 2011.

EVENTS

The largest event was a part of the *Researchers' Night 2011* project supported by FP7. It took place on September 23th. Another big event, organised together with the Vilnius municipality department of culture and education, took place on June 18. Each of them attracted about 500 visitors.

Altogether 591 lectures were offered to the visitors of the Planetarium. More than 25 500 people attended Planetarium during 2011.