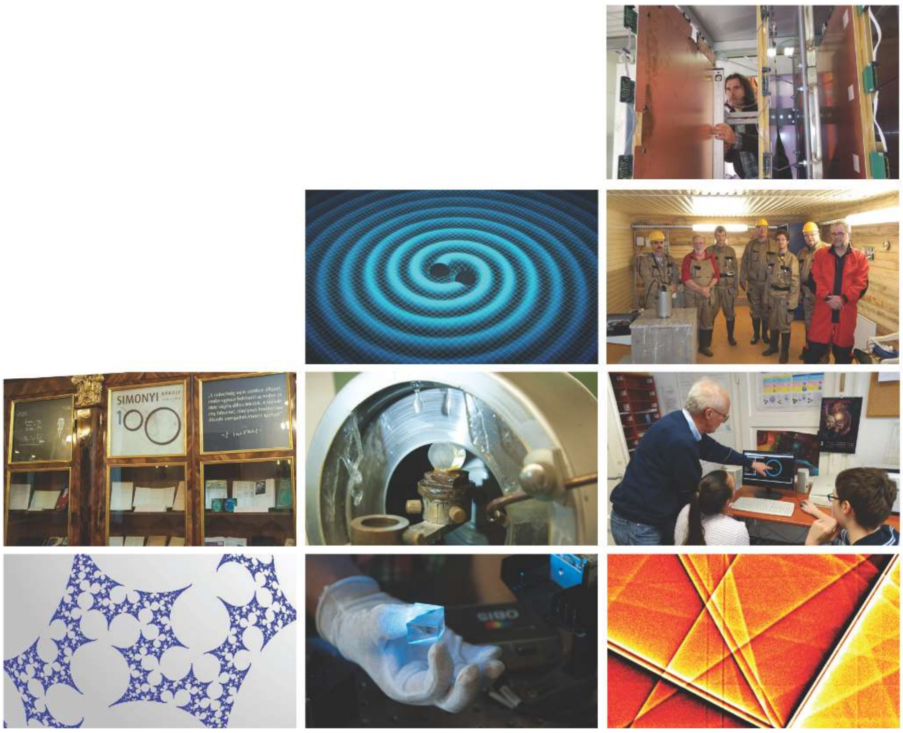
Wigner 2016

Annual Report



Wigner Research Centre for Physics
Hungarian Academy of Sciences
Budapest, Hungary

Wigner RCP 2016

Annual Report

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Wigner RCP 2016 – Annual Report

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Proofreaders: I. Bakonyi, P. Ván

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DEAR READER,

We have completed the fifth year of the Wigner Research Centre for Physics (Wigner RCP). The year 2013 was the year of exploring new ways and new directions for the activities of the research groups and the whole institute. We can consider 2014 and 2015 as a years of strengthening, when we improved and extended our activities. In 2016 we had to prepare a 5 years report, which was evaluated by different committees of the Hungarian Academy of Sciences. At the end of the evaluation we have received the “excellent” mark for the Wigner RCP’s activity and for both of the two member institutes’ activity. In this Annual Report 2016 we display and summarize the scientific achievements of the research groups, which gave the basis of this important result.

The prestigious MTA Momentum Research Groups, all of the eight, continued their well supported and visible research activity with excellent results, as well as the one group supported in the framework of the National Brain Project (“NAP: Nemzeti Agy Program”). The Wigner scientific community has selected seven Wigner Research Groups on the basis of excellence criteria and awarded with extra financial support for one year. (Their results are presented in the first part of the Annual Report, indicating their importance.)

We continuously explored the opportunities in the EU HORIZON 2020 Framework. Until the end of 2016 we submitted 65 proposals and awarded the financing for 9 projects. The success rate of 13 % is an outstanding result. These EU-supported projects will determine strongly the activity of the involved research groups in the near future, as well as the strategy of the Wigner RCP itself. At the same time the requested high level of performance will strengthen the position of the participating research groups in the international competition. On the basis of the received EU financial support combined with the extra financial support of the Hungarian Academy of Sciences, we started to modernize the local infrastructure, especially our Open Laboratories. This is very important, since our mission is to increase the readiness and the research potential of these local infrastructures and support internal and external research and R&D requests, because they will become the cornerstones of the national research activities in the near future.

Hungary joined to the European Space Agency (ESA) in February 2015. Following the restructuring and widening of the related space research and R&D activities, ESA awarded the Wigner RCP by the opportunity to open the ESA Broker Network Point in close collaboration with the local Technology Transfer Office. The ESA BNP is serving the whole Hungarian community and even institutes and companies from the whole Carpathian Basin.

During 2016 we had to farewell Ágnes Buka, Deputy Director General and the Director of Institute for Solid State Physics and Optics (she was replaced by Aladár Czitrovszky) and Ilona Deme, Financial Director (she was replaced by Péter Bányász) because of retirement process. Both of them have been decorated by the Officer's Cross of the Order of Merit of Hungary. I would like to thank for both of them for their more than 40 years long activity and the service of Wigner's and Hungarian scientific community.

Thereby I thank all colleagues for their continuous enthusiasm and participation in the research projects, for their hard work and devotion to science. The year 2016 was a year full with challenges and also a successful one for the Wigner RCP. This Annual Report shows examples of this hard work and prove the excellence of the research activities accomplished at Wigner RCP.

Lévai Péter József

Director General

FOREWORD

from the Director of the Institute for Solid State Physics and Optics

Engagement in the scientific endeavour is not merely an everyday activity, but requires commitment and sacrifice from its participants, with complete dedication towards realizing their goals. From the diversity of research, through the freedom of expression, until the euphoria of discovery, the researcher gains countless experiences which cannot be duplicated and are perhaps more valuable than material rewards.

Despite using different scientometric parameters and indices, sometimes it is difficult to judge the true value of a given scientific activity and correctly compare and rank various colleagues and research groups working in different areas. Nobody is infallible, hence in our opinion the fairest approach is that we appoint multiple expert committees for given tasks, and jointly make important decisions, set priorities, and develop research strategies, as well as use a system of rotation to enable support for the development of every worthy group in a balanced manner. This traditional approach alongside with the coordinated choice of research topics was the driving force for the management of the institute throughout the decades, and perhaps thanks to this approach the Research Institute for Solid State Physics and Optics (SZFKI and later the SZFI) grew to have the leading research groups with excellent academic indicators for a long period now.

The present yearbook is a collection of information which showcases the structure that was developed throughout the years, and briefly summarizes the 2016 scientific activities and results of our 20 research groups. This is done through listing selected publications, grants, and contracts, and in addition their applications as well as related educational activities putting higher emphasis on the 4 "MTA Momentum" and 4 "Wigner " research teams. In addition a number of other data of general interest are listed – like participation in international committees, awards, scientific events, etc.

As we can also see from the papers written in 2016, about two-thirds of the institute's 219 publications have a foreign co-author. It shows that there are strong ties with colleagues from over 35 countries, mainly in European but also from overseas universities and research institutions. The institute has cooperation with 39 foreign universities, among those 17 are with German universities. They are followed in line by 6 American, 4 French, 3 Austrian, and 3 Japanese universities. Among the 20 research institutions 16 are located in the EU and associated countries, 1 in both the US and China, as well as 1 in Russia and the Ukraine.

As a result, the mobility of our young scientists follows the international trend and more and more of our young scientists get short or long-term invitations, postdoctoral scholarships or positions and hopefully even more Marie Curie scholarships in the future. Long-term employment and scholarship opportunities are vital, especially for the professional development of young scientists, and provide them with ample networking opportunities. During the course of the year, 40 researchers spent time doing research abroad for periods of over six months. In the year 2016 we also had 81 foreign visitors at the institute.

The coordination of our everyday work and administration is greatly enhanced by the operational system developed in-house – the Wigner Administration Protocol (WÜR - Wigner Ügyintéző Rendszer), covering the full spectrum of the institute's activity starting from the attendance and holiday register to the official visits and other databases supporting the activity of the Financial Department.

We pay attention to keeping up-to-date of different regulations supporting our work, and, of course, to their adherence. At the same time, we try to support an impartial, humane, and creative atmosphere where mutual support and a healthy tone characterises the work environment.

In addition to the theoretical activities in the field of solid state physics and optics, the Institute's activities also branch into a variety of table-top experiments, so we focus efforts on infrastructural developments which serve this purpose. In the past years the Hungarian Academy of Sciences has allocated various sources of funding, based on which we were able to upgrade our laser, optical, and experimental solid state infrastructure.

Considering all of the above, in the Yearbook of 2016 we try to give the readers a documentation of our scientific activity of the period with an overview of the recent developments and the main achievements in solid state physics, laser physics, applied and nonlinear optics, quantum optics, complex fluids, neutron spectroscopy and a number of applications – e.g. in environmental science, biology, pharmacology, toxicology, etc. By doing so, we hope to facilitate spreading word of the research groups' activities and their evaluation.

We offer our publication not only to the scientific community, but to all interested readers in Hungary and abroad who would like to catch a glimpse of the activity of our institute and witness milestones in the history of Hungarian science.

Aladár Czitrovszky

Director of the Institute of Solid State Physics and Optics

Wigner Research Centre for Physics

AWARDS AND PRIZES

Awards of the State of Hungary and Government of Hungary

Á. Buka: Officer's cross of the Order of Merit of Hungary (civil division)
G. Beke, A. Csóré: Scholarship of the Ministry of Human Capacities

Awards of the Hungarian Academy of Sciences

F. Siklér: Academy Prize of the Hungarian Academy of Sciences, 2016
I. Hagymási: Excellence Award of the Young Researchers of the Hungarian Academy of Sciences, 2016
Á. Pekker, Junior Prize of the Hungarian Academy of Sciences
I. Korolov, Junior Prize of the Hungarian Academy of Sciences

International professional awards

D.L. Nagy, EPS Gero Thomas Commemorative Medal 2016
T. S. Biró: Member of Academia Europaea, 2016
I. Hagymási, Humboldt Research fellowship
Z. Zimborás: Selected by the Editorial Board of the Journal of Physics in its Special Issue ``Emerging Talents'' 2016
M. Vasúth, D. Barta, G. Debreczeni: 2016 Special Breakthrough Prize in Fundamental Physics (as authors of the LIGO Scientific Collaboration and Virgo Collaboration)
M. Vasúth, D. Barta, G. Debreczeni: 2016 Gruber Cosmology Prize (as part of The LIGO Discovery Team)
K. Krajczár, CMS Achievement Award 2016: "For his outstanding work on High Level Trigger menu development for Heavy Ion data taking"

National professional awards

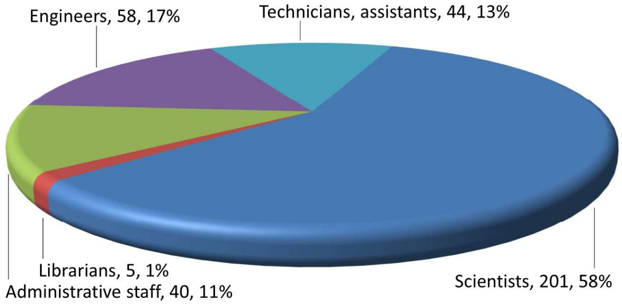
D.L. Nagy, Medal of the Loránd Eötvös Physical Society 2016
A. Kiss, Pál Gombás award of the Loránd Eötvös Physical Society
V. Ivády, Junior Prima Award
N. Kroó: Popular Science Prize awarded by the Club of Science Journalists
Á. Pekker, Wigner Postdoctoral Fellowship
Katalin Kamarás, "Honorary Professor", BME
V. Csajbók, B. Nagy, L. Bencs: Applied Research Prize of the Wigner RCP SZFI
L. Temleitner: Publication Prize of the Wigne RCP SZFI

Bolyai János Scholarship of the H.A.S. granted in 2016

K. Lengyel	D. Nagy	Á. Pekker
G. Szirmai	S. Tóth	R. Vértesi
A. Vukics		

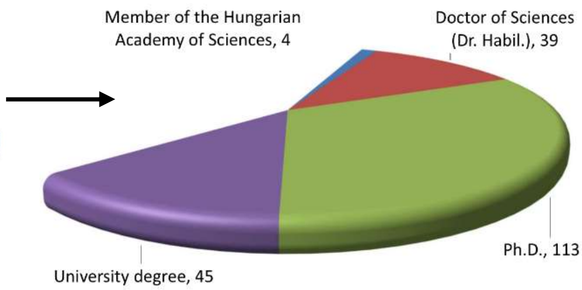
Permanent staff by profession

Total: 348



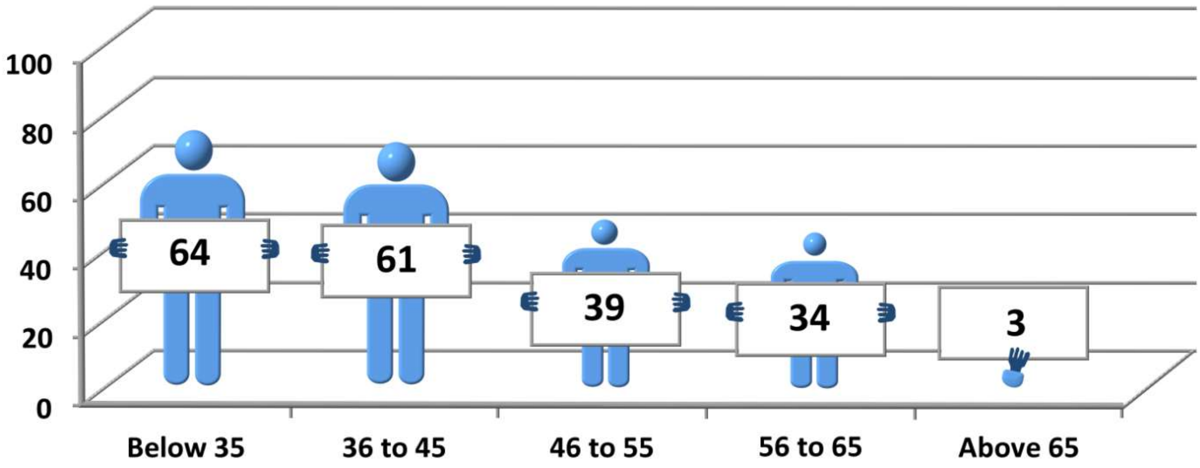
Scientists by degree/title

Total: 201

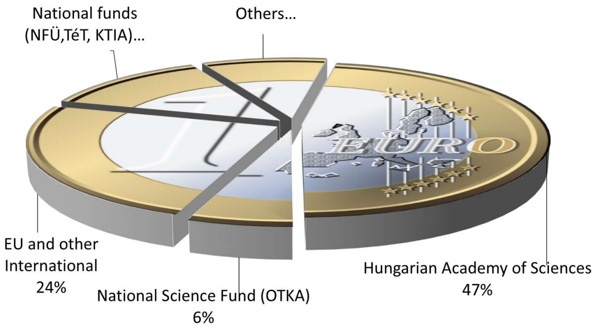


Scientists by age group

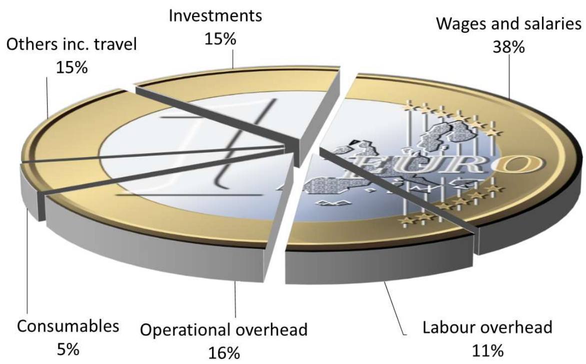
Total: 201



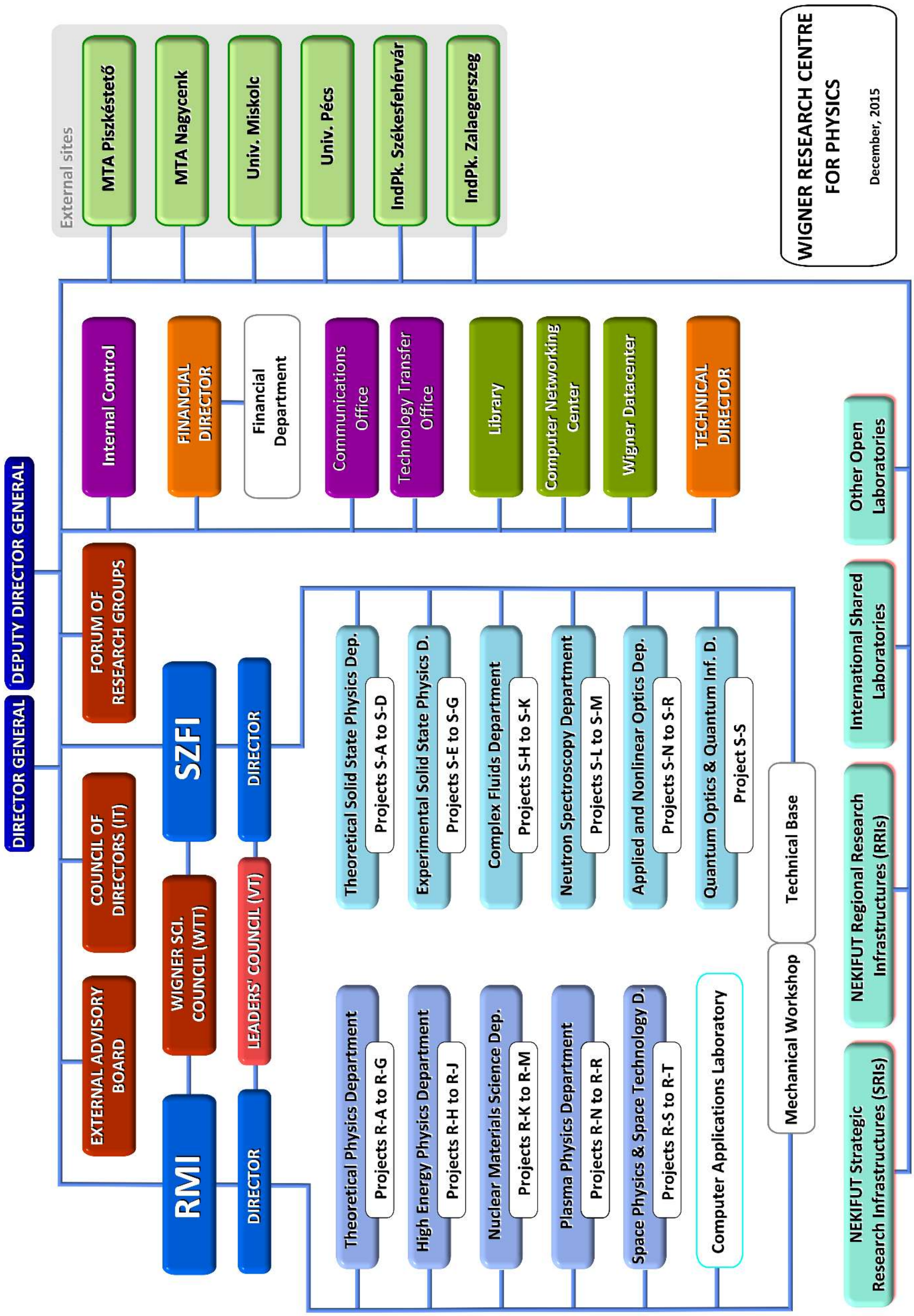
Income*



Expenditure*



*V.A.T not included.


WIGNER RESEARCH CENTRE FOR PHYSICS
December, 2015
DIRECTOR GENERAL
DEPUTY DIRECTOR GENERAL
EXTERNAL ADVISORY BOARD
COUNCIL OF DIRECTORS (IT)
FORUM OF RESEARCH GROUPS
RMI
WIGNER SCI. COUNCIL (WTT)
SZFI
DIRECTOR
LEADERS' COUNCIL (VT)
DIRECTOR
Theoretical Physics Department
Projects R-A to R-G
High Energy Physics Department
Projects R-H to R-J
Nuclear Materials Science Dep.
Projects R-K to R-M
Plasma Physics Department
Projects R-N to R-R
Space Physics & Space Technology D.
Projects R-S to R-T
Computer Applications Laboratory
Theoretical Solid State Physics Dep.
Projects S-A to S-D
Experimental Solid State Physics D.
Projects S-E to S-G
Complex Fluids Department
Projects S-H to S-K
Neutron Spectroscopy Department
Projects S-L to S-M
Applied and Nonlinear Optics Dep.
Projects S-N to S-R
Quantum Optics & Quantum Inf. D.
Project S-S
Mechanical Workshop
Technical Base
Internal Control
FINANCIAL DIRECTOR
Financial Department
Communications Office
Technology Transfer Office
Library
Computer Networking Center
Wigner Datacenter
TECHNICAL DIRECTOR
External sites
MTA Piszkéstető
MTA Nagycenk
Univ. Miskolc
Univ. Pécs
IndPk. Székesfehérvár
IndPk. Zalaegerszeg
NEKIFUT Strategic Research Infrastructures (SRIs)
NEKIFUT Regional Research Infrastructures (RRIs)
International Shared Laboratories
Other Open Laboratories

MOST IMPORTANT EVENTS OF THE YEAR 2016

Csilla Dovicsin-Péntek, communication secretary

In our research centre the dissemination and the science outreach is a priority activity by tradition. It is really important to us that the next generation and the general public have a chance to meet with our new and outstanding results presented directly by our colleagues. We organise lectures, scientific road shows and open days. Our colleagues participate in writing articles, making films and interviews popularizing science every year.

Our most important open days that we organise yearly are the Wigner Open Day, the Girls' Day and the CERN-Wigner Open Days. The Wigner Open Day is an interactive program for high school students offering lectures and laboratory visits. This program is part of the Hungarian Science Festival (organised by the Hungarian Academy of Sciences). In 2016, approximately 140 students and teachers visited our research centre and about 30 colleagues helped the implementation of the program. The Girls' Day is also a similar outreach program but focusing on high school girls. In Hungary it is coordinated by the Association of Women in Science. The third one, the CERN-Wigner Open Days is somewhat different, as it is not only for schools. During this programme anybody can meet with our research groups working closely with CERN and they can visit the Wigner Datacenter, too. We have one more interactive program for high school students: the High Energy Physics School Lab. It is an international program with lectures, data analysis and a short video conference with students from other countries.

CERN-Wigner Open Days

2016 was the third year that our exhibition bus with its interactive „All Colors of Physic Roadshow" run in Hungary and the second time that Wigner could participate on the sciences festival in Serbia. Many programs were organised for high schools and some of our colleagues took part in the Night of the Museums in Szeged.

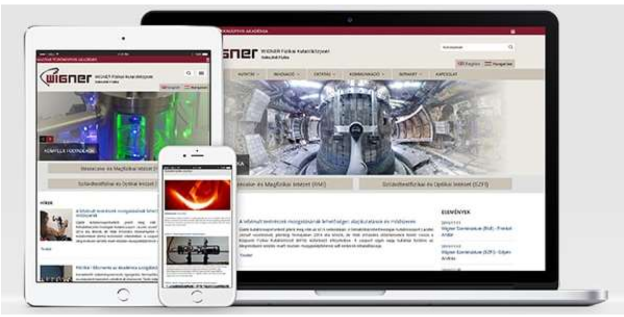
Our young researchers from the Plasmaphysics Department represented science at the biggest festivals for young people organised in Hungary like Sziget and VOLT.

Plasmaphysicist colleagues on the SZIGET festival

For the most talented students we continue on mentoring programs and we participate in trainings organised by the CERN for high school teachers.

2016 was the memorial year of the famous Hungarian physicist, Charles Simonyi. On this occasion, many programs were organised and our research centre had an important role in the coordination of these programs.

Simonyi Memorial Exhibition and the wreathing of the Simonyi memorial plaque



In 2016, our website was renewed. We would like to give more useful information for the public and for researchers too.

LISTENING TO THE COSMIC WHISPER

Mátyás Vasúth

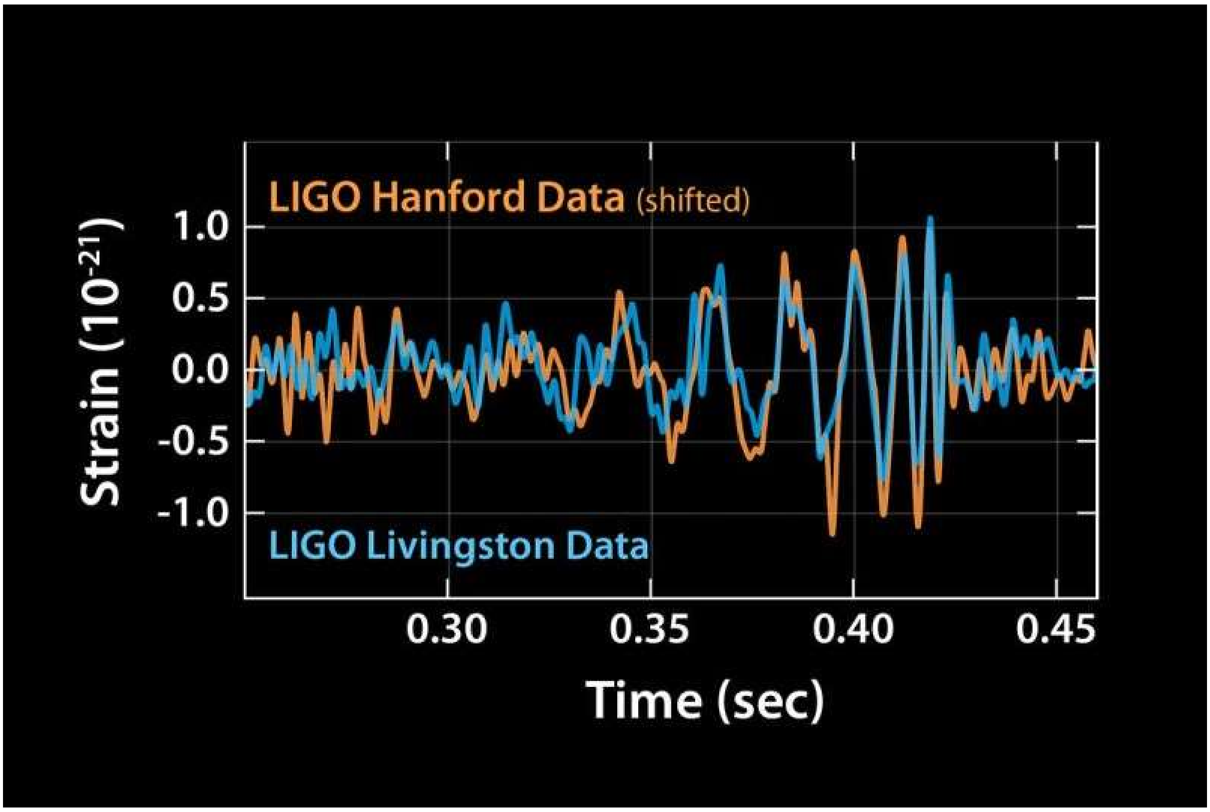
Newton's law of universal gravitation is very effective in describing our everyday celestial observations. The motion of heavenly bodies is precisely represented within the theory in a way that even the planet Neptune was mathematically predicted before its direct observation as a dramatic confirmation of Newtonian gravitational theory itself. Aside from the unusual motion of planet Mercury, it seemed to be no reason to doubt the validity of the theory.

After announcing the special theory of relativity in his miracle year 1905, Albert Einstein started to work on the incorporation of gravitation into his new relativistic description. He needed 10 more years to formulate general relativity, the geometric theory of gravitation. The theory connects the curvature of spacetime with its matter content through the nonlinear field equations, the Einstein equations. Matter is the source of spacetime curvature while its motion is taking place in this non-trivial, curved geometry. An additional prediction of general relativity is the time dependent nature of the curvature. As a natural solution of the weak field approximation of general relativity, gravitational waves (GWs) emerge as simple wave solutions propagating with the speed of light. They are ripples in spacetime, the time dependent variations of the curvature itself, and represent the finite velocity of the gravitational interaction itself not present in Newtonian theory. GWs are generated by the accelerating motion of masses, e.g. the inspiral of two heavy stars around each other. Propagating GWs change the spatial distance between test masses in time, though this change is extremely small even for heavy astrophysical sources and very sensitive instruments required for their detection.

GW detection experiments were started in the 1970s. Large, kilometre-scale laser interferometer observatories, i.e. LIGO and Virgo are operating from the beginning of 2000s. The original sensitivity of these first generation detectors were not enough for direct observation, however, they have demonstrated their working principle. The community decided to initiate an intense upgrade period in 2010/2011 to increase the sensitivity of the detectors. In summer last year the upgrade of the two LIGO detectors in the US have been completed and they started their first scientific data-taking period of 6 month in September 2015.

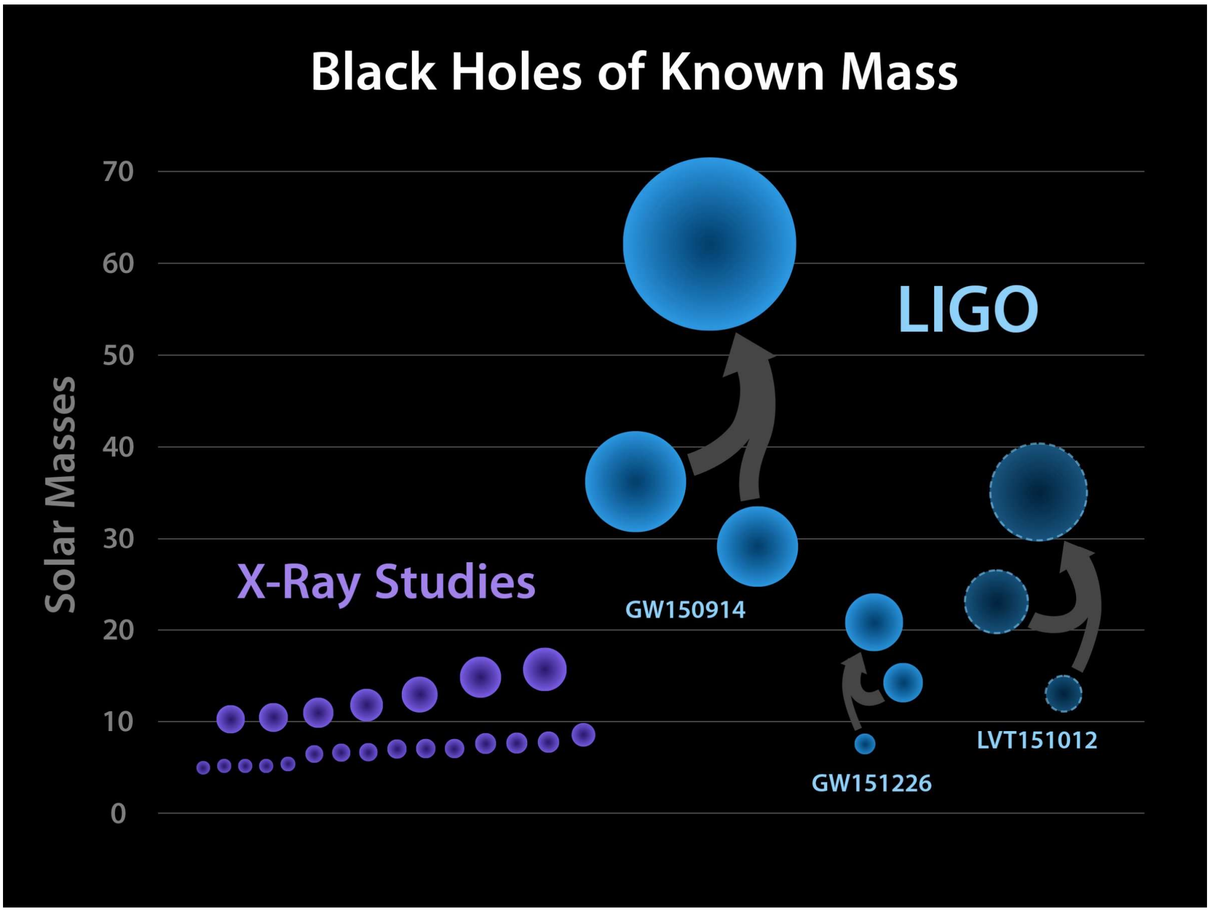
2016 marks the discovery of GWs, the historical moment of the century. The upgrade process of the observatories was a success of the community and resulted in the direct observation of two real GW events. The first direct detection occurred at September 14, 2015, only two weeks after the LIGO-Virgo collaboration meeting organized by Wigner RCP in Budapest. However, the community needed a few months analyzation of the data and the detector itself for certainly claim the detection before the public announcement in February 11, 2016. In the recorded data, there is an additional strong candidate, but its signal to noise ratio is low to claim detection positively.

The upgrade process of the European Virgo detector is expected to finish in 2017. Moreover, the KAGRA detector in Japan can start its operation in 2018. There are plans to install another detector in India with the support of the LIGO Scientific Collaboration. Following the announcement of the first direct detection of GWs, the Indian prime minister expressed his support for the project, which, similarly to the LIGO detectors, is planned to be a laser interferometer with 4 km arm length. With all of these detectors, a worldwide network of GW observatories is about emerging.



First direct observation of a gravitational wave. The signal, labeled GW150914, appeared in the data streams of both of Ligo's detectors near 30 Hz and rose to roughly 300 Hz in 0.2 second. The time separation between the signal's arrival in the L1 and H1 detectors was 7 milliseconds. The signals came from two merging black holes, each about 30 times the mass of our sun, lying 1.3 billion light-years away. The event would not have registered in LIGO's first-generation detectors; the fact that it appeared with striking clarity in both L1 and H1 indicates the leap in detector performance that the Advanced LIGO program has produced. (Source: Advanced LIGO News)

During the first direct observation of GWs the observatories were recorded the last tenth of seconds of the inspiral and merger of two black holes. It is interesting to note that due to the high sensitivity achieved by the LIGO detectors the GW signals were directly visible in the recorded data. The GW, originating from the merger of two heavy black holes of the famous detection event travelled 1.3 billion years and hitting the Earth generated a change in distances comparable to 1/1000 of a single proton. Equivalently, due to the passage of the wave the distance between the Sun and Earth changed approximately by the diameter of a single atom. This extremely small change was generated by an exceptionally energetic merger event during which the energy released in the form of GWs was equivalent with 3 solar masses. This huge amount of energy is approximately equivalent with the energy production of all the stars of our galaxy in 500 years. An interesting fact that the frequency of the detected signal lies within the audible sound range and one can play and hear the sound of GWs. The original frequency of the detected signal covers the 20 – 300 Hz range, below the normal A-sound of 440 Hz.



LIGO has already significantly increased the number of black holes with known masses. The observatory has definitively detected two sets of black hole mergers (bright blue). For each event, LIGO determined the individual masses of the black holes before they merged, as well as the mass of the black hole produced by the merger. The black holes shown with a dotted border represent a LIGO candidate event that was too weak to be conclusively claimed as a detection. (Source: LIGO Gallery)

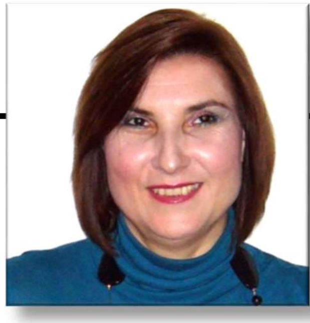
The first direct observation of GWs is a historical event. Its importance can be compared to the moment when Galilei first looked into his telescope, started the systematic observation of the solar system, and recorded interesting phenomena unknown before. Optical telescopes observe the sky in the entire electromagnetic spectrum, however, with GWs a totally new window has been opened to the Universe. This new window is marked by the new field of GW astronomy, and as a result, rapid development in our astrophysical and cosmological knowledge is expected. For an accurate description of GW sources and present measurements, the knowledge of strong gravitational fields is indispensable.

During data analysis, the detected signal is compared with theoretical wave templates. These templates are depending on several source parameters, e.g. the mass, separation and rotation of the inspiralling black holes. The theoretical description is very sensitive to the change of the involved parameters, both the frequency and amplitude of the wave changes significantly during the evolution of the source. The analysis of these data is an extremely calculation intensive task.

For the development of the operating detectors, it is inevitable to map the low frequency noises and their sources. With the initiation of the Mátra Gravitational and Geophysical Laboratory, the main objective was to join the international efforts aiming this research field. The initial measurements with several instruments, e.g. a seismograph, a Polish seismic sensor, an infrasound detector, an electromagnetic sensor and a muon detector, were concluded this year. With the long-term observations, our institute can contribute to the development of future GW observatories.

Before the start of the first observation period of the advanced LIGO detectors, the Virgo collaboration started to update its public outreach website. As a part of the upgrade process, the outreach team asked the whole Virgo collaboration for a good slogan for the new site to catch the very essence of the research field. There have been many excellent suggestions, e.g. “Lighting the dark Universe”, and “The whole universe within an arm length away”. Receiving the majority of the votes the winner became the sentence chosen as the title of this summary: “Listening to the cosmic whisper”.

RESEARCH GRANTS AND INTERNATIONAL SCIENTIFIC COOPERATION



Valéria Kozma-Blázsik, scientific secretary

We can measure the scientific output of a research institution using various indicators, such as the number of publications which in 2016 this was about 220 for SZFI, income from national funds, international grants, or even though looking at successful academic or academic-industry collaborations.

National Funds. — In 2016, the amount of OTKA funding received increased even further. Researchers of the institute started a total of 11 new projects with a combined funding of 299.7 million HUF for the entire funding period. Four of these were Post-Doctoral fellowships for young scientists worth a total of 60,3 million HUF. Another four were theoretical projects, as well as two experimental projects are aimed at developing new materials and procedures. During 2016 the National Research Development and Innovation Office (NKFIH) financed a two-year-long project VEKOP2.3.3.-15-2016-0001 in the field of determining the atomic structure of nanosystems.

Scientific excellence via international cooperation. — Internationality is a general characteristic of research, and in many cases is a key factor in its success. Researchers of the institute developed strong ties with their counterparts from over 35 countries. The institute's international partnerships consist of several types of EU FP7, H2020, ESA, IAEA, and COST scientific collaborative projects, in addition to other international projects, bilateral agreements with the Hungarian Academy of Sciences, intergovernmental contracts (TéT), and a wide range of informal partnerships.

There is a common assignment with the International Atomic Agency and with American institutions, such as Oak Ridge National Laboratory.

International Grants. — At the Institute of Solid State Physics and Optics there were 12 bilateral Scientific and Technological Projects (TéT). Four of the previously funded TéT projects concluded this year, while four new projects began in partnership with two French, one Slovenian and one Austrian research group. The "JST V4" consortium was set up between Japan and the four Visegrád countries. This project involves both theoretical and experimental research in the field of advanced materials: Nanophotonics with metal - group IV-semiconductor nanocomposites: from single nanoobjects to functional ensembles.

Collaborative research became more difficult in H2020 this is why it is even more significant that the institute won two grants in 2016. The first winning FET-Open proposal of the institute, NEURAM – H2020-FETOPEN-2014-2015-RIA, (No. 712821, 2016 - 2019), received 4,271,481.25 Euro (1300 million HUF) of funding for a period of 3 years. Within the framework of the NEURAM project, 4 institutions in 3 countries are working together on developing methods for the investigation and monitoring of brain cells without markings, and for learning processes occurring in cells during DNS transcription. The new method and the microscope under development is based on stimulated Raman-deviation. Wigner's share is 712,250.00 Euro, and as a beneficiary is responsible for the development and optimization of an instrument applying stimulated Raman-deviation and the mapping of Raman-zones that describe nerve cells.

There is one new H2020-MSCA-RISE-2016 project: VISGEN 734862 Transcribing the Processes of Life: Visual Genetics with a total budget of 1,269,000 Euro, here Wigner has the second largest budget of 211,500 Euro among the 11 participants. The other participants are research institutes, universities, and industrial partners from 6 different countries (UK, HU, G, F, NL, NO).

Since the Treaty of Lisbon the goal of European Research Area (ERA) is included in the EU's primary laws. Within the EU's boundaries „researchers, scientific knowledge and technology circulate freely". The strengthening of ERA became one of the priorities of H020 together with other cross-cutting issues that include widening participation, which in some cases also contains some controversial questions. As the potential of the EU13 is not properly explored the German Government made an initiative to integrate these countries more, and in 2016 initiated the ERA Fellow Program as a pilot project in which EU13 Fellows participated who are currently working at the middle administrative management level at scientific organisations located in the EU13 member states.

The program's objectives were to improve collaboration with the EU13 member states and to contribute to the European Research Area (ERA). This is why the German Federal Ministry of Education and Research (BMBF) also offered theoretical training with a focus on science management in the framework of two on-campus weeks to the ERA Fellows. Main topics of these lectures, presentations and workshops were preparing applications to Horizon2020, the internationalization strategies of the research institutions, international research infrastructures, and the identification of further funding sources.

Valéria Kozma-Blázsik, responsible for EU projects at the Wigner Research Centre for Physics of the Hungarian Academy of Sciences participated in this six-week stay in Germany, including a guest stay of four weeks at Max Planck Institute of Quantum Optics (MPQ).

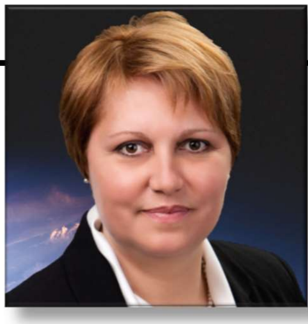
She gave a presentation on September 14, 2016, describing the role of Wigner RCP in the Hungarian scientific landscape, organised and hosted by her counterpart Julia Epp, Head of Third-Party-Funds/EU Office of Max Planck Institutes in Regional Cluster Bavaria, working on developing training concepts providing support to her counterpart for an effective grant office and administrative system.

At MPQ, the focus was on procedures and processes in EU proposal consulting and project management. Valéria Kozma-Blázsik was hosted in MPQ's Third-party funds department/EU Office Bavaria, which will serve as a starting point to explore further cross-cutting issues in the institute's administration and in Max Planck Society's administrative headquarters. Besides the effect of capacity-building, which will benefit the EU13 member states according to the program's aims, the German hosts also expect the exchange to prove advantageous. "In view of future scientific collaborations and projects we are also interested in a smooth collaboration at the administrative level", outlines Prof. Ferenc Krausz, Managing Director at MPQ.

The program was concluded by a campus week in Berlin with participation at the National Conference on the European Research Area. The Federal Ministry of Education and Research hosted this conference at the Berlin Congress Center (BCC) (For further information, please visit www.eubuero.de/era-conference.htm). This high-level conference focused on the Strategy of the Federal Government on the European Research Area (ERA). It provided a forum to exchange views on current developments and emerging challenges regarding research and innovation in Europe. Professor Dr. Wanka, Federal Minister of Education and Research, opened the conference. She was joined by a number of high-ranking national and international guests from EU politics, research and business.

INNOVATION ACTIVITIES OF WIGNER RCP

Zsuzsanna Tandi, innovation adviser



The MTA Wigner RCP is continuously developing its international industrial relations, looking for investment opportunities and endeavors to strengthen internal support processes, which contribute to the implementation of an effective technology transfer activity. As a result of the efforts of the previous years, the processes of the Intellectual Property Rules have been strengthened, regular sessions of the Evaluation Commission for IP Results were held and professional partners have been involved to promote our marketable projects.

The ESA Technology Transfer Office was established at the end of 2016. The mission of the European Space Agency (ESA) technology transfer network is aimed at working on facilitating innovations, systems and know-how of space technology in non-space areas and thus, also in the everyday life throughout Europe. The MTA Wigner RCP represents Hungary in the network of the ESA Broker Network Points, see details on the WEB-page "wigner.mta.hu/esa".

The Wigner RCP is an active member of the CERN-supported organization of HepTech, which is performing technology transfer of leading HEP technologies to the industry. HepTech submitted joint grant proposals for EU H2020 Calls to support these activities, they are under evaluation. The Innovation Advisor of Wigner has been invited to participate in the next 4 years in the Innovation Work Package of the 28 million euro Project by the Accelerator Research and Innovation European Science and Society (ARIES), supported by the EU. The aim of the work package is to support new startups to utilize the research results.

OUTSTANDING RESEARCH GROUPS

MTA's "Momentum" Research Teams

Lendület program 2014

The goal of the "Momentum" Program of the Hungarian Academy of Sciences (HAS) is to renew and replenish the research teams of the Academy and participating universities by attracting outstanding young researchers back to Hungary. The impact and success of this application model is highly acclaimed and recognised by the international scientific community. Initiated by the former HAS President József Pálinkás, the "Momentum" Program aims to motivate young researchers to stay in Hungary, provides a new supply of talented researchers, extends career possibilities, and increases the competitiveness of HAS' research institutes and participating universities.

Wigner Research Groups

The "Wigner Research Group" program is introduced to provide the best 3-3 research groups from both institutions of the Centre with extra support for a year. Its primary goal is to retain in science and in the Research Centre those excellent young researchers who are capable of leading independent research groups. It aims to energize research groups, and to recognize, support and raise the profile of the leader of the group. During the support period the research group should make documented efforts to perform successfully on domestic R&D tenders and international tenders of the EU and its member states.

R-C. Gravitational physics

Wigner research group

Mátyás Vasúth, Dániel Barta[#], Károly Zoltán Csukás[#], Máté Ferenc Egri-Nagy[#], István Rácz, László Somlai

The members of the Gravitational Physics Research Group of the Wigner RCP have solid background in experimental and theoretical physics, in particular, general relativity and/or particle physics. They also have experience in developing optimal numerical algorithms and coding these algorithms into efficient computer procedures that can run on grid and GPU clusters. One of the main motivation of our research interest originates in gravitational wave (GW) physics as our group is a member of the Virgo Scientific Collaboration operating the Virgo detector, the European gravitational wave observatory. The scientific results of last year are summarized below.

Gravitational wave data analysis. — Interferometric gravitational wave detectors such as LIGO and Virgo are sensitive to compact astrophysical objects with time-varying quadrupole moment. The start of the advanced LIGO detectors in fall of 2015 has opened the very interesting era of gravitational wave astronomy. The first direct detection of GWs and their subsequent observation have important consequences on various fields of science and modern technology. It opens a totally new window to the Universe as our current knowledge is entirely based on observations of electromagnetic radiation. Despite its weakness gravity is believed to be the dominant force governing the evolution of astrophysical objects and the entire cosmos. With the help of the developing GW astronomy scientists will be able to probe the nature of dark energy and matter and, in turn, increase our knowledge about the universe considerably. Joining not only to the European efforts but also the international LIGO-Virgo collaboration our research projects aimed to analyze important and interesting compact binary sources of GWs and study the astrophysical and cosmological implications of the observations.

For ground-based interferometric GW detectors compact binary systems of low mass black holes are the most important sources for detection considering their present sensitivity. The dynamics and the emitted radiation of these binaries are commonly described by the post-Newtonian expansion. Specific waveform templates are ready for offline searches and parameter estimation studies for these kind of sources within the software package of the LIGO-Virgo Collaboration, e.g. the *PyCBC* and *GstLAL* packages. In data analysis processes the matched template filtering method is considered to be the most optimal one for the identification of theoretically predicted waveforms that are significantly suppressed by a noisy background. Matched filtering for compact binary sources are implemented in the *PyCBC* software package. The members of the Gravitational Physics Research Group have learnt the use of the *PyCBC* toolkit and we are utilizing this knowledge during the upcoming GW observations. Using Institutional computational resources we are performing data analysis runs on *Wigner Cloud*. We have successfully installed clusters of virtual machines

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and set up a Condor task manager system. From a central computer all of the virtual machines are accessible through Condor. Test result for running basic *PyCBC* scripts are successful. As an important application we have implemented high precision waveform match calculations for a wide range of the parameter space using in-built *PyCBC* waveforms.

Reduced basis for GWs. — The large dimensionality of the parameter space for binary sources makes GW searches, parameter estimation, and modeling expensive and computationally unsuitable with most of the methods. This problem is called the "curse of dimensionality", and, as a solution, the reduced basis approach was introduced in GW physics. We have developed an interpolation technique for the reduction of the required gravitational waveforms. For a given parameter space of compact binary systems it is possible the appropriately choose a system of basis waveforms in a way that an arbitrary gravitational waveform can be faithfully represented by this basis. The method is available for circular binaries. In our work we have demonstrated the applicability of this procedure for binaries on eccentric orbit resulting in the reduction of the required computational capacity.

The effect of the cosmological constant. — The presence of a non-zero cosmological constant Λ makes the Universe globally a de Sitter space-time. The smallness of the cosmological constant may imply that it is unobservable except at large distances. Gravitational waves of the first direct detection fit to the current ΛCDM cosmological model and to Einstein's prediction of gravitational waves. In the linearized approximation of general relativity, the metric tensor is the sum of the flat metric and a perturbative term, which can be interpreted as the sum of gravitational waves and background perturbation involving Λ. In order to study the effect of the cosmological constant on the linearized theory a different gauge choice was considered. This allowed us to write the equations of motion in terms of the two perturbation part separately and order by order in Λ. With these equations the earlier results of gravitational waveforms calculated in the usual transverse-traceless gauge can be used to study the effect of the cosmological constant Λ. It was shown that the presence of the cosmological constant modifies both the phase and the amplitude of the original quadrupole GW signal.

Continuous gravitational waves. — Within the science exchange program of the NewCompStar EU COST action our Polish colleague Michal Bejger visited our department for 3 weeks. Our common interest is in the analysis of continuous GWs. These waves are produced by systems that have almost constant and well-defined frequency. Example of these are rotating single stars with a large mountain or other irregularity. These sources are expected to produce weak gravitational waves since they evolve over longer periods of time and are usually less catastrophic than sources producing inspiral or burst gravitational waves. The aim of our project was to develop a new version of an all-sky data-analysis pipeline which was initially developed by the Polish Virgo-POLGRAW group aiming at a targeted search for almost-monochromatic gravitational-wave signals from rotating, non-symmetric, isolated neutron stars. During our joint work we have enhanced the existing GPU implementation of the pipeline. Our initial discussions led to riding the code of dead parts, obsolete dependencies, etc. making it generally more flexible. In hope of acquiring a larger user base, we have moved from GCC/Linux/CUDA-only support to using open standards, such as C11 and OpenCL.

With the contribution of Tuan Máté Nguyen our group is actively engaged in the development of analysis software for the analysis group in Rome. The Rome group have concluded that the bottleneck in their Wolfram Mathematica script toolchain was the Hough-transform they implemented in Mathematica’s own scripting language, hence the goal of its acceleration was set. First time around a native C++ implementation was devised, both serial and parallel. The results are positive and can be put to use immediately. Further collaboration may target a GPU-parallel implementation as well as porting other parts of the toolchain.

Neutron star interiors. — Neutron stars (NS) are interesting and important sources of gravitational waves. Despite of the fact that the present sensitivity of GW observatories does not allow the detection of neutron star coalescences future upgrades will enable the analyzation of such processes. The most intense part of the observed GW signal is coming from the merger part of the coalescence carrying essential information about the neutron star characteristics and the merger itself. In our work we have analyzed neutron star interiors of ideal and non-ideal fluids. Assuming spherical symmetry the metric tensor is time dependent and the equations characterizing the neutron star interior are decouple to the TOV equation and a differential equation for the time evolution of the radius. For a two-component polytrophic equation of state we have analyzed the Mass-Radius relation for neutron stars. The analysis was extended to other equation of states. Without GW observation of neutron stars present bounds for NS mass and radius can limit the parameter ranges of possible equation of states.

Matra Gravitational and Geophysical Laboratory. — The lower frequency bound of present Advanced GW observatories are around 20 Hz. The fundamental limitations at low frequency of the sensitivity are given by the seismic noise, the related gravitational gradient noise (so-called Newtonian noise) and the thermal noise of the mirrors. To circumvent these limitations new infrastructures are necessary: an underground site for the detector, to limit the effect of the seismic noise, and cryogenic facilities to cool down the mirrors to directly reduce the thermal vibration of the test masses. To accurately predict the seismic noise variation and behavior it is inevitable to perform long term seismic monitoring underground. The Mátra Gravitational and Geophysical Laboratory was constructed 88 m deep below the surface in an unused mine near Gyöngyösoroszi in 2016. In a collaboration of several Institutes the aim of the Laboratory is to perform long term seismic, infrasound and electromagnetic noise measurements, and monitor the variation of the cosmic muon flux. The members of our group were involved in the preparation of the first data taking period between March and August, 2016. In preparation for the subsequent measurements, we have performed preliminary unification of the measured data coming from different devices.

Constraint equations as evolutionary systems. — Seven decades ago the constrains of Einstein's theory of gravity were converted to a semilinear elliptic system by the seminal work of Lichnerowicz and York. All the currently applied techniques developed to solve the constraints are based on this approach which, as it involves conformal rescaling of the basic variables, also referred as the conformal method. A new alternative approach was proposed which endows the constraints with a radically new evolutionary character. In particular, it is shown that the constraints may be put either to a parabolic-hyperbolic system or to a strongly hyperbolic system subsided by an algebraic relation. The proposed new approach is expected to yield new techniques to solve the constraints, because local (in some cases global) existence and uniqueness of solutions to these evolutionary systems are guaranteed.

Numerical relativity research. — In hope of investigating the perturbations of near spherically symmetric processes on various space-times we are developing a numerical library keen in making use of series expansion of spin-weighted spherical harmonics. We would like to simulate the perturbations of spinning black holes with unprecedented accuracy. The solution of the arising constraint equations have been accounted for with CPU parallel calculations. Our future plans involve devising the equations governing the evolution in a similar formalism as well completing the GPU-accelerated back-end of the library.

Concurrently to previous efforts and consulting with members of the GPU-Lab we are working on a visualization module to GridRipper, the subject of our theoretical work. Our aim is to develop a ray caster (in the computer graphics sense), to visualize various volumetric density functions, implemented in a fully templated manner in modern C++ for maximum flexibility. Similar to other developments in the Lab, his work is relying on portable and open standards.

Outreach. — The announcement of the first direct detection of gravitational waves in February 2016, 100 years after Einstein's original prediction, was generated a very intense public interest and attention to this research field. Our group members were actively participated in the preparation of the Press Kit for the announcement. Moreover, we have given several scientific and public lectures, radio interviews about the first direct detection of gravitational waves and its implications.

In 2016 our group members were actively participated in the organization of the national scientific conference "100 éves az általános relativitáselmélet" in Budapest.

Grants

OTKA K 115434: Developing and applying new methods to solving the Cauchy problem in general relativity (I. Rácz, 2015-2019)

International cooperation

Virgo Scientific Collaboration (M. Vasúth, D. Barta, M.F. Egri-Nagy, L. Somlai)

NewCompStar EU COST MP1304 action, (Hungarian Representatives: G.G. Barnaföldi – QCD Topic Leader WG2, M. Vasúth, 2013-2017)

Long term visitor

Michal Bejger (M.F. Egri-Nagy, 3 weeks)

Publications

Articles

1. Rácz I: Constraints as evolutionary systems. ***CLASSICAL QUANT GRAV*** 33:(1) 015014/1-18 (2016)

See also: R-B.1, R-B.7

R-E. Theoretical neuroscience and complex systems

Wigner research group

Zoltán Somogyvári, Fülöp Bazsó, Tamás Bábel, Zsigmond Benkő#, Jennifer Csatlós, Dorottya Cserpán#, Péter Érdi, Tamás Kiss, László Négyessy, László Zalányi

We have been implementing **a new causal measure** – which can determine causal relations between time series generated by dynamical systems-based on manifold dimensions. We used frequentist statistical tools and we have been developing a Bayesian inference algorithm to detect hidden common causes between apparently directly related variables. Simultaneously, we have been validating our method on model systems and have applied on multivariate electrical recordings from epileptic patients to develop our understanding on seizure onset, propagation and to get better epileptic focus localization.

We proved that **the combination of in vivo multichannel neural recording and controlled tracer injection using a single implanted microdevice is feasible**, and therefore it can be a powerful tool for studying the connectome of the brain. This new microprobe allows the simultaneous electric recording of the activity of a neuronal pool and the labelling of its connectivity.

Based on our quantitative analyses of the distribution of the **connectivity in the region of the primate cortex responsible for tactile functions** we proposed that intra-areal connections are important in integrating information across fingers, while inter-areal connections are important in maintaining input localization during hand movement. This finding significantly contribute to our understanding about the role of intra-areal and inter-areal cortical interactions in information processing.

We proposed **a new feedback model** of the dynamics of gene expression and protein synthesis on the basis of experimental findings. We built a stochastic kinetic model to investigate and compare the "traditional" and the feed-back model of genetic expression processes. Qualitative and quantitative changes in the shape and in the numerical characteristics of the stationary distributions of proteins and RNA molecules suggest that more combined experimental and theoretical studies should be done to uncover the details of the kinetic mechanisms of gene expressions.

A **statistical learning based visual solution** developed and applied for fault detection in industrial environment. As a mobile vision system the area of use was the automatic detection of rare faults in complex assembled objects. The object detection, the fore- and background separation, and the multi-model database enables the system to manage irregular batches of the different objects. A multi-model database guarantees that the object is compared with the statistically most relevant model, therefore it reduces the number of false alarms. The developed system is able to detect faults with the size of 2% of the total picture based on previously learned models (Fig. 1).

Ph.D student

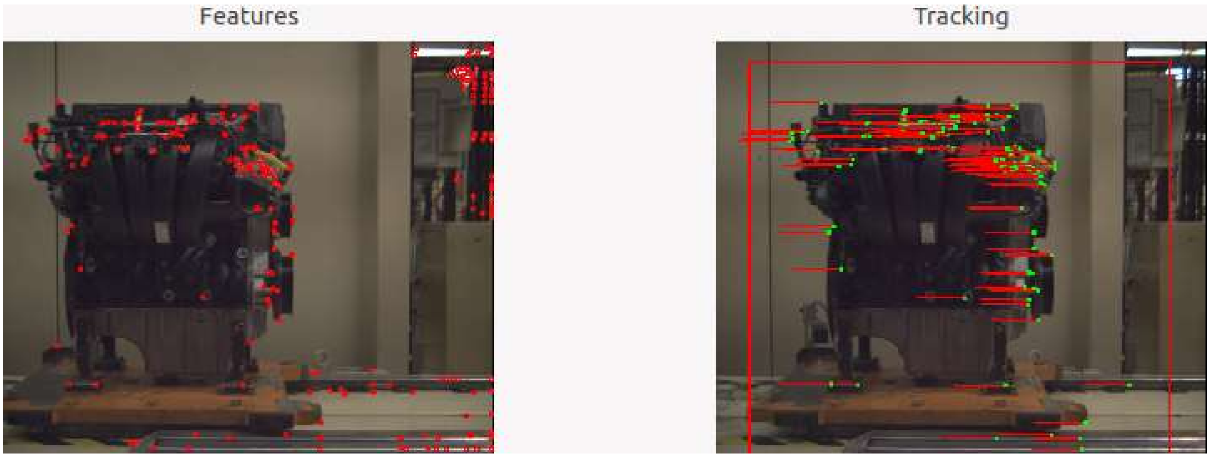

Figure 1. *Identification and tracking of the features on an engine running on the conveyor track, based on statistical learning.*

Starting in August, 2016 our group expanded its interest from purely theoretical work in the field of neuroscience to be capable of **generating in-house data** used in model creation and validation. Supported by the Wigner Research Group Grant and the Department of Anatomy, Histology and Embryology of Semmelweiss University (SU) we have been setting up an experimental electrophysiology laboratory at SU. Data collection for developing an animal model of cognitive symptoms associated with Schizophrenia started in October and recording of the first of two major datasets was completed in December. Besides collecting original data students are also trained in this newly formed laboratory to learn the necessary techniques to handle data acquisition equipment, work with experimental animals and analyze data.

Using the formal apparatus of concentration inequalities we clarified the **asymptotic behaviour of regularity-based model fitting** in graphs. We proved that the fitting and model selection procedure converges and gives either optimal result or ends in a result close to the optimal solution.

We applied regularity-based classification of detrended fMRI voxel time series in healthy young adults and have found significant overlaps in partitions corresponding to resting and 2-back states, suggesting task-related structured activity in the resting state.

International cooperations

Stem Cell and Brain Research Institute, French Institute of Health and Medical Research, (Lyon, France) Multiscale and multimodal analyses of brain signals using new neuro-probes (Emmanuel Procyk - László Négyessy, Zoltán Somogyvári)

VTT Technical Research Centre of Finland (Espoo, Finland), Regular structure in networks and graphs (Hannu Reittu – Fülöp Bazsó)

Oregon Health & Sciences University, (Portland, OR, USA) és Interdisciplinary Institute of Neuroscience and Technology Yuquan Campus, Zhejiang University (38 Zheda Road, Hangzhou, Zhejiang, China) Imaging and mapping sensorimotor circuits in the primate (Anna Wang Roe – László Négyessy).

Neuroscience Research Unit, Pfizer Global Research and Development, Cambridge, MA, USA. Tau-pathology in Alzheimer’s disease (Liam Scott – Tamás Kiss)

Translational Neuropharmacology, Section of Comparative Medicine, Yale University School of Medicine, New Haven, CT 06520, USA. Tau-pathology in Alzheimer’s disease (Mihály Hajós – Tamás Kiss)

Universiteit van Amsterdam, Netherland. Investigating the canonical organization of neocortical circuits for sensory integration (Conrado Bosman and Unberto Olcese – László Négyessy, Zoltán Somogyvári)

Institut national de la santé et de la recherche médicale, INSERM, Lyon, France. Investigating the canonical organization of neocortical circuits for sensory integration (Luc Gentet – László Négyessy, Zoltán Somogyvári)

Danish Research Institute of Translational Neuroscience, DANDRITE, Aarhus, Danish Kingdom. Electrophysiological recordings and manipulation of single neurons in behaving animals (Duda Kvitsiani – Zoltán Somogyvári)

Grants

NKFIH OTKA K-113145, Micro-electric imaging: modeling, source reconstruction and causality analysis for multi-electrode arrays. (Zoltán Somogyvári, 2015-2018)

ERA-NET FLAG-ERA, Human Brain Project, NKFIH NN-118902: “CANON – Investigating the canonical organization of neocortical circuits for sensory integration”. (L Négyessy & Z Somogyvári Pis, 2016-2018)

NIH: „Neural basis of tactile object perception in SI cortex” (consortial subaward to L Négyessy, 2016-2019)

French-Hungarian Bilateral Intergovernmental S&T Cooperation TET14FR_C85E25D3_eBrain:

Publications

Articles

1. Bruck P, Réthy I, Szente J, Tobochnik J, Érdi P: Recognition of emerging technology trends: class-selective study of citations in the U.S. Patent Citation Network. ***SCIENTOMETRICS*** 107:(3) 1465-1475 (2016)

2. Érdi P, Bruck P: Patent citation network analysis: Ranking: From web pages to patents. ***LECT NOTES ARTIF INT*** 9886 544 (2016) In: 25th International Conference on Artificial Neural Networks, ICANN 2016. Barcelona, Spain,: 06-09-2016 – 09-09-2016

3. Érdi P: Patent citation network analysis: Topology and evolution of patent citation networks. ***LECT NOTES ARTIF INT*** 9886 543 (2016) In: 25th International Conference on Artificial Neural Networks, ICANN 2016. Barcelona, Spain,: 06-09-2016 – 09-09-2016

4. Fekete Z, Pálfi E, Márton G, Handbauer M, Bérces Zs, Ulbert I, Pongrácz A, Négyessy L: Combined in vivo recording of neural signals and iontophoretic injection of pathway

tracers using a hollow silicon microelectrode. ***SENSOR ACTUAT B-CHEM*** 236: 815-824 (2016)

5. Kamalaldin K, Salome A, Érdi P: Modelling ebola. ***SCI PROG*** 99:(2) 200-219 (2016)

6. Kantor O, Mezey S, Adeghate J, Naumann A, Nitschke R, Enzsoly A, Szabo A, Lukats A, Nemeth J, Somogyvari Z, Volgyi B: Calcium buffer proteins are specific markers of human retinal neurons. ***CELL TISSUE RES*** 365:(1) 29-50 (2016)

7. Kantor O, Benko Z, Enzsoly A, David C, Naumann A, Nitschke R, Szabo A, Palfi E, Orban J, Nyitrai M, Nemeth J, Szel A, Lukats A, Volgyi B: Characterization of connexin36 gap junctions in the human outer retina. ***BRAIN STRUCT FUNCT*** 221: 2963-2984 (2016)

8. Scott L, Kiss T, Kawabe TT, Hajós M: Neuronal network activity in the hippocampus of tau transgenic (Tg4510) mice. ***NEUROBIOL AGING*** 37: 66-73 (2016)

9. Érdi P: Kémiai kinetika, ahogy azt látni kell és lehet (Chemical kinetics, as should and can be seen, in Hungarian) ***ALKALMAZOTT MATEMATIKAI LAPOK*** 33:(2) 121-128 (2016)

10. Pálfi E, Ashaber M, Palmer C, Friedman RM, Roe AW, Négyessy L: Neuronális összeköttetések a szomatoszenzoros kérgi area 3b és area 1 kézreprezentációs területén főemlősökben (Neuronal connections within the hand representation in areas 3b and 1 of the somatosensory cortex in primates, in Hungarian). ***ORVOSI HETILAP*** 157:(33) 1320-1325 (2016)

Conference proceeding

11. File B, Klimaj Z, Somogyvári Z, Kozák LR, Gyebnár G, Tóth B, Kardos Z, Ulbert I, Molnár M: Age-related changes of the representative modular structure in the brain. In: *Proc. 6th International Workshop on Pattern Recognition in Neuroimaging, PRNI Trento, Italy, 2016 22-06-2016 – 24-06-2016*. IEEE, Seattle, (ISBN:9781467365307) Paper 7552346, pp. 1-4, 2016

Book chapters

12. Érdi P, Bányai M: Introduction to cognitive systems. In: Angelov (ed.): *Handbook on Computational Intelligence*. Singapore: World Scientific (ISBN:978-981-4675-00-0) pp. 317-356, 2016

13. Somogyvári Z, Érdi P: Forward and backward modelling: from single cells to neural population and back. In: Kozma R, Freeman WJ (eds*.): Cognitive Phase Transitions in the Cerebral Cortex - Enhancing the Neuron Doctrine by Modeling Neural Fields. (Studies in Systems, Decision and Control; 39)* Springer International Publishing. (ISBN:9783319244068) pp. 135-146, 2016.

Others

14. Somogyvári Z, Zalányi L: Biofizika (Biophysics, in Hungarian). In: *Simon-Székely Attila (ed.): Lélekenciklopédia: A lélek szerepe az emberiség szellemi fejlődésében.* Budapest: Gondolat Kiadó, (ISBN:978 963 693 710 2) pp. 355-374 (2016).

R-F. Holographic quantum field theory

"Momentum" research team

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Subtitle. — Gluon scattering amplitudes in the simplest interacting 4D gauge theory and exact mass-coupling relation for the homogeneous sine-Gordon model

The electromagnetic, weak, strong and gravitational forces are the four fundamental interactions of Nature: The first two are unified by the electro-weak quantum gauge theory and have been tested with very high precision. The strong interaction is also formulated as a quantum gauge theory but tested analytically at high energies only, where the interaction is effectively weak. The gravitational interaction can be formulated as a classical gauge theory but does not allow a satisfactory quantum field-theoretical formulation. Thus the language of Nature seems to be gauge theories, but there is no analytically solved strongly interacting quantum gauge theory yet.

The unification of all fundamental forces into one single theory is a dream of theoretical physicists. String theory, which replaces point particles with one-dimensional string-like objects could provide such a unification. Strings move in space-time such that they minimize the area of the two dimensional (2D) surface they sweep: the worldsheet. The theory can be formulated as a 2D quantum field theory on this worldsheet; however, consistent quantization requires the space-time to be 10 dimensional. In order to understand how 4D Minkowski space and the Standard Model emerge from this theory, one has to solve string theory on compactified curved backgrounds, which is one of the most relevant unsolved problems in this field. It includes the determination of the masses of string excitations, such as gauge bosons and matter particles, and their interaction strengths. Ideally, it would explain the origin of the parameters of the Standard Model.

The holographic duality conjecture gives a hope to understand the strong interaction and quantum gravity in one turn, as it relates strongly-coupled gauge theories to semi-classical string theory, and the deeply quantum string theory to perturbative gauge theory. The duality is a kind of holography, as it proposes an equivalence between string theory in an open curved space and a strongly-coupled gauge theory living on the boundary of this space, in a way that is reminiscent of an optical hologram which stores a 3D imagine on a 2D holographic plate. The best established correspondence relates the maximally supersymmetric 4D quantum gauge theory to superstring theory on the product of the 5D anti de Sitter (AdS) space and the 5D sphere (AdS5×S5) (Fig. 1).

The evolution of string states are calculated in the path integral formulation by summing up all string configurations connecting the initial to the final string state. The action is proportional to the area of the worldsheet and the proportionality constant, g, is a

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combination of the string tension and the AdS radius. It plays the role of the inverse of the Planck constant as quantum corrections go with inverse powers of g.

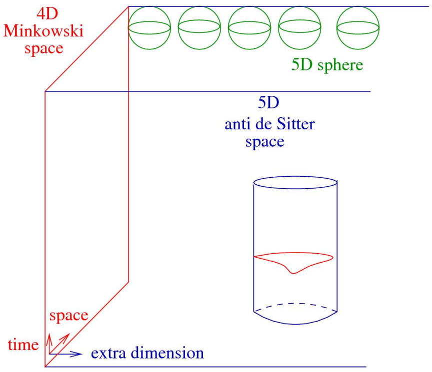

Figure 1. *In the holographic description our 4D Minkowski space, indicated by red on the figure, is the holographic boundary of the 5D anti de Sitter space (blue):* AdS_5*. Above each point a 5D sphere is added (green):* S^5*. The evolution of a closed string state is shown. The 2D surface swept by the moving strings is called the worldsheet. The dynamics tries to minimize the area of this worldsheet.*

On the other side of the duality we have the simplest interacting 4D *SU(N)* gauge theory, where *N* denotes the number of colors (3 for QCD). It has the maximal amount of (super) symmetry and considered to be the hydrogen atom of all gauge theories. Due to the large amount of symmetry all fields are *N* by *N* traceless matrices, which create massless particles, whose couplings are completely fixed up to an overall coupling constant g_{YM}. The theory is invariant not only under scale transformations but also under conformal transformations, i.e. coordinate transformations that preserve angles. In conformal invariant theories the small volume, ultraviolet, and the large volume, infrared scales can be mapped to each other thus they manifest the same physical phenomena. In particular, the scattering matrices of the massless particles can be mapped to the vacuum expectation values of light-like Wilson loops. These Wilson loops can be obtained by drawing consecutively the particles' momenta and momentum conservation guaranties, that the lines close forming a light-like polygon.

In perturbation theory the 't Hooft coupling, $\lambda=N(g_{YM})^2$ measures the number of loops, while 1/*N* the genus, that is adding one more handle on the surface introduces a factor *1/N*. For weak couplings it is enough to sum a few diagrams with a few vertex, however at strong couplings dense surfaces of Feynman graphs contribute dominantly. The intuitive understanding of the duality is that the gauge theory dynamics tries to minimize the surface of dense Feynmann graphs like if it were a string worldsheet in the AdS_5xS^5 background. It is conjectured that the 't Hooft coupling is related to the string tension as $g=\lambda/(2\pi)$. This actually shows why the duality is a conjecture, since perturbative gauge theory provides an expansion for small *g*, while the quantization of classical strings is an expansion in *1/g*.

In the case of gluon scattering amplitudes perturbative calculations are reliable at small couplings. At strong couplings, however, we can use the dual picture and calculate the vacuum expectation value of the light-like polygonal Wilson loop. This is equivalent to the determination of the minimal surface, which can be spanned over the polygon, similarly how, the soup film stretches over the frame (Fig.2).

The shape of the two dimensional surface is dictated by the dynamics of strings. As string theory on the AdS background is integrable, the determination of the minimal surface can be obtained by solving the thermodynamic Bethe ansatz equations of the string sigma model. The analytic expansion of these equations requires the calculation of the *mass-coupling relation in a multi-scale model*.

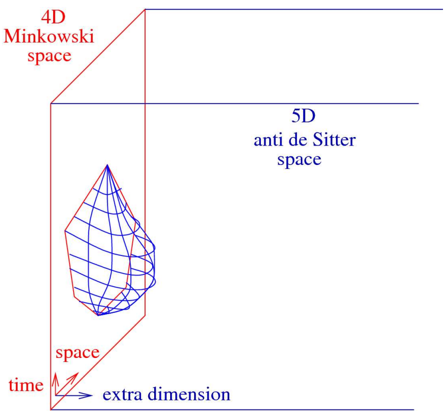

Figure 2. *Gluon scattering amplitudes are equivalent to the vacuum expectation values of light-like polygonal Wilson loops, indicated by a red polygon at the Minkowski boundary of AdS space. At strong coupling the amplitude can be calculated by evaluating the area of the minimal surface in AdS space with the boundary polygon, drawn by the blue net.*

One of the most difficult problems in a quantum field theory is to determine the mass-coupling relation i.e. the relation between the renormalized couplings related to the Lagrangian definition of the theory and the physical masses. Such an exact relation would express for example the dynamically generated nucleon mass in the chiral limit of quantum chromodynamics in units of the perturbative Lambda-parameter Λ. The difficulty lies in the fact that the Lagrangian is defined at short distances (or –UV– scale), while the masses are the parameters at large distances (or –IR– scale).

There is one family of models where such a relation can be found exactly, namely, two dimensional integrable models. The mass/Λ ratio was indeed exactly determined in the non-linear sigma (NLS) model. To this end, one adds an external field coupled to one of the conserved charges, calculates the free energy perturbatively on the UV side, and compares it to the large field expansion from the Bethe Ansatz integral equation/the thermodynamic Bethe Ansatz (TBA) equation on the IR side.

In contrast to the NLS model with marginally relevant perturbations, there is also a large class of integrable models which can be defined as perturbations of their UV-limiting conformal field theories (CFTs) by strictly relevant scaling operators. In this case, coupling constants are dimensional, and one can show that they are not renormalized in the perturbative CFT scheme and hence are physical themselves. When a model in this class has only one perturbing operator, the relation between the coupling constant and the (lowest) physical mass boils down to a single proportionality constant. This non-trivial constant was determined as well by the method described above for the sine-Gordon and affine-Toda field theories and their reductions.

A common feature of all these models is that they have only one mass scale. In some of these models the particles have a non-trivial spectrum but all mass ratios are encoded in the scattering (S) matrix: the UV/IR relation is complete once the lowest mass is expressed by Λ, the coupling, or some other physical dimensionful parameter related to the Lagrangian. However, when the models have several independent perturbing operators, the particle spectrum continuously depends on the couplings and not fixed by the S-matrix. In this sense, such models can be called multi-scale, to which the method in the single-scale case is not applicable, and hence there are no results for multi-scale mass-coupling relations in the literature.

The aim of our work was therefore to provide a novel method which can fill this gap. Though our method is conceptually more general, we focused on a class of multi-scale quantum integrable models with strictly relevant perturbations, i.e., the homogenous sine-Gordon (HSG) model. We presented our ideas in particular for its simplest case with two scales. The mass-coupling relation gives the one-point functions of the perturbing operators, encoding all the non-perturbative information which is not captured by the CFT perturbation. Via the gauge/string duality, it is applied to the four-dimensional maximally supersymmetric gauge theory at strong coupling, which is one of the recent main subjects in field and string theories: it provides the missing link to derive an analytic expansion of the strong-coupling gluon scattering amplitudes.

Grants

OTKA K 109312: Holographic solutions of gauge theories (Á. Hegedűs 2013-2016)

OTKA K 116505: Integrability and the holographic duality (Z. Bajnok 2016-2019)

HoloGrav ESF Network: Holographic methods for strongly coupled systems (Z. Bajnok 2012-2016)

“Momentum” Program of the HAS (Z. Bajnok 2012-2017)

International cooperations

MTA Hungarian-Japanese bilateral: Integrability in gauge gravity duality and strong coupling dynamics of gauge theory II; Kyoto, Tokyo and Tsukuba (Z. Bajnok, 2015-2017)

MTA Hungarian-Polish bilateral: Gauge string duality and its applications; Krakow (Z. Bajnok 2013-2015)

Long term visitor

Ines Aniceto, Krakow, 2016.11.12-2016.12.10

Publications

Articles

1. Aoki S, Balog J, Onogi T, Weisz P: Flow equation for the large N scalar model and induced geometries. ***PROG THEOR EXP PHYS*** 2016:(8) 083B04/1-18 (2016)

2. Bajnok Z, Balog J, Ito K, Satoh Y, Tóth GZ: Exact mass-coupling relation for the homogeneous Sine-Gordon model. ***PHYS REV LETT*** 116:(18) 181601/1-5 (2016)

3. Bajnok Z: How integrability works (for AdS/CFT. ***ACTA PHYS POL B*** 47:(12) 2451-2477 (2016)

4. Bajnok Z, Holló L: On form factors of boundary changing operators. ***NUCL PHYS B*** 905 96-131 (2016)

5. Bajnok Z, Balog J, Ito K, Satoh Y, Tóth GZ: On the mass-coupling relation of multi-scale quantum integrable models. ***J HIGH ENERGY PHYS*** 2016:(6) 71/1-54 (2016)

6. Bajnok Z, Janik RA: The kinematical AdS(5) x S-5 Neumann coefficient. ***J HIGH ENERGY PHYS*** 2016:(2) 138/1-25 (2016)

7. Bajnok Z, Lajer M: Truncated Hilbert space approach to the 2d φ 4 theory. ***J HIGH ENERGY PHYS*** 2016:(10) 050/1-41 (2016)

8. Bajnok Z, Nepomechie RI: Wrapping corrections for non-diagonal boundaries in AdS/CFT. ***J HIGH ENERGY PHYS*** 2016:(2) 024/1-23 (2016)

9. Balog J, Zhang P: Effective potential from zero-momentum potential. ***PROGR THEOR EXP PHYS*** 2016:(10) 103B02/1-21 (2016)

10. Gombor T, Palla L: Algebraic Bethe Ansatz for O(2N) sigma models with integrable diagonal boundaries. ***J HIGH ENERGY PHYS*** 2016:(2) 158/1-33 (2016)

11. Hegedűs Á, Konczer J: Strong coupling results in the AdS 5 /CF T 4 correspondence from the numerical solution of the quantum spectral curve. ***J HIGH ENERGY PHYS*** 2016:(8) 061/1-56 (2016)

12. Tóth GZ: Weak cosmic censorship, dyonic Kerr-Newman black holes and Dirac fields. ***CLASSICAL QUANT GRAV*** 33:(11) 115012/1-23 (2016)

Other

13. Pusztai BG, Gorbe TF: Lax representation of the hyperbolic van Diejen dynamics with two coupling parameters. arXiv:1603.06710v1/1-38 (2016)

R-G. Computational systems neuroscience

"Momentum" research team

Gergő Orbán, Mihály Bányai, Merse Előd Gáspár, Dávid Gergely Nagy[#], Balázs Török[#]

Hierarchical computations in the visual system. — Understanding how the brain processes visual information requires computational models that decompose images in a way that facilitates object recognition. To validate such models, we need to derive predictions from them that may be compared to experimental recordings, while controlling for measurement confounds.

A critical aspect of modelling neural response is to assess the sources of variability in the measurable spike trains. We compared two widely used models of neural spiking in terms of predictive power regarding higher-order statistics of neural responses. Comparing our simulation results to publicly available recordings from awake monkeys revealed that the Doubly Poissonian model, which assumes that the source of variability is at he level of spike generation, is not consistent with observed changes in the correlations in response to changes in stimulus features including contrast and orientation. On the other hand, a model that assumes noise to emerge at the level of membrane potential, the Rectified Gaussian model, was demonstrated to account for stimulus-dependent modulations in repsonse statistics. We presented these results in two international conferences, and they are under review at an international journal.

The key prediction of the hierarchical model of visual responses we developed earlier is that trial-to-trial correlations of evoked spike counts in the primary visual cortex (V1) are dependent on the stimulus content. Importantly, a part of this stimulus dependence of correlations is assumed to originate from areas processing higher-level percepts. A critical consequence of this assumption is that stimulus-dependence of correlations are present when complex, highly structured stimuli are precessed by the visual system, but vanish when higher-level structure is absent from images. We designed experiments that specifically test whether visual stimuli eliciting higher-order percepts elicit more specific correlational patterns than stimuli containing independent features. We recorded neural responses from the V1 of macaques performing an attention task at the Ernst Strüngmann Institute in Frankfurt. The results confirmed the prediction of our model. We also investigated what types of image structure elicit similar specificities without photorealistic information, revealing intermediate stages of cortical processing. Our results corroborated the earlier finding that the secondary visual cortex is involved in the representation of textures. The results are currently being prepared for publication.

Normative analysis of memory processes. — In the preceding years we have developed a theory of the interactions of episodic a semantic memory, according to which the dynamics of these memory systems is optimised for dealing with the problem of iterative structure learning and model selection in high dimensional data and complex model spaces. Our

[#] Ph.D. student

sequential Monte Carlo approximation algorithm made it possible to apply this model to larger datasets. We have published these results in a proceedings article, while also presenting them in multiple international and Hungarian conferences. The scaling up made possible by the approximation revealed that the selection of episodes from the contents of episodic memory to integrate into the statistical model is critical. Consequently, we have developed a procedure for the optimisation of this selection, however this requires further analysis.

It would be an important extension of our model if we were able to show that episodic memory makes structure learning possible in the more realistic situation where episodes are compressed in a non-invertible way. For modelling this compression, we propose an encoding where the brain uses latent state variables in a hierarchical probabilistic model of the environment, and higher level variables are prioritised over lower level details. This gives diverging predictions from current accounts of episodic reconstruction, which can be tested experimentally.

Perception in the brain, especially the visual processing, what we have studied mainly, has a hierarchical structure. The role of a cortical area, representing a hierarchical level, is essentially the re-representation of information in a form to facilitate recognition and classification of higher level complex objects. To achieve these complex representations the nervous system utilizes non-linear transformations at all levels. Previous studies have characterized this process with the full extent of the information at each level. We put the emphasis on the structure of the information. Easily decodable information is considered to be a more relevant quantity. We quantify this by linear decodability which can be plausibly realized by a neuronal layer at the next hierarchical level.

Contribution of firing rate nonlinearity to optimal cortical computations. — Processing of visual information in the brain is performed in a hierarchical structure. The role of a cortical area that forms a level of the processing hierarchy can be phrased as the re-representation of information in a form to facilitate recognition and classification of higher level, or more complex features. To achieve these complex representations the nervous system utilizes non-linear transformations at all levels. Previous studies have characterized this process with the full extent of the information at each level. We put the emphasis on the structure of the information. Easily decodable information is considered to be a more relevant quantity. We quantify this by linear decodability of information, since a linear decoder can be plausibly realized by a neuronal layer at subsequent levels of the hierarchy.

Recently, several studies have shown that the structure and the statistical characteristics of the nervous system adapt to the statistics of the environment. The subject of our investigation is the adaptation of the dynamics at the cellular level. We examined this through the effect of the so-called firing rate nonlinearity on the quality of information that can be decoded from a population of neurons. A critical feature of sensory neurons is their mixed sensitivity: a neuron is sensitive to multiple features of the stimulus, which in the case of simple cells of V1 comprises orientation, phase, spatial frequency and contrast. These mixed sensitivities pose a critical challenge for decodability: when some of these parameters are unknown, areas downstream in the processing hierarchy need to integrate over these features. We point out, however, that when integration occurs, linear decoding becomes ineffective: orientation cannot be decoded while other parameters are unknown. In our investigations we have pointed out that in the absence of unknown parameters decoding from membrane potential is effective and no nonlinearity is required. However, in the presence of any of these so-called nuisance parameters a nonlinearity is necessary for efficient decoding. At higher levels of the computational hierarchy the number of nuisance parameters grows, therefore the importance of nonlinearity becomes even more pronounced.

Beyond demonstrating the necessity of a non-linearity in the processing we have also shown quantitatively that the form of the nonlinearity implemented by cortical neurons is optimal for decoding. Based on the form of firing rate nonlinearity we have derived a prediction for the optimal firing threshold of V1 neurons that could be contrasted with intracellular measurements for V1 simple cells. We found a qualitative match between predicted and measured thresholds. Our results were presented on a poster at an international conference and in Hungary and at a prestigious international conference in the US. A publication is in preparation. In the future, we plan to study consistency between shapes of non-linearities at adjacent hierarchical levels on the basis of our normative linear decoding principle. We plan to extend our investigations on higher level with more realistic non-local decoding tasks connected to pattern recognition.

Disentangling learning-dependent and learning-independent processes in human implicit learning. — Investigating human learning and decision making in dynamical environments in a general setting could allow one to understand the common principles relating intuitive physics, natural language understanding and theory of mind. Higher-level representations in temporal domains could then be measured for each individual.

We contributed to developing and improving methods for inferring human representations. To gather information in high-dimensional spaces, one requires a large number of data points during a learning process to identify the model forms individuals use during a learning task. The generative process of behavioural responses is, however, highly confounded with learning-independent effects. We developed a method for segregating the variation in response time measurements that are related to such confounds from the variation induced by learning. As a result of our analysis, we concluded that the confounds may impose a much larger effect on the response times than learning itself, rendering filtering or other form of accounting for confounds essential for inference. We could demonstrate that using the method developed in this study can increase the predictive power a learning-based model. Our work was presented at two international conferences and is now in review at a journal for publication.

Grants

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NAP-B National Programme for Brain Research (G. Orbán, 2015-)

International cooperation

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Central European University (Budapest), J. Fiser

Ernst Strüngmann Institute (Frankfurt, Germany), W. Singer, A. Lazar

Publications

Article

1. Orbán G, Berkes P, Fiser J, Lengyel M: Neural variability and sampling-based probabilistic representations in the visual cortex. ***NEURON*** 92:(2) 530-543 (2016)

Conference proceeding

2. Nagy DG, Orbán G: Episodic memory as a prerequisite for online updates of model structure. In: Proc. 38th Annual Meeting of the Cognitive Science Society, Philadelphia, Pennsylvania, USA, 10-08-2016 – 13-08-2016. Eds.: Papafragou A, Grodner D, Mirman D, Trueswell J, Cognitive Science Society, 2016. pp. 2699-2704. (ISBN:978-0-9911967-3-9)

See also: R-E.12

R-I. "Lendület" innovative gaseous detector development

"Momentum" research team

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After the infrastructure developments of the previous years, the activities of the group were focused on detector development and detector physics research. This includes contributions to specific CERN experiments, such as the ALICE, NA61 and RD51. Relevant detector physics projects were financed by H2020 grants. In the field of cosmic muon imaging, novel methods and novel detector systems were established, leading to a Japanese-Hungarian utility patent.

Contributions to CERN Collaborations. — The group's participation, along with the Hungarian ALICE Group, is now clearly established within the Time Projection Chamber (TPC) Upgrade Collaboration. Budapest will be one of the two Advanced Quality Assurance testing sites, that is, half of the foils which will be built into the new ALICE TPC readout will pass through our lab. Within the framework of the NA61 Collaboration, new TPC-s will be built to capture the forward particles, highly relevant for neutrino factories. The RD51 Collaboration establishes the basis for R&D for gaseous detectors, and is correlated with the AIDA-2020 participation of the group.

Detector physics results. — The most relevant results of the group are related to detector physics, that is, the fundamental questions in the operation of gaseous detectors. Gas Electron Multipliers (GEM-s) are particularly interesting, both as a highly relevant Micro-Pattern Gaseous Detector (MPGD) type with very confined amplification region, and as a popular actual advanced detector technology (also used in the ALICE TPC Upgrade).

By understanding the cascaded steps in the multiplication process (Fig. 1, left), one can trace the energy resolution of GEM-s, dominated by avalanche fluctuations. The inverse of the energy resolution can be experimentally found to linearly increase with the inverse of the effective GEM gain (Fig. 1, right), to first order independently from absolute gain and from gas type.

A statistical calculation leads to an analytic formula for the effective gain fluctuations, as a function of the true avalanche fluctuation f (ratio of spread over mean) as well as transfer and collection parameters, which explicitly predicts the resolution dependence on the inverse of the effective gain G:

$$f_{all}^2 = (\frac{1+f^2}{c} - 1) + \frac{1}{G}(1 - t + F^2)$$

[#] Ph.D. student

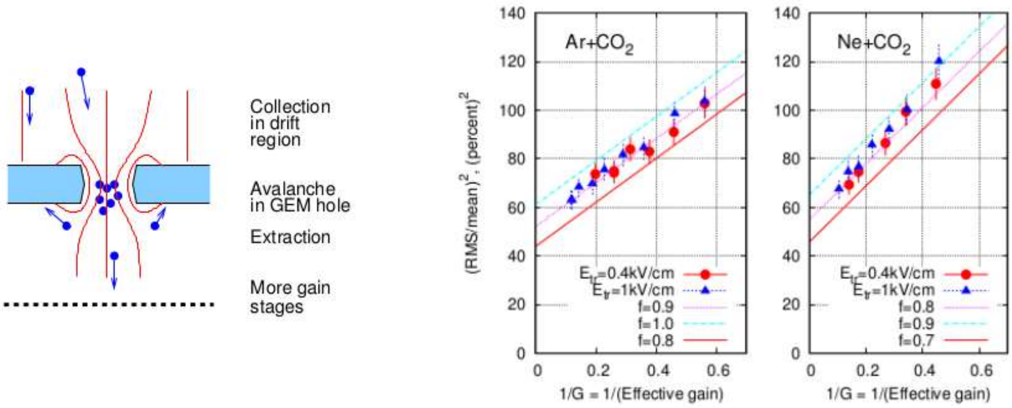

Figure 1. *Relevant cascaded processes in a GEM amplification stage (left panel), including collection, avalanche fluctuation and extraction before subsequent gain stages. Analytic calculation predicts that the inverse of the resolution (right panel) linearly depends on the inverse of the effective gain G.*

Even more interesting is to establish the *avalanche size distribution initiated by single electrons,* as this has been directly measured in various gases. Fig. 2 left panel shows a typical pulse height distribution for very low UV photon irradiation: if there is no photo-electrons induced, a sharp peak appears, whereas a single photo-electron distribution clearly departs from the noise peak. In this measurement, 2 or more photo-electrons (Poissonian) contribution is very small, thus making this measurement very clear for the first time.

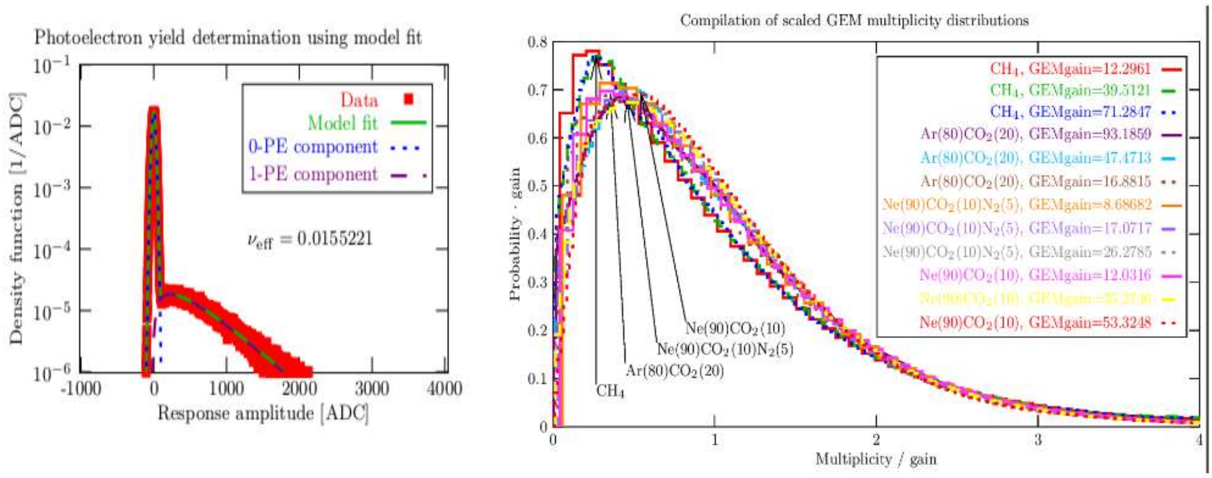

Figure 2. *Signal amplitude (left panel) from UV photons, showing typically 0 (sharp peak) and 1 photo-electron responses. The amplitude distribution clearly departs from the typical exponential distribution. For various gases, the signal amplitude (right panel) shows similar non-exponential feature, strongly depending on gas composition.*

On the right panel of Figure 2, the extracted single electron avalanche distributions are shown, normalized to a mean of 1, in different gases. There is a clear trend indicating that gases with higher ionization potential show stronger departure from a pure exponential distribution, observed regularly in Multi-Wire Proportional Chambers (MWPC).

Imaging with cosmic muons. — The application of cosmic muons for large scale imaging has been a research direction in the group in the previous years. Collaboration with the Novi Sad University (Serbia) has led to a novel imaging technique, which utilizes secondary emission. When cosmic particles, mainly muons, cross any material, a gamma photon (with energies from few keV up to few MeV) may be emitted coincidentally. Registering the particle trajectory along with the energy deposit in a gamma counter, one can visualize those tracks which were responsible for the emission: this possibility is demonstrated on the left panel of Figure 3. A key advantage of the approach in comparison to earlier techniques is that it is sensitive for low atomic number materials as well. The method may find its application in imaging where X-ray irradiation is undesirable.

An important application for cosmic muons detectors, developed in the last years by the group, is imaging the interior of volcanos. This direction was pursued by Japanese and various European groups. Given the fact that gaseous tracking detectors, and in our case, a specific type of an MWPC, are highly competitive with the traditional scintillators in terms of cost, weight and power consumption, a utility patent has been filed in Japan, owned jointly by Wigner RCP and Tokyo University, for the so called "Muography Observation Instrument". A first prototype of the detector, installed at the Wigner campus, is shown on the right panel of Figure 3. The detector shows excellent long term performance, sustaining high efficiency at varying environmental conditions.

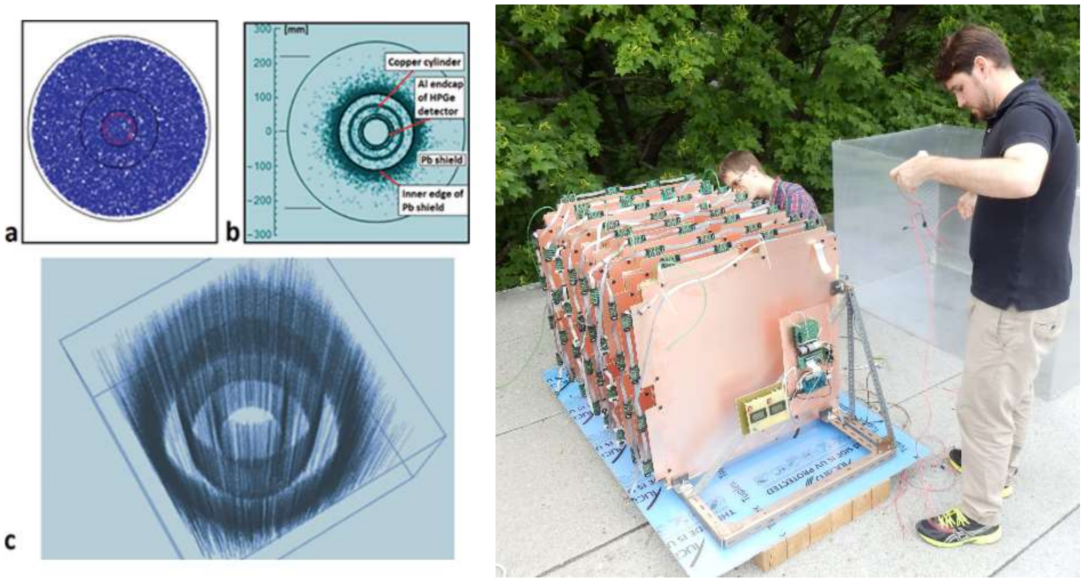

Figure 3. *A new imaging technique involving secondary emission can be used to visualize low atomic number materials: on the left panel, the middle ring appears for those tracks which had a coincident gamma photon in the HPGe detector. The right panel shows the prototype of a large size imaging system installed outdoor.*

Grants

"Momentum" Program of the HAS (D. Varga, 2013-2017)

AIDA-2020 (Advanced European Insfrastructures for Detectors at Accelerators), H2020 support (D. Varga, 2015-2018)

BrightnESS (Research Infrastructure for ESS), H2020 support (D. Varga)

International cooperation

CERN NA61 Collaboration (A. László), CERN RD51 Collaboration (D. Varga), CERN ALICE TPC Upgrade Collaboration (D. Varga)

Earthquake Research Institute, Tokyo Uni., Muography for Volcano Monitoring (L. Oláh, D. Varga)

University of Novi Sad (Serbia), Novel Imaging Methods (L. Oláh, D. Varga)

Publications

Articles

1. Bikit I, Mrdja D, Bikit K, Slivka J, Jovancevic N, Oláh L, Hamar G, Varga D: Novel approach to imaging by cosmic-ray muons. ***EUROPHYS LETT*** 113:(5) 58001/1-4 (2016)

2. László A: A natural extension of the conformal Lorentz group in a field theory context. ***INT J MOD PHYS A*** 31:(28-29) 1645041/1-11 (2016)

3. László A: Convergence and error propagation results on a linear iterative unfolding method. ***SIAM J UNCERTAIN QUANT*** 4:(1) pp. 1345-1371. (2016)

4. László A, Hamar G, Kiss G, Varga D: Single electron multiplication distribution in GEM avalanches. ***J INSTRUM*** 11: Paper P10017. 25 p. (2016)

5. Magnani A et al. (158 authors) incl. Bencze G, Endrőczi G: Impact of the GE1/1 upgrade on CMS muon system performance. ***NUOVO CIMENTO C*** 39:(1) 260 (2016)

6. Mitra J, Khan SA, Marin MB, Cachemiche J-P, David E, Hachon F, Rethore F, Kiss T, Baron S, Kluge A, Nayak TK: GBT link testing and performance measurement on PCIe40 and AMC40 custom design FPGA boards. ***J INSTRUM*** 11:(3) C03039/1-13 (2016)

7. Mrdja D, Bikit I, Bikit K, Slivka J, Hansman J, Oláh L, Varga D: First cosmic-ray images of bone and soft tissue. ***EUROPHYS LETT*** 116:(4) 48003/1-5 (2016)

8. Oláh É, Ádám P, Béni N, Hamar G, Horváth Á, Horváth D, Jancsó G, Jarosievitz B, Lévai P, Péntek C, Sükösd C, Szillási Z, Trócsányi Z, Újvári B, Vámi T, Varga D: Particle physics education in Hungary. ***NUCL PART PHYS P*** 273-275: 2569-2571 (2016)

9. Oláh L, Surányi G, Barnaföldi GG, Bemmerer D, Hamar G, Melegh HG, Varga D: Cosmic background measurements at a proposed underground laboratory by the REGARD muontomograph. ***J PHYS CONF SER*** 665:(1) 012032/1-4 (2016)

10. Vai I e al. (156 authors) incl. Bencze G, Endroczi G: Development and performance of triple-gem detectors for the upgrade of the muon system of the cms experiment. ***NUOVO CIMENTO C*** 39:(1) 269/1-3 (2016)

11. Varga D: Analytic approximation of energy resolution in cascaded gaseous detectors. ***ADV HIGH ENERGY PHYS*** 2016 8561743/1-8 (2016)

12. Varga D, Nyitrai G, Hamar G, Oláh L: High efficiency gaseous tracking detector for cosmic muon radiography. ***ADV HIGH ENERGY PHYS*** 2016 1962317/1-11 (2016)

13. Abbaneo D et al. incl. Bencze G, Endrőczi G (158 authors): Status report of the upgrade of the CMS muon system with Triple-GEM detectors. ***NUCL INSTRUM METH A*** 824: 521-525 (2016) Frontier Detectors for Frontier Physics: Proceedings of the 13th Pisa Meeting on Advanced Detectors.

14. Abbaneo D et al. incl. Bencze G, Endrőczi G (159 authors): Design of a constant fraction discriminator for the VFAT3 front-end ASIC of the CMS GEM detector. ***J INSTRUM*** 11:(1) C01023/1-10 (2016)

15. Abbaneo D et al. incl. Bencze G, Endrőczi G (161 authors): Fiber Bragg Grating (FBG) sensors as flatness and mechanical stretching sensors. ***NUCL INSTRUM METH A*** 824: 493-495 (2016)

Conference proceeding

16. Ortiz A, Bencédi Gy, Bello H, Jena S: Jet effects in high-multiplicity pp events. In: Proc. of the workshop MPI@LHC 2015 Trieste, Italy, 23-11-2015 – 27-11-2015, Eds.: Gunnellini P, Diehl M, Jung H Verlag Deutsches Elektronen-Synchrotron, Hamburg, 2016. pp. 215-219. (ISBN:978-3-945931-01-1)

Other

17. László A: A tanítómester (The master teacher, in Hungarian) ***FIZIKAI SZEMLE*** 66:(9) 301-302 (2016)

See also: R-B.1,R-B ALICE Collaboration, R-H NA49 Collaboration, R-H NA61 Collaboration

R-K. Femtosecond spectroscopy and X-ray spectroscopy

“Momentum” research team

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Pump-probe experiments are powerful structural dynamics tools, which apply an ultrashort laser excitation pulse, and study the time evolution of the system with a probe pulse at chosen time delays. Unveiling the details of the relaxation processes that follow the light excitation can lead to a complete understanding of the involved mechanisms, which, for instance, shall promote the design of more efficient functional molecules. Here we report on experimental results and technical developments using femtosecond X-ray probes in time-resolved investigations of transition metal complexes that are model systems for molecular switches or chromophores of light harvesting systems. The experimental work is aided by quantum chemistry and quantum dynamics calculations.

Photoswitching of the spin state in transition metal complexes: separating the different time responses for the changes in the electronic structure, in the molecular structure, and in the molecular environment. — Photoswitchable molecular compounds have great potential in information technology as molecular switches or storage systems. The typical model system for these compounds is the $[Fe(bpy)_3]^{2+}$ complex (bpy: 2,2’-bipyridine), where the molecule of a $3d^6$ electron configuration can be excited to a quintet state from its singlet ground state, by populating antibonding orbitals, leading to a large expansion. This multi-step process has been intensively studied in pump-probe experiments. We have revisited this system using X-ray probes with subpicosecond time resolution, combining the spin momentum sensitivity of X-ray emission spectroscopy (XES) and the structural sensitivity of X-ray diffuse scattering (XDS), to simultaneously probe changes in the electronic and molecular structure, as well as in the solvent environment. The experimental setup and the results are summarized in Fig. 1. Although the time resolution in this experiment was smeared to about 500 fs by the large time jitter between the laser and X-ray pulses, the time scale of the mentioned changes could be obtained, as shown in the right side of Fig. 1. More importantly, the experiment also revealed the consecutive nature of these processes: the change of the molecular structure follows the almost prompt change of the electronic structure with a substantial lag of 400 fs, while the density and temperature increase of the solvent surrounding the molecule takes place almost 1 ps after the excitation. This result demonstrates the potential of the combination of femtosecond X-ray techniques, and future experiments, with better resolution can shed more light on the intricate details of the transition processes on the femtosecond time scale.

[#] Ph.D. student

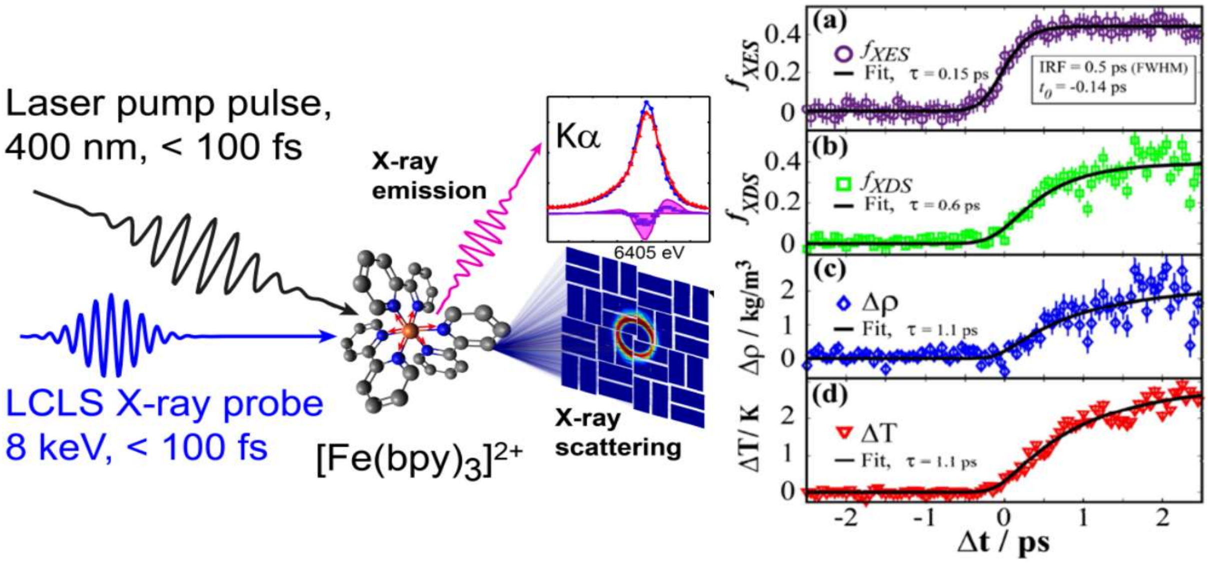


Figure 1. *(Left) Time resolved X-ray techniques applied to photoexcited $[Fe(bpy)_3]^{2+}$. (Right) The XES intensity variation shows **(a)** the change of the electronic structure (the increase of the total spin momentum on the Fe), while **(b)** the changes of the molecular structure (i. e., the expansion of the molecule due to the 10% elongation of the Fe–N bond length) are shown to occur with a lag of a few hundred fs. The density **(c)** and temperature **(d)** increase of the solvent environment follows the molecular changes with a larger delay, ca. 1 ps after the excitation.*

Photoswitching of the spin state in transition metal complexes: monitoring the wavepacket dynamics when reaching the high spin state. — Several complexes of Co^{2+}, having a $3d^7$ electron configuration, can also be switched between their doublet ground state and quartet excited states. This includes $[Co(terpy)_2]^{2+}$, (2,2':6',2"-terpyridine) whose excited state cannot be studied at synchrotrons due to the relatively short, 7 ps lifetime of the quartet. (The typical X-ray pulse length at synchrotrons is 50–100 ps.) Similar to the case of $[Fe(bpy)_3]^{2+}$, the spin state change induces a structural change, since in the quartet state also the e_g^* antibonding molecular orbitals are populated leading to significant Co–N bond length elongation. We have performed a similar XES+XDS investigation on this complex at the XPP instrument of the LCLS, now with improved time resolution, focussing on the short time scales. XDS not only revealed the expansion of the molecule upon the spin state transition, but an oscillatory pattern has also been observed on the subpicosecond time scale in the scattering signal, as it is seen in Fig. 2. A Fourier-transformation using a narrow sliding time window unveiled that the initial oscillation fades after 1 ps, and another pattern appears (see the inset of Fig. 2). The time behaviour of the two oscillations suggest a sequential activation of the two vibrational modes during the relaxation. These oscillations are assumed to arise from coherent vibratory relaxation into the quartet state. The oscillatory data can be fitted with two frequencies; the fit and the characteristic times are also displayed in Fig. 2. We have carried out a density functional study, which allowed us to unambiguously identify these modes. The first one agrees with the frequency of the breathing mode, while the second one corresponds to an asymmetric combined Co–N stretching mode (in which the nitrogens of the two middle and the four side rings move out of phase). Mapping of the active modes of the relaxation significantly contributes to the full understanding of the fine details of the structural dynamics of the system.

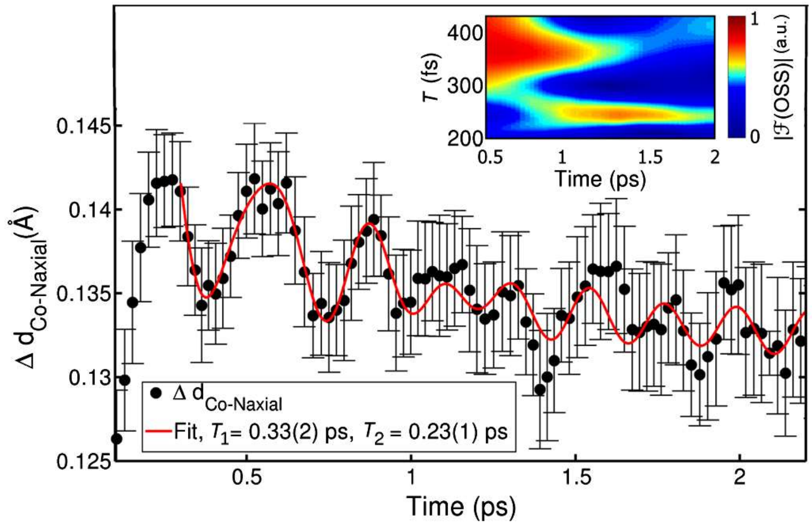
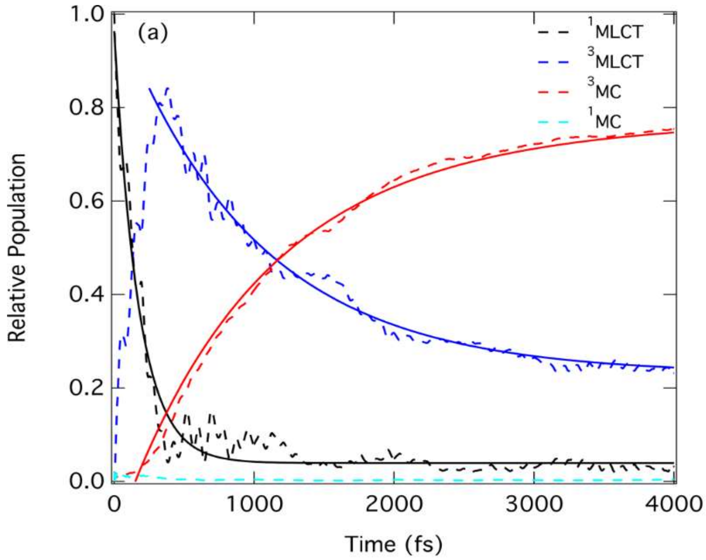


Figure 2. *Time evolution of the Co-N bond lengths in $[Co(terpy)_2]^{2+}$ upon photoexcitation as determined from XDS. The inset shows a time-resolved Fourier transform of the oscillatory part of the difference scattering signal, indicating sequential activation of two vibrational modes. The red line shows a fit, incorporating the sequential activation.*

Figure 3. *Relative populations of the ^{1}MLCT, ^{3}MLCT, ^{1}MC, and ^{3}MC states. The solid lines are exponential fits of the populations kinetics.*



Quantum nuclear wavepacket simulations of the photoexcited $[Fe(bmip)_2]^{2+}$ complex. — Quantum chemical calculations can provide potential energy surfaces; however, these alone will not permit us to unambiguously determine the relaxation pathways and to estimate lifetimes in excited molecules. An effective technique to treat the dynamics of an excited molecular system is the Multiconfigurational Time-Dependent Hartree (MCTDH) method. This has been successfully used to study singlet-triplet transitions in organic molecules; however, from the relatively large transition metals only the simpler Cu(I) ($3d^{10}$) complexes were studied before our work, which have a closed 3d shell. We have used MCTDH to study the $[Fe(bmip)_2]^{2+}$ complex, which is the first iron-based system with real potential to substitute the expensive and environmentally unfriendly Ru and Ir complexes in photosensitizers of photocatalysts or light-harvesting systems. Fe complexes have long been assumed unsuitable as photosensitizers because of their low-lying nonemissive metal-centered (MC) states, which rapidly drain the excited metal-to ligand charge transfer (MLCT) states, inhibiting electron transfer. The bmip (2,6-bis(3-methyl-imidazole-1-ylidine)-pyridine) ligand was designed to increase the ligand field and thus destabilize the MC states, which lead to an ^{3}MLCT lifetime of about 9 ps, two orders of magnitude larger than that of the vast majority of low-spin Fe(II) complexes.

Using first-principles quantum nuclear wavepacket simulations in the MCDTH framework, we have achieved a detailed understanding of the unusual photoexcited decay mechanism. We have identified 4 relevant modes as most important for the excited-state dynamics associated with relaxation into the ^{3}MC state, and performed the simulation in the four-dimensional space spanned by them.

We have found that the relaxation is dominated by an ultrafast intersystem crossing (~100 fs) from ^{1}MLCT–^{3}MLCT, proceeded by slower kinetics associated with the conversion into the ^{3}MC states. The time evolution of the state populations are shown in Fig. 3; the fitted lifetimes (100 fs, 4 ps) are in good agreement with the experimental values (100 fs, 9 ps). We were also able to identify why the ^{3}MLCT decay, important in the context of photosensitizers, is much longer than in related Fe(II) complexes. The evolution of the wavepacket density, displayed in Fig. 4, sheds a light on this. It is obvious from the figure that the wavepacket does not readily reach the crossing between the states; therefore, population transfer occurs in the region of the potential energy surface where the energy gap between the ^{3}MLCT and ^{3}MC states is large, making it inefficient.

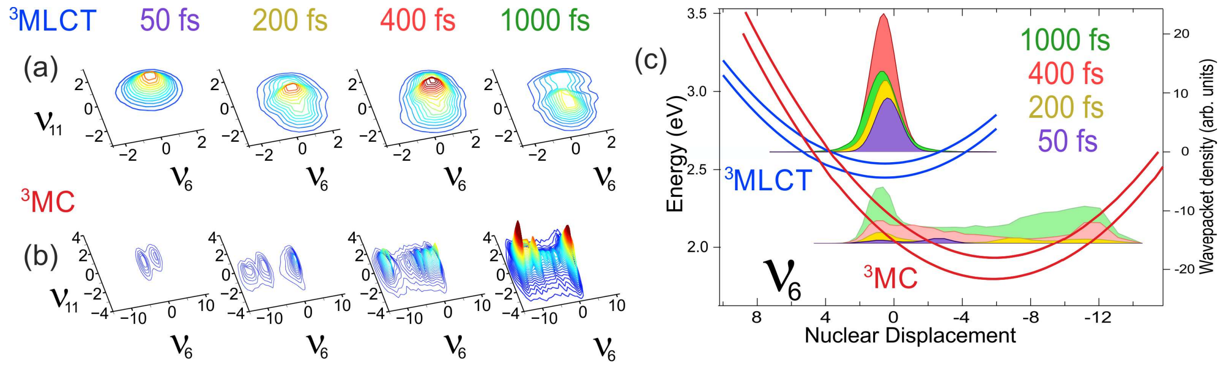


Figure 4. *Snapshots of the wavepacket density of the ^{3}MLCT (a) and ^{3}MC states (b) at 50, 200, 400 and 1000 fs after the excitation, over the ν_6 breathing and ν_{11} asymmetric combined stretching modes. (c) The one-dimensional projections over the corresponding potential surfaces.*

Laboratory X-ray absorption spectroscopy for routine measurements. — High energy resolution hard X-ray absorption and emission spectroscopies are powerful element selective probes of the electronic and local structure of matter, with diverse applications in materials science, chemistry, physics and biology. These techniques were revitalized with the appearance of third generation synchrotrons, as their intensive and focussed X-ray beams provide us with sufficient photon flux density to enable frontier studies in the forefront of materials science, physics, chemistry and biology even at extreme conditions and minuscule sample quantities, concentrations or sizes. However, these techniques could not become wide-spread general tools, as their routine applications have been hindered by the complicated and slow access to synchrotron radiation facilities. Nevertheless, due to the progress in monochromatization, detection technology and laboratory X-ray sources, new powerful table-top instruments could be realized.

We have developed a new, economic, easily-operated laboratory high-energy-resolution von Hámos type X-ray spectrometer, which offers rapid transmission experiments for X-ray absorption. The use of a conventional X-ray tube, a cylindrical analyzer crystal and a position sensitive detector enabled us to build an almost maintenance free, flexible setup with low operational costs, while delivering spectra with a good signal to noise ratio in reasonable acquisition times (few hours). The instrument does not contain any scanning components and does not need special sample environment such as vacuum or He atmosphere. Experiments with this table-top instrument are not direct competitors to those at synchrotron radiation sources, but this device can be used in laboratories at universities or research institutes for rapid routine characterisation of bulk and concentrated samples for a wide range of applications, making X-ray spectroscopy available to a significantly broader community. Also, it can serve as a valuable tool that can assist the preparations for synchrotron and XFEL experiments.

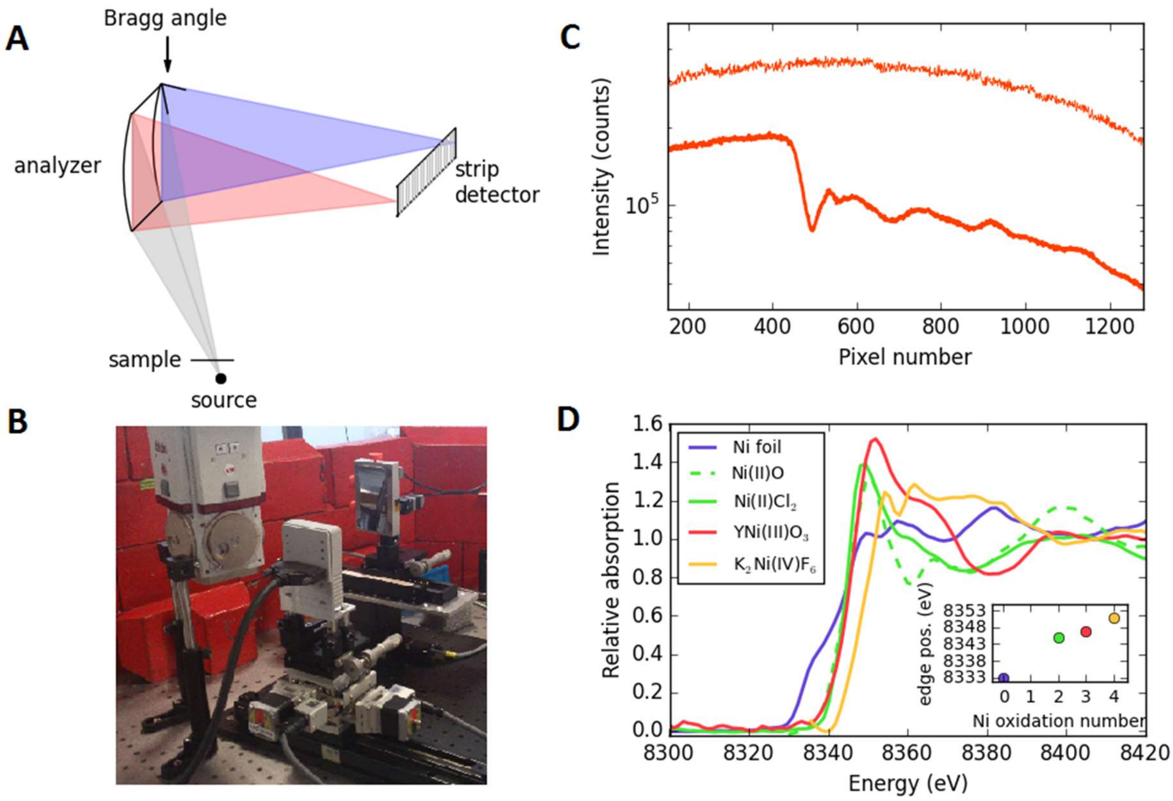


Figure 3. A*: The schematic diagram of the von Hámos arrangement.* ***B****: A photo of the actual setup of the spectrometer with the X-ray tube (left), the back side of the detector (middle) and the Si(111) analyzer crystal (right top).* ***C****: The raw, focused transmission signal on the Mythen detector with and without a NiO sample (red thick and thin curves, 120 and 130 min acquisition times, respectively).* ***D****: Laboratory X-ray absorption near edge spectra of different Ni compounds. Inset: deduced K edge positions vs. oxidation number. Error bars are smaller than the dot size.*

Grants

"Lendület" (Momentum) Programme of the Hungarian Academy of Sciences: Functional molecules caught in the act: Electronic structure – function relationships studied by femtosecond spectroscopy (G. Vankó, 2013 – 2018)

International cooperation

Main cooperations: Prof. C. Bressler (Hamburg), Prof. F. M. F. de Groot (Utrecht), Dr. Kelly Gaffney (SLAC), Dr. A. Juhin (Paris), Dr. K. Knízek (Prague), Prof. M. M. Nielsen (Copenhagen), Prof. F. Renz (Hannover), Dr. S. H. Southworth (Argonne), Prof. V. Sundström (Lund), Dr. Jakub Szlatchetko and Dr. Chris Milne (SwissFEL, PSI), Dr. Thomas Penfold (Newcastle)

Publications

Articles

1. Biasin E, van Driel TB, Kjær KS, Dohn AO, Christensen M, Harlang T, Chabera P, Liu Y, Uhlig J, Pápai M, Németh Z, Hartsock R, Liang W, Zhang JX, Alonso-Mori R, Chollet M, Glownia JM, Nelson S, Sokaras D, Assefa TA, Britz A, Galler A, Gawelda W, Bressler Ch, Gaffney KJ, Lemke HT, Møller KB, Nielsen MM, Sundström V, Vankó Gy, Wärnmark K, Canton SE, Haldrup K: Femtosecond X-Ray scattering study of ultrafast photoinduced structural dynamics in solvated $[Co(terpy)_2]^{2+}$. ***PHYS REV LETT*** 117:(1) 013002/1-6 (2016)

2. Haldrup K, Gawelda W, Abela R, Alonso-Mori R, Bergmann U, Bordage A, Cammarata M, Canton SE, Dohn AO, van Driel TB, Fritz DM, Galler A, Glatzel P, Harlang T, Kjær KS, Lemke HT, Moller KB, Németh Z, Pápai M, Sas N, Uhlig Jens, Zhu Diling, Vankó Gy, Sundstrom V, Nielsen MM, Bressler Ch: Observing solvation dynamics with simultaneous femtosecond X-ray emission spectroscopy and X-ray scattering. ***J PHYS CHEM B*** 120:(6) 1158-1168 (2016)

3. Li XN, Yuan LH, Wang JH, Jiang LH, Rykov AI, Nagy DL, Bogdan Cs, Ahmed MA, Zhu KY, Sun GQ, Yang WS: A "copolymer-co-morphology" conception for shape-controlled synthesis of Prussian blue analogues and as-derived spinel oxides. ***NANOSCALE*** 8:(4) 2333-2342 (2016)

4. Németh Z, Szlachetko J, Bajnóczi ÉG, Vankó Gy: Laboratory von Hámos X-ray spectroscopy for routine sample characterization. ***REV SCI INSTRUM*** 87:(10) 103105/1-10 (2016)

5. Pápai M, Vankó Gy, Rozgonyi T, Penfold TJ: High-efficiency iron photosensitizer explained with quantum wavepacket dynamics. ***J PHYS CHEM LETT*** 7 2009-2014 (2016)

6. Pápai M, Penfold ThJ, Moller KB: The effect of tert-butyl functionalization on the photoexcited decay of a Fe(II)-N-heterocyclic carbene complex. ***J PHYS CHEM C*** 120:(31) 17234-17241 (2016)

7. Penfold ThJ, Papai M, Rozgonyi T, Moller KB, Vanko Gy: FDDYNAM16 probing spin-vibronic dynamics using femtosecond X-ray spectroscopy. ***FARADAY DISCUSS*** 194: pp. 731-746. (2016)

8. Rozsályi E, Verger L, Cabaret D, Juhin A: DFT+U calculation of the Cr K pre-edge structures in $ZnCr_2O_4$. ***J PHYS CONF SER*** 712:(1) 012011/1-5 (2016)

9. Spiering H, Ksenofontov V, Leupold O, Kusz J, Deák L, Németh Z, Bogdán C, Bottyán L, Nagy DL: Line shape of ^{57}Co sources exhibiting self absorption. ***HYPERFINE INTERACT*** 237 58. 9 (2016)

10. Verger L, Dargaud O, Rousse G, Rozsályi E, Juhin A, Cabaret D, Cotte M, Glatzel P, Cormier L: Spectroscopic properties of Cr^{3+} in the spinel solid solution $ZnAl_{2-x}Cr_xO_4$. ***PHYS CHEM MINER*** 43:(1) 33-42 (2016)

11. Zhang J, Pápai M, Hirsch A, Jennings G, Kurtz CA, Møller KB, Lomoth R, Gosztola D, Zhang X, Canton SE: Elucidating the ultrafast dynamics of photoinduced charge separation in metalloporphyrin-fullerene dyads across the electromagnetic spectrum. ***J PHYS CHEM C*** 120:(35) 19537-19546 (2016)

12. Zhang XY, Papai M, Moller KB, Zhang JX, Canton SE: Characterizing the solvated structure of photoexcited [Os(**terpy**)$_2$]$^{2+}$ with X-ray transient absorption spectroscopy and DFT calculations. ***MOLECULES*** 21:(2) 235/1-9 (2016)

Conference proceeding

13. Britz A, Assefa T, Diez M, Galler A, Gawelda W, Khakhulin D, Zalden P, Torres-Alacan J, Németh Z, Bajnóczi E, Szemes D, Doumy G, March AM, Szlachetko J, Sato T, Nozawa S, Katayama T, Adachi S, Milne C, Vankó G, Vöhringer P, Bressler C: Synchrotron and X-Ray free electron laser studies of high-valent iron formation with X-ray absorption spectroscopy. In: Proc. International Conference on Ultrafast Phenomena 2016 (Santa Fe, USA, 17-07-2016 – 22-07-2016) OSA Technical Digest, Optical Society of America Washington, 2016. Paper UF1A.4. (ISBN:978-1-943580-18-7)

R-R. Pellet and video diagnostics

Wigner research group

Tamás Szepesi, Gábor Cseh[#], Gábor Kocsis, Tamás Szabolics

Video diagnostics system at the Wendelstein 7-X stellarator (W7-X) — A 10-channel overview video diagnostic system was developed for W7-X superconducting stellarator, based on self-developed EDICAM cameras. The main aim of the system is to monitor almost the entire inner wall at a frame rate in the 100 Hz range, and detect dangerous events automatically. Additionally, making use of the non-destructive feature of the EDICAM's sensor, scientific observations with up to 50 kHz frame rate can be simultaneously carried out, without affecting the low frame rate overview. In the first campaign of W7-X (OP1.1), spanning from December 2015 to March 2016, EDICAMs were installed in 7 channels. One channel was equipped with an ultra-fast framing Photron SA5 camera, another channel hosted a low-noise PCO PixelFly CCD camera, while the last channel was not used due to a leak in the port tube.

A special piece of software "VIDACS" was developed to operate the EDICAM system, which was running flawlessly during the whole first experimental campaign of W7-X. The EDICAM system recorded the first plasma discharge and displayed the images real-time for the audience in the control room. Based on first experiences, many improvements were implemented to the software during the campaign: performance and GUI optimizations were carried out, as well as new features were built in, necessitated by a new camera firmware release.

EDVIS (Extended Data Visualisation Software) was designed and developed especially to visualize the recordings of the EDICAM cameras. EDVIS is capable to display the images of the ten cameras installed on W7-X simultaneously. Its beta version was successfully used during the first campaign of W7-X, demonstrating the basic features such as reading, synchronized displaying of the videos, applying colour tables, gamma correction and threshold. Learning from the usage experiences there, many improvements and new features were added to the software. One of the most important new features is that EDVIS can now read movies of plasma sequences from the W7-X Archive System, which is a central storage system containing all the data of the measurements during a plasma pulse. Another improvement is the possibility of rotating the videos during display, zooming, defining regions of interest (ROIs) from the software with their own colour tables, exporting parts of the movies into different file formats. A logging system was also introduced to help the developers hunt for bugs and to inform the users about the current state of EDVIS. To speed up the video processing, EDVIS is now capable of calculating the different derived signals (such as the integrated brightness of the frames) in different threads using multiple processor cores. The software is continuously under development, but it is already well prepared for the next campaign of W7-X, starting in the summer of 2017.

[#] Ph.D. student

A spatial calibration system was also developed for the complete video diagnostic system, which uses control points on the wall elements to determine the calibration parameters. The individual cameras have to be calibrated separately. Using the calibration, it is possible to linearly project any 3D coordinate onto the given camera view, i.e. provide the image pixel coordinate for the given 3D point.

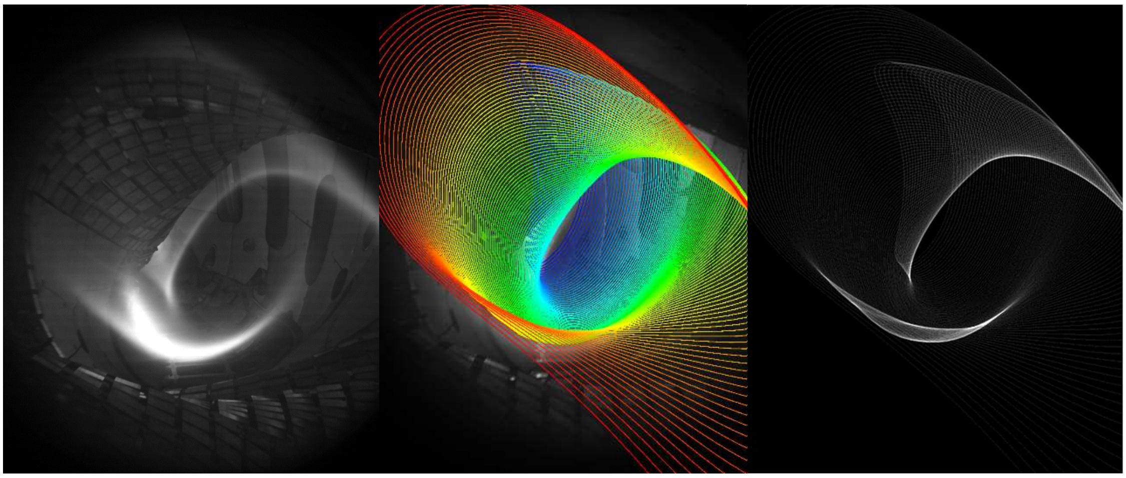


Figure 1. *Left: EDICAM camera image. Middle: spatially calibrated image with Last Closed Flux Surface curves overplotted at several toroidal positions (denoted by colors: toroidal angle 161-216° red-blue). Right: synthetic image.*

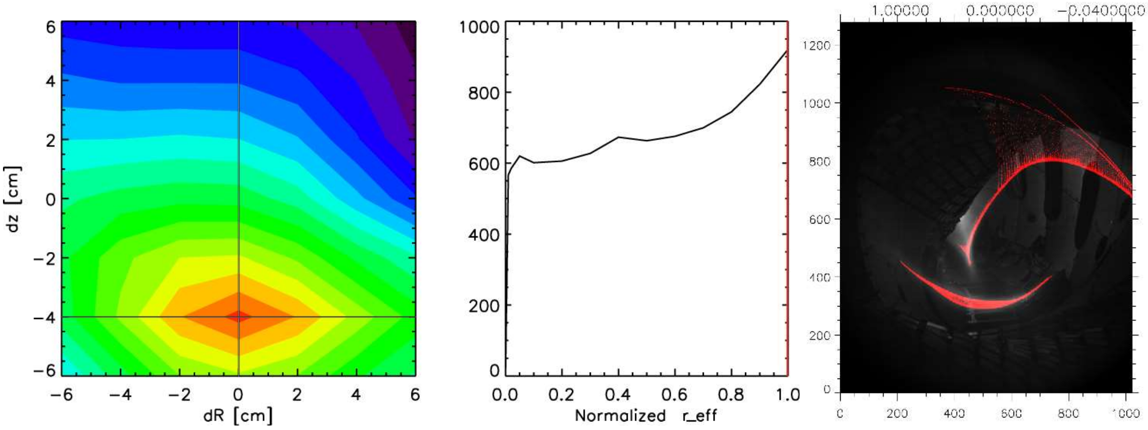


Figure 2. *The process of fitting the synthetic image onto the measurement. The contour plot on the left shows the total weighted brightness as a function of displacement in the R-z directions (resolution: 2 cm), while the middle figure shows the same as a function of plasma size. The result is shown on the right: the camera image is overplotted by the fitted synthetic image in red, the numbers on the top are reff, dR [m] and dz [m], respectively.*

Another important aspect at the investigation of the recordings is the determination of the position of the observed structures (brightness distributions) with respect to the magnetic field lines and magnetic flux surfaces. To achieve this, the central magnetic field line simulation code of the stellarator was used, with which the magnetic data can be calculated on the W7-X servers, providing us the desired number of field lines and flux surfaces from a given starting point for different magnetic configurations. To access this system an interface was developed, which can be used to generate the magnetic field lines and the needed flux surfaces, and – using the spatial calibration system – they can be projected onto the camera images. After that, it can be determined e.g. whether a structure is outside or inside the last closed flux surface, or whether is it elongated along the magnetic field lines or follow a different path, or whether the observed structure is the effect of uniform radiation on multiple flux surfaces.

Determining plasma position and size using the video diagnostics system at W7-X — Utilizing the spatial calibration, EDICAM images can be used to determine the size of the plasma (characterized by the effective minor radius, r_{eff}) and its displacement in the R-z plane relative to the ideal vacuum field position. Since W7-X is a stellarator, the plasma is not toroidal-symmetric, and hence the observed edge radiation detected by the tangentially viewing cameras is the superposition of light intensities coming from a flux surface with a shape depending on the toroidal position. The resulting radiation pattern does not resemble any of the flux surface shapes; therefore a straightforward conversion to plasma size is not possible. Instead, a synthetic radiation image is produced by projecting the 3D coordinates of a flux surface in toroidal positions covered by the view onto the 2D plane of the camera sensor, and "summing up" the light intensity along each camera pixel (equivalent to a line-of-sight in the machine reference frame). To account for the possible plasma position changes, at each r_{eff} additional synthetic images are produced by shifting the coordinates of the flux surface in 2 cm steps in both the R and the z-direction (maximum displacement ±6 cm), resulting in 49 possible variations for each r_{eff}. The synthetic images are used as a mask: each pixel value of a camera image is multiplied by the pixel intensity of the synthetic image, resulting in a weighted image. By summing up the pixel values of the weighted image, the total weighted brightness is calculated. This process is repeated for all synthetic images, and the one with the largest total weighted brightness corresponds to the best fitting flux surface (hence the plasma size) and displacement in the R-z directions. Each segment of W7-X is equipped with a trim coil, which, in addition to error field correction, can be used to modify the plasma position. This set of trim coils was used to investigate effect of plasma positioning on the heat load onto the five limiters. The applied n=1 perturbation is supposed to displace the plasma as a rigid body. It can be seen on Figure 3 that the plasma responds to the magnetic field perturbation. The result fits to prior expectations: more displacement in the radial direction is observed. Additionally, the largest displacement is found when the maximum coil perturbation is one module away (72° toroidally) from the observed location, which is consistent with other diagnostics' findings.

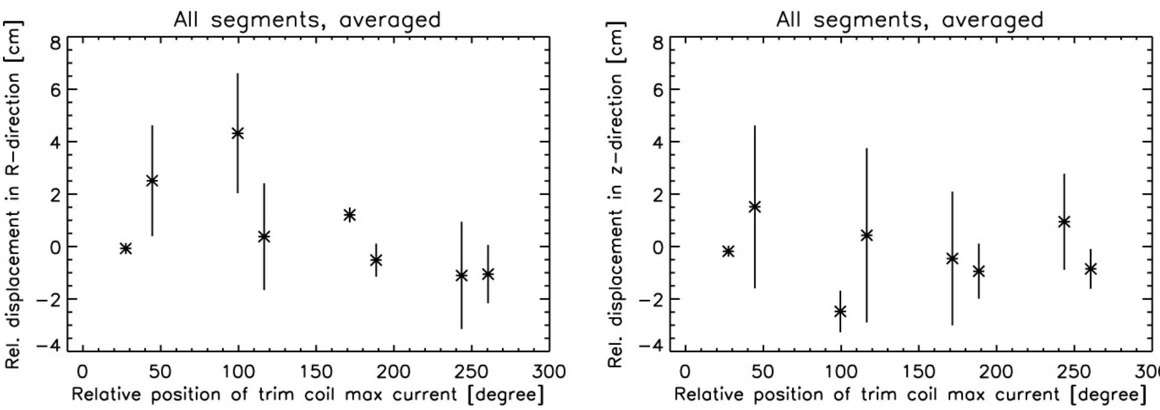


Figure 3. *Relative displacement of the LCFS as a function of the relative position of the maximum trim coil current location.*

Investigation of turbulent filamentary structures in W7-X limiter plasmas — The typical evolution of a discharge observed by the video cameras starts with a small radiating magnetic surface around the hot plasma core where the ECRH is absorbed. The radiating surface expands until the last closed flux surface. The discharge is terminated by either switching off the heating or by impurity accumulation released by the first wall components causing a radiation collapse. Taking images with short exposure time, filamentary structures can be observed at the plasma edge (Fig. 4). The frames are sampled in series of 5x5 pixel regions of interest, ROIs, ("channels") located poloidally around the plasma. The spatiotemporal correlation of the channel data showed that the filaments are ~200 µs lifetime turbulent structures elongated along the magnetic field lines, rotating poloidally with a velocity which is consistent with an ExB advection with a negative radial electric field of ~5 kV/m if they are in the confined plasma. During Nitrogen gas puff, where the filaments are seen probably in the scrape off layer (SOL) plasma, positive radial electric field could be observed. The correlation properties of the filaments resemble SOL turbulence observed in Wendelstein 7-AS. As correlation analysis also revealed them in fast ROIs of the standard EDICAM cameras their toroidal and poloidal structure can be studied in detail.

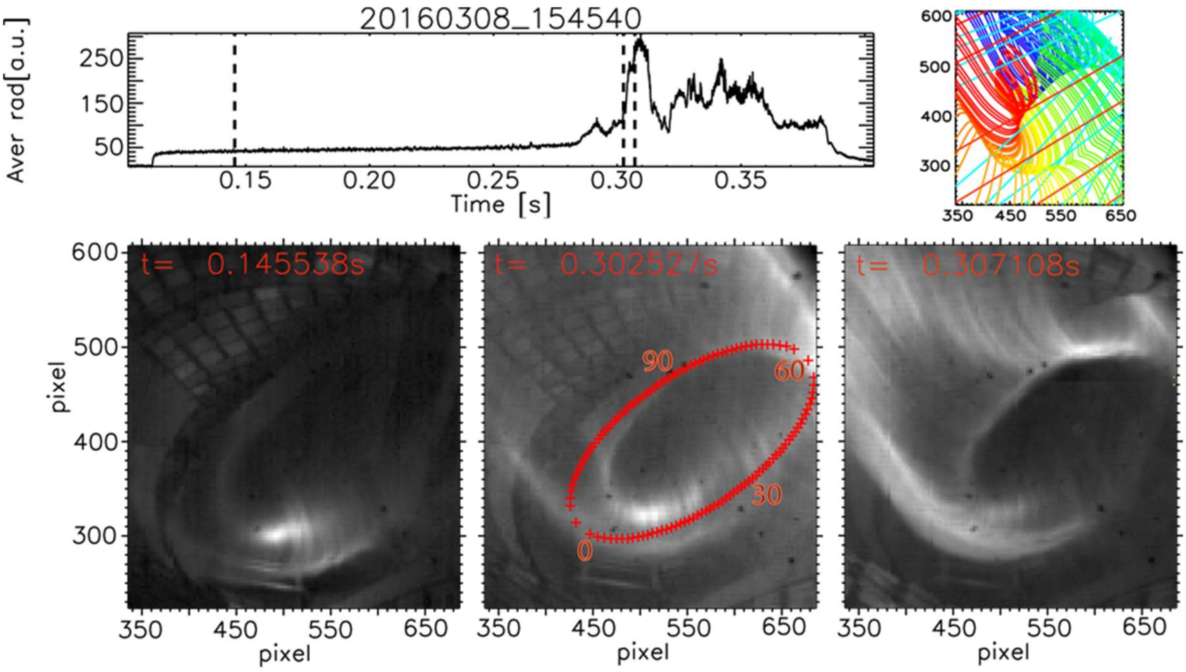


__Figure 4.__ A discharge with Nitrogen gas puff (101-303 ms). Images detected by 46.5 kHz frame rate are plotted on the lower part of the figure at selected times: during the gas puff (left), at the end of the gas puff (middle) and after the gas puff (right). The red crosses represent the middle of 5x5 pixel ROIs used to determine the radiation in a full poloidal circle. The time trace on the top shows the averaged radiation detected by the camera pixels. The result of the field line tracing projected to the camera sensor is also shown on the upper right corner.

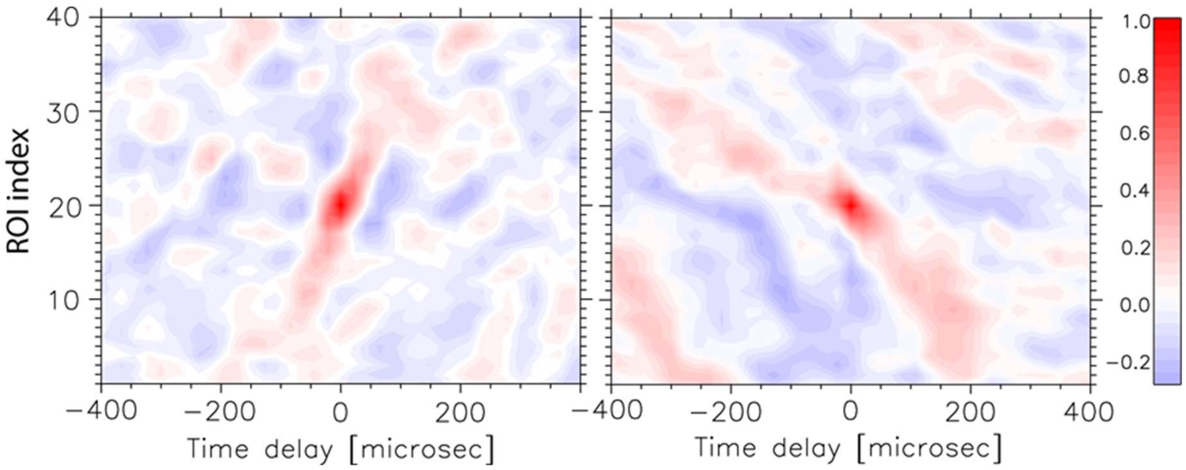


Figure 5. *Taking channel No. 20 as reference (see Fig.4.), the spatiotemporal correlation function of the surrounding channels as a function of the time lag for two time windows: during the Nitrogen gas puff (0.293-0.299s, left) and at the later phase of the discharge (0.305-0.311s, right).*

Investigation of pellet cloud evolution on ASDEX Upgrade tokamak — Cryogenic pellet injection is one of the prime candidates to fuel large scale fusion devices like ITER and DEMO. To allow for an efficient use of the pellet injection tool, the predictive understanding of the underlying processes of the pellet ablation is indispensable. Theoretical and experimental investigations performed in the last decades revealed that pellet ablation is a complex 3D process - taking place on the µs timescale -, which is still not satisfactorily explained. Recently, pellet ablation dynamics was experimentally investigated by recording fast framing movies (up to 600 kHz frame rate) during cryogenic pellet ablation through a radial port. This year these movies were analyzed and the results confirmed our earlier findings that the reason of the light fluctuation emitted by the pellet cloud is the repetitive release of drifting clouds. The flux tube approach – which takes into account that the pellet cloud is elongated along the magnetic field lines – gives a good separation of the radiation of the different clouds (cloud around the pellet vs drifting cloud). The observed radiation distribution of the field aligned pellet cloud was compared with modelled ones (synthetic diagnostics), revealing the time evolution of the pellet cloud distribution. Because of the dominant role of the cold pellet electrons, the developed pellet cloud has two maxima along the magnetic field lines before erupting a cloudlet. The erupted cloudlet typically has one maximum caused by the homogeneously distributed target plasma electrons which – in the absence of the pellet as particle source – dominate the atomic processes.

Grants

EUROfusion: WP Medium-Size Tokamak 1 (G. Kocsis, 2015-2016)

EUROfusion: WP JET 1 (G. Kocsis, 2015-2016)

EUROfusion: WP Stellarator 1 (T. Szepesi, 2015-2016)

EUROfusion: WP SA (T. Szepesi, 2015-2016)

International cooperation

Max-Planck-Institut für Plasmaphysik, Garching, Germany (G. Kocsis)

Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald, Germany (T. Szepesi)

Culham Centre for Fusion Energy, Oxfordshire, UK (G. Kocsis)

Japan Atomic Energy Agency, Naka, Japan (T. Szepesi)

Publications

ASDEX Upgrade Team

Due to the vast number of publications of the large collaborations in which the research group participated in 2016, here we list only a short selection of appearances in journals with the highest impact factor. Wigner-authors in these publications are Cseh G, Erdős B, Kálvin S, Kocsis G, Nemes-Czopf A, Réfy D, Szepesi T, Tál B.

1. Wagner D et al. incl. ASDEX Upgrade Team: Status, operation, and extension of the ECRH system at ASDEX Upgrade. ***J INFRARED MILLIM TE*** **37:**(1) 45-54 (2016)
2. Martinov S et al. incl. ASDEX Upgrade Team: Three novel software tools for ASDEX Upgrade. ***FUSION ENG DES*** 112: 839-844 (2016) Proc. 10th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, Ahmedabad, India, 20-04-2015 – 24-04-2015
3. Treutterer W et al. incl. ASDEX Upgrade Team: Configuration-defined control algorithms with the ASDEX Upgrade DCS. ***FUSION ENG DES*** 112: pp. 999-1002. (2016) Proc. 10th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, Ahmedabad, India, 20-04-2015 – 24-04-2015
4. Beurskens MNA et al. incl. ASDEX Upgrade Team, EUROfusion MST1 team: The role of carbon and nitrogen on the H-mode confinement in ASDEX Upgrade with a metal wall. ***NUCL FUSION*** **56:**(5) 056014/1-10 (2016)
5. Birkenmeier G et al. incl. ASDEX Upgrade Team: Magnetic structure and frequency scaling of limit-cycle oscillations close to L- to H-mode transitions. ***NUCL FUSION*** **56:**(8) 086009/1-15 (2016)
6. Bobkov V et al. incl. ASDEX Upgrade Team: First results with 3-strap ICRF antennas in ASDEX Upgrade. ***NUCL FUSION*** **56:**(8) Paper 084001. 5 p. (2016)
7. Burckhart A et al. incl. ASDEX Upgrade Team: ELM behaviour and linear MHD stability of edge ECRH heated ASDEX Upgrade plasmas. ***NUCL FUSION*** **56:**(5) 056011/1-6 (2016)
8. Fable E et al. incl. ASDEX Upgrade Team:Transport simulations of the pre-thermal-quench phase in ASDEX Upgrade massive gas injection experiments. ***NUCL FUSION*** **56:**(2) 026012/1-19 (2016)
9. Happel T et al. incl. ASDEX Upgrade Team: Turbulence intermittency linked to the weakly coherent mode in ASDEX Upgrade I-mode plasmas. ***NUCL FUSION*** **56:**(6) 064004/1-7 (2016)
10. Hubbard AE et al. incl. ASDEX Upgrade Team: Multi-device studies of pedestal physics and confinement in the I-mode regime. ***NUCL FUSION*** **56:**(8) 086003/1-14 (2016)
11. Jacquet P et al. incl. ASDEX Upgrade Team: Maximization of ICRF power by SOL density tailoring with local gas injection. ***NUCL FUSION*** **56:**(4) 046001/1-14 (2016)
12. Kasparek W et al. incl. ASDEX Upgrade Team: NTM stabilization by alternating O-point

EC current drive using a high-power diplexer. ***NUCL FUSION*** **56:**(12) 126001/1-16 (2016)

13. Liu YQ et al. incl. ASDEX Upgrade Team, EUROfusion MST1 team: Toroidal modelling of RMP response in ASDEX Upgrade: coil phase scan, q(95) dependence, and toroidal torques. ***NUCL FUSION*** **56:**(5) 056015/1-21 (2016)
14. Meisl G et al. incl. ASDEX Upgrade Team: Experimental analysis and WallDYN simulations of the global nitrogen migration in ASDEX Upgrade L-mode discharges ***NUCL FUSION*** **56:**(3) Paper 036014. 15 p. (2016)
15. Salewski M et al. incl. ASDEX Upgrade Team: High-definition velocity-space tomography of fast-ion dynamics. ***NUCL FUSION*** **56:**(10) 106024/1-15 (2016)
16. Schweinzer J et al. incl. ASDEX Upgrade Team, EUROfusion MST1 team: Development of the Q=10 scenario for ITER on ASDEX Upgrade (AUG). ***NUCL FUSION*** **56:**(10) 106007/1-10 (2016)
17. Valovic M et al. incl. ASDEX Upgrade Team: Pellet refuelling of particle loss due to ELM mitigation with RMPs in the ASDEX Upgrade tokamak at low collisionality. ***NUCL FUSION*** **56:**(6) 066009/1-9 (2016)
18. Vezinet D et al. incl. ASDEX Upgrade Team, EUROfusion MST1 team: Non-monotonic growth rates of sawtooth precursors evidenced with a new method on ASDEX Upgrade. ***NUCL FUSION*** **56:**(8) 086001/1-26 (2016)
19. Zhang W et al. incl. ASDEX Upgrade Team: 3D simulations of gas puff effects on edge density and ICRF coupling in ASDEX Upgrade. ***NUCL FUSION*** **56:**(3) 036007/1-11 (2016)

W7X Collaboration

1. Krychowiak M et al. incl. Cseh G, Kocsis G, Szabolics T, Szepesi T, Zoletnik S (102 authors): Overview of diagnostic performance and results for the first operation phase in Wendelstein 7-X (invited). ***REV SCI INSTRUM*** **87:**(11) 11D304/1-7 (2016)
2. Marushchenko NB et al. incl. Cseh G, Kocsis G, Szabolics T, Szepesi T, Zoletnik S (85 authors): Main results of the first experimental campaign in the stellarator W7-X. ***PROBL AT SCI TECH*** **106:**(6) 3-8 (2016)
3. Pedersen TS et al. incl. Cseh G, Kocsis G, Szabolics T, Szepesi T, Zoletnik S (297 authors): Confirmation of the topology of the Wendelstein 7-X magnetic field to better than 1:100,000. ***NAT COMMUN*** **7:** 13493/1-8 (2016)

S-A. Strongly correlated systems

"Momentum" research team

Örs Legeza, Gergely Barcza, Imre Hagymási, Mihály Máté[#], Jenő Sólyom[E], Szilárd Szalay

Tensor factorization in high-dimensional problems and applications to strongly correlated systems in condensed matter physics and quantum chemistry.

In this year, we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG), *Matrix Product State* (MPS) and *Tree Tensor Network State* (TTNS) algorithms. In addition, we have further developed our scientific softwares (**Budapest QC-DMRG program package**), which have been used with great success in numerous research institutes and universities around the world for, e.g., simulating material properties of solid state systems or molecules, or for the quantum simulation of the information technology itself. Major algorithmic developments have also been carried out concerning the *quantum chemistry DMRG* and *Coupled-Cluster* (CC) algorithms. As will be presented below, among many others, we have examined strongly correlated electrons in magnetic materials in several quantum phases, exotic quantum phases in ultracold atomic systems, and we have determined the correlation and entanglement patterns in molecules, playing important role in chemical reactions.

Entanglement, excitations and correlation effects in narrow zigzag graphene nanoribbons. — We have investigated the low-lying excitation spectrum and ground-state properties of narrow graphene nanoribbons with zigzag edge configurations. Such nanoribbons have been synthesized very recently, and their descriptions require more sophisticated methods since in this regime conventional methods like mean-field or density-functional theory with local density approximation fail to capture the enhanced quantum fluctuations. Using the unbiased DMRG algorithm, we have calculated the charge gaps with high accuracy for different widths and interaction strengths and compared them with mean-field results. It turned out that the gaps are much smaller in the former case due to the proper treatment of quantum fluctuations. Applying the elements of quantum information theory, we also revealed the entanglement structure inside a ribbon and examined the spectrum of subsystem density matrices to understand the origin of entanglement. We examined the possibility of magnetic ordering and the effect of magnetic field. Our findings are relevant for understanding the gap values in different recent experiments and the deviations between them.

Characterization of a correlated topological Kondo insulator in one dimension. — We have investigated the ground-state of a p-wave Kondo-Heisenberg model introduced by Alexandrov and Coleman with an Ising-type anisotropy in the Kondo interaction and with correlated conduction electrons. Our aim was to understand how they affect the stability of the Haldane state obtained in the SU(2) symmetric case without the Hubbard interaction. By

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applying the DMRG algorithm and calculating the entanglement entropy, we have shown that in the anisotropic case a phase transition occurs and a Néel state emerges above a critical value of the Coulomb interaction. These findings were also corroborated by the examination of the entanglement spectrum and the spin profile of the system which clarify the structure of each phase.

Optical phonons for Peierls chains with long-range Coulomb interactions. — We have considered a chain of atoms that are bound together by a harmonic force. Spin-1/2 electrons that move between neighboring chain sites (Hückel model) induce a lattice dimerization at half band filling (Peierls effect). We have supplemented the Hückel model with a local Hubbard interaction and a long-range Ohno potential, and calculate the average bond-length, dimerization, and optical phonon frequencies for finite straight and zigzag chains using the DMRG method. We have checked our numerical approach against analytic results for the Hückel model. The Hubbard interaction mildly affects the average bond length but substantially enhances the dimerization and increases the optical phonon frequencies whereas, for moderate Coulomb parameters, the long-range Ohno interaction plays no role.

Coupled-cluster method with single and double excitations tailored by MPS wave functions. — In the last decade, the quantum chemical version of the DMRG method has established itself as the method of choice for calculations of strongly correlated molecular systems. Despite its favourable scaling, it is not suitable for computations of dynamic correlation in practice. We have presented a novel method for accurate "post-DMRG" treatment of dynamic correlation based on the tailored CC theory, in which the DMRG method is responsible for the proper description of non-dynamic correlation, whereas dynamic correlation is incorporated through the framework of the CC theory. We have illustrated the potential of this method on prominent multireference systems, in particular N_2, Cr_2 molecules and also oxo-Mn(Salen) for which we have performed the first "post-DMRG" computations in order to shed light on the energy ordering of the lowest spin states.

The correlation theory of the chemical bond. — The quantum mechanical description of the chemical bond is given in terms of delocalized bonding orbitals, or, alternatively, in terms of correlations of occupations of localized orbitals. However, in the latter case, multiorbital correlations were treated only in terms of two-orbital correlations, although the structure of multiorbital correlations is far richer; and, in the case of bonds established by more than two electrons, multiorbital correlations represent a more natural point of view. For the first time, we have introduced the true multiorbital correlation theory, consisting of a framework for handling the structure of multiorbital correlations, a toolbox of true multiorbital correlation measures, and an algorithm for the multiorbital correlation clustering. These make it possible to characterize quantitatively how well a bonding picture describes the chemical system. As proof of concept, we have applied the theory for the investigation of the bond structures of several molecules. We have shown that the non-existence of well-defined multiorbital correlation clustering provides a reason for debated bonding picture.

Method of Increments (MoI). — We have further developed the method of increments (MoI) that allows one to successfully calculate cohesive energies of bulk materials with high accuracy, but it encounters difficulties when calculating whole dissociation curves. The reason is that its standard formalism is based on a single Hartree-Fock (HF) configuration whose orbitals are localized and used for the many-body expansion. Therefore, in those situations where HF does not allow a size-consistent description of the dissociation, the MoI cannot yield proper results either. We have addressed the problem by employing a size-consistent multiconfigurational reference for the MoI formalism. This led to a matrix equation where a coupling derived by the reference itself is employed. In principle, such approach allows one to evaluate approximate values for the ground as well as excited states energies. While the latter are accurate close to the avoided crossing only, the ground state results are very promising for the whole dissociation curve, as we have shown by the comparison with DMRG benchmarks. We tested this two-state constant-coupling (TSCC)-MoI on beryllium rings of different sizes and studied the error introduced by the constant coupling.

On the Multi-Reference Nature of Plutonium Oxides: PuO_2^{+2}, PuO_2, PuO_3 and $PuO_2(OH)_2$. — Actinide-containing complexes present formidable challenges for electronic structure methods due to the large number of degenerate or quasi-degenerate electronic states arising from partially occupied 5f and 6d shells. Conventional multi-reference methods can treat active spaces that are often at the upper limit of what is required for a proper treatment of species with complex electronic structures, leaving no room for verifying their suitability. We have addressed the issue of properly defining the active spaces in such calculations, and introduce a protocol to determine optimal active spaces based on the use of the DMRG algorithm and concepts of quantum information theory. We applied the protocol to elucidate the electronic structure and bonding mechanism of volatile plutonium oxides (PuO_3 and $PuO_2(OH)_2$), species associated with nuclear safety issues for which little is known about the electronic structure and energetics. We have shown how, within a scalar relativistic framework, orbital-pair correlations can be used to guide the definition of optimal active spaces which provide an accurate description of static/non-dynamic electron correlation, as well as to analyze the chemical bonding beyond a simple orbital model. From this bonding analysis, we were able to show that the addition of oxo- or hydroxo-groups to the plutonium dioxide species considerably changes the pi-bonding mechanism with respect to the bare triatomics, resulting in bent structures with considerable multi-reference character.

Analysis of two-orbital correlations in wavefunctions restricted to electron-pair states. — Wavefunctions constructed from electron-pair states can accurately model strong electron correlation effects and are promising approaches especially for larger many-body systems. We have analyzed the nature and the type of electron correlation effects that can be captured by wavefunctions restricted to electron-pair states. We focused on the Antisymmetric Product of 1-reference orbital Geminal (AP1roG) method combined with an orbital optimization protocol whose performance was assessed against electronic structures obtained from DMRG reference data. Our numerical analysis covered model systems for strong correlation: the one-dimensional Hubbard model with periodic boundary condition as well as metallic and molecular hydrogen rings. Specifically, the accuracy of AP1roG was benchmarked using the single-orbital entropy, the orbital-pair mutual information as well as the eigenvalue spectrum of the one-orbital and two-orbital reduced density matrices. Our study indicated that contributions from singly occupied states become important in the strong correlation regime which highlights the limitations of the AP1roG method.

Furthermore, we have examined the effect of orbital rotations within the AP1roG model on correlations between orbital pairs.

Fermionic orbital optimization in tensor network states. — We have further developed and implemented the novel fermionic mode transformation algorithm in the Budapest QC-DMRG code and performed additional large scale calculations by keeping more than 8000 block states. For the investigated chemical systems we have obtained significantly more optimal basis sets compared to those generated by conventional approaches.

Nuclear structure theory. — We have further improved the nuclear shell variant of the DMRG algorithm that includes an optimal ordering of the proton and neutron orbitals and an efficient expansion of the active space, utilizing various concepts of quantum information theory. We have generalized the implementation of non-Abelian symmetries.

Post-DMRG methods. —We have developed algorithms that rely on the MPS representation of the wave function obtained by the DMRG procedure. These so-called post-DMRG algorithms allow one to calculate expectation values of arbitrary operators between wave function generated by independent DMRG calculations. These methods were applied to various spin and fermionic models.

Multipartite correlations in fermionic systems. — We have started to investigate the theoretical foundations of the notions of correlations in second-quantized fermionic systems, mostly in the Jordan-Wigner representation. The results of our investigations make possible to use the main parts of the correlation theory of distinguishable systems for fermionic systems, providing firm theoretical grounds for the projects dealing with fermionic systems, e.g., in molecular physics or fermionic lattice models.

N-heterocyclic carbenes. — The N-heterocyclic carbenes are one of the most important "experimental tools" of the modern main group chemistry, which can be applied to stabilize compounds with unidentified bonds. Nowadays, the understanding of the stabilization (whether the process is realized through dative or covalent bond) is in the focus of theoretical literature to shed light on the unidentified bonds. This year we began to study various carbenes, using our previously developed quantum information theory based analysis which is capable to distinguish covalent and dative structures.

Ultracold atomic systems. — The interest in the gas of optically trapped ultracold atoms rapidly increases due to the high controllability and tunability of the experimental setups and the versatility of the realized quantum phases. We have studied the interacting system of atoms with spin 3/2 trapped in a square lattice using different numerical approaches. In the strongly repulsive limit, the system can be described by a generalized bilinear-biquadratic Heisenberg model. We have investigated this model in terms of mean field approaches, exact diagonalization, DMRG and cluster mean field approximation. Our primary goal is to understand the conflicting results published so far for SU(4) symmetric couplings, and to extend the analysis to general cases.

Graphene nanoribbons. — We have investigated the effect of long-range interaction on graphene nanoribbons and their low-lying excitation spectrum. We have also studied triangular-shaped graphene nanoflakes to reveal the correlation effects and magnetic properties induced by the electron-electron interaction.

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Universidad Autonoma de Madrid, and Instituto de Estructura de la Materia, CSIC (Madrid, Spain), Development of the nuclear shell version of the DMRG method (A. Poves, J. Dukelsky)

Publications

Articles

1. Boguslawski K, Tecmer P, Legeza Ö: Analysis of two-orbital correlations in wave functions restricted to electron-pair states. ***PHYS REV B*** 94:(15) 155126/1-8 (2016)

2. Hagymási I, Legeza Ö: Characterization of a correlated topological Kondo insulator in one dimension. ***PHYS REV B*** 93:(16) 165104/1-6 (2016)

3. Hagymási I, Legeza Ö: Entanglement, excitations, and correlation effects in narrow zigzag graphene nanoribbons. ***PHYS REV B*** 94:(16) 165147/1-8 (2016)

4. Krumnow C, Veis L, Legeza Ö, Eisert J: Fermionic orbital optimization in tensor network states. ***PHYS REV LETTERS*** 117:(21) 210402/1-6 (2016)

5. Timár M, Barcza G, Gebhard F, Veis L, Legeza Ö: Hückel-Hubbard-Ohno modeling of π-bonds in ethene and ethyne with application to *trans*-polyacetylene. ***PHYS CHEM CHEM PHYS*** 18:(28) 18835-18845 (2016)

6. Veis L, Antalík A, Brabec J, Neese F, Legeza O, Pittner J: Coupled cluster method with single and double excitations tailored by matrix product state wave functions. ***J PHYS CHEM LETTERS*** 7:(20) 4072-4078 (2016)

Other

7. Sólyom J, Zaránd G: A kvantumtérelmélettől a szilárdtest-fizikáig. Zawadowski Alfréd tudományos életútja (From Quantum field theory to Solid State Physics. The scientific carreer of Alfréd Zawadowski, in Hungarian). ***FIZIKAI SZEMLE*** 66:(5) 146-150 (2016)

S-B. Complex systems

Wigner research group

Róbert Juhász, Ferenc Iglói, István Kovács[A], Gergő Roósz[#], András Sütő[E], Attila Virosztek

The Complex Systems research group is interested mainly in the cooperative behavior, phase transitions, equilibrium and nonequilibrium dynamics of systems with many degrees of freedom. Our research activity in 2016 covered various interrelated topics of this broad area, which are subjects of intensive research currently.

The *non-equilibrium quench dynamics*, i.e., the time evolution of a closed or open quantum system after a sudden change of global or local parameters is in the focus of current research. Such phenomena are important because they are experimentally accessible in systems of cold atoms trapped in optical lattices. We studied these phenomena in integrable models under different circumstances such as in the presence of a global noise or quenched spatial disorder. The investigation of *quantum correlations*, especially the entanglement properties of the ground state of extended quantum systems with inhomogeneities or at first-order phase transitions also constituted an important part of our activity. An almost inevitable feature of real systems is the presence of *quenched disorder*, which has striking effects both on the static and dynamic properties especially at phase transition points. Another feature of many real systems, which affects the critical behavior, is that the interactions between particles are *long-ranged*, i.e. their strength decays as an inverse power of the distance. We were interested in the interplay of the above two features in theoretical models, which turned out to result in new types of critical behavior characterized by a Kosterlitz-Thouless type of essential singularity or by a *mixed-order* of the phase transition. The latter means that the transition resembles first-order ones in that the order parameter is discontinuous, but, at the same time, the correlations diverge, which is a property of second-order transitions. Mixed-order transitions occur typically in systems with long-range interactions. We have found that simple short-range models can also exhibit this phenomenon locally under a special geometry, namely, near junctions of chains. Besides, we have a contribution to the solution of the long-standing problem of *crystallographic phase retrieval* as well, by introducing a new method called volumic omit map. The results obtained in the above fields are described in detail in the following.

Non-equilibrium quench dynamics of noisy quantum systems. — We continued our work on the nonequilibrium dynamics of the quantum Ising chain in the presence of a stochastically varying global transverse field. The dynamics of entanglement entropy and magnetization can be understood by a semi-classical theory of the spreading of quasiparticle excitations, which are described by a continuous-time random quantum walk with stochastic transition amplitudes. In general, the stochastic noise gives rise to decoherence

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and a diffusive behavior of excitations. For the special case of a dichotomous noise, there can also be coherent modes, which give a ballistic contribution beside the diffusive one and result ultimately in a superdiffusive behavior. We extended these investigations in several directions. We considered a dichotomous noise which changes in discrete times steps with a frequency that decays algebraically in time as $p(t) \sim t^{-\kappa}$. We found that the excitations spread ballistically for $\kappa>1$, while the spreading is anomalous with a κ-dependent dynamical exponent for $\kappa<1$. We also considered different aperiodic modulations such as the Fibonacci sequence, where the spreading of excitations is found again to be anomalous with a non-universal dynamical exponent z. In the high frequency limit, for sequences with a non-positive wandering exponent, z is found to be close to 1, while, for a positive wandering exponent, it is considerably less than 1. We studied the effect of a point-like source of dichotomous noise on the dynamics of an excitation initially localized near the source. Here, the distributions of the position at different times still follow the ballistic scaling, which is characteristic of the noiseless quantum walk. However, a depletion zone with nearly zero probability develops around the origin, the width of which increases linearly in time.

Critical quench dynamics of random quantum spin chains. - By means of free-fermion techniques combined with multiple-precision arithmetic, we studied the time evolution of the average magnetization, m(t), of the random transverse-field Ising chain after global quenches. We observed different relaxation behaviors for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow described by $m(t) \sim \ln^a t$, and in a finite sample of length L, the average magnetization saturates at a size-dependent plateau $m_p(L) \sim L^{-b}$; here, the two exponents satisfy the relation $b/a = \psi = 1/2$. Starting from a fully disordered initial state, the magnetization stays at zero for a period of time until $t = t_d$ with $\ln t_d \sim L^{\Psi}$ and then starts to increase until it saturates to an asymptotic value $m_p(L) \sim L^{-b'}$, with $b' \approx 1.5$. For both quenching protocols, finite-size scaling is satisfied in terms of the scaled variable $\ln t/L^{\Psi}$. Furthermore, the distribution of long-time limiting values of the magnetization shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behavior of the magnetization is explained through a semi-classical theory.

Entanglement entropy of the Q ≥ 4 quantum Potts chain. -- The entanglement entropy, S, is an indicator of quantum correlations in the ground state of a many-body quantum system. At a second-order quantum phase-transition point in one dimension, S generally has a logarithmic singularity. We considered quantum spin chains with a first-order quantum phase transition, the prototype being the Q-state quantum Potts chain for Q > 4 and calculated S across the transition point. According to numerical density matrix renormalization group results, at the first-order quantum phase transition point S shows a jump, which is expected to vanish for $Q \to 4^+$. This jump was calculated in leading order as $\Delta S = \ln Q[1-4/Q-2/(Q\ln Q)+ O(1/Q^2)]$.

Long-range random transverse-field Ising model in three dimensions. — We considered quantum magnets with long-range interactions in the presence of quenched disorder. Such a system is realized by the compound $LiHo_{1-x}Y_xF_4$, in which a fraction x of the magnetic Ho atoms are replaced by non-magnetic Y atoms. A related but somewhat simplified model, which describes the low-energy properties is the three-dimensional random transverse-field Ising model with long-range ferromagnetic interactions, which decay as a power α of the distance. Using a variant of the strong-disorder renormalization group method we studied numerically the phase-transition point and the paramagnetic phase. The schematic flow diagram in terms of the dynamical exponent z and the ratio r of the frequency of coupling and field decimations can be seen in Fig. 1. We found that the fixed point controlling the transition is of the strong-disorder type, and based on experience with other similar systems, we expect the results to be qualitatively correct, but possibly not asymptotically exact. The distribution of the (sample dependent) pseudocritical points is found to scale with 1/lnL, L being the linear size of the sample. Similarly, the critical magnetization scales with $(\ln L)^{\chi}/L^{d}$ and the excitation energy behaves as $L^{-\alpha}$. Using extreme-value statistics, we argued that, extrapolating from the ferromagnetic side, the magnetization approaches a finite limiting value and thus the transition is of mixed order.

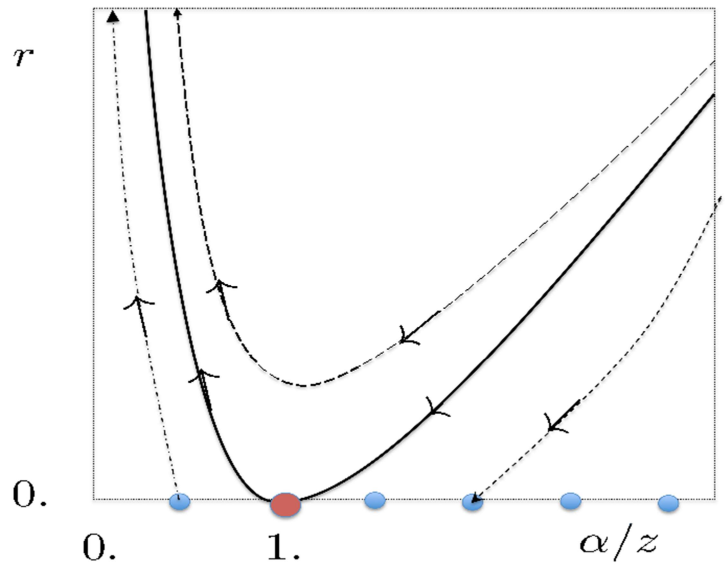

Figure 1. *RG flow diagram of the long-range random transverse-field Ising model. At r=0, the line of stable (α/z>1) and unstable (α/z<1) fixed points is separated by the critical fixed point indicated by the red dot.*

Random-bond Potts chain with long-range interactions. — We studied phase transitions of the ferromagnetic q-state Potts chain with random nearest-neighbor couplings having a variance Δ^2 and with homogeneous long-range interactions, which decay with the distance as a power $r^{-(1+\sigma)}$, $\sigma > 0$. In the large-q limit, the free energy of random samples of length $L \leq 2048$ was calculated exactly by a combinatorial optimization algorithm. The phase transition remains of first order for $\sigma < \sigma_c(\Delta) \leq 0.5$, while the correlation length becomes divergent at the transition point for $\sigma_c(\Delta) < \sigma < 1$. In the latter regime, the average magnetization is continuous for small enough Δ, but, for larger Δ, it is discontinuous at the transition point, thus the phase transition is of mixed order. A schematic phase diagram showing the short-range (SR), long-range (LR), first-order (FO), second-order (SO), and mixed-order (MO) phases can be seen in Fig. 2.

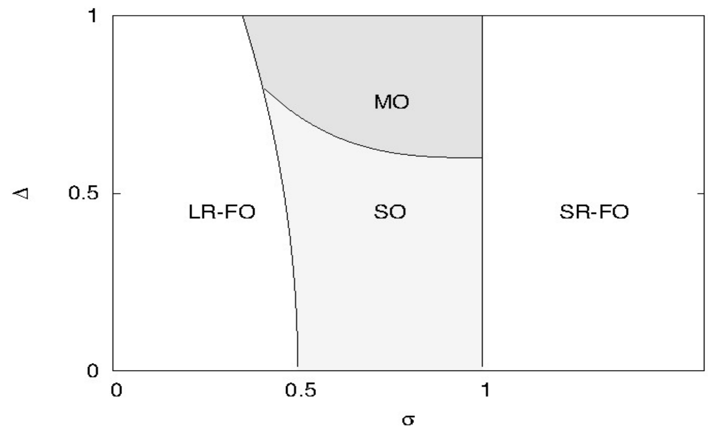

Figure 2. *Schematic phase diagram of the long-range random Potts model.*

Critical behavior of the contact process near multiple junctions. — The contact process is a basic stochastic lattice model of epidemic spreading or population dynamics. It displays a nonequilibrium phase transition between a fluctuating active phase and an absorbing phase, which is continuous in any dimensions and falls into the robust universality class of directed percolation. Discontinuous transitions are rare in low dimensional fluctuating systems; for the particular case of one-dimensional systems with short-range interactions, they are conjectured to be impossible since fluctuations destabilize the ordered phase. We demonstrated by numerical simulations that a suitable topology of the underlying lattice is able to induce a discontinuous local transition even with a simple dynamics such as the contact process. We have considered, namely, a multiple junction of M semi-infinite chains. As opposed to the continuous transitions of the translationally invariant (M=2) and the semi-infinite (M=1) system, the local order parameter is found to be discontinuous for M>2. The temporal correlation length diverges algebraically at the critical point, thus the transition is of mixed order. Interestingly, the corresponding exponents on the two sides of the transition are different. We proposed a scaling theory, which is compatible with the numerical results and explains the exponent asymmetry by the presence of an irrelevant local variable, which is harmless in the active phase, but becomes dangerous in the inactive phase. Quenched spatial disorder is found to make the transition continuous, in agreement with earlier renormalization group results.

Phase problem of crystallography. – In the framework of our study of the problem of crystallographic phase retrieval, we introduced a new method called “volumic omit map”, to accelerate slowly converging dual space iterative procedures. Alternating-projection-type dual-space algorithms have a clear construction, but are susceptible to stagnation and, thus, inefficient for solving the phase problem ab initio. To improve this behavior, new omit maps were introduced, which are real-space perturbations applied periodically during the iteration process. The omit maps are called volumic because they delete some predetermined subvolume of the unit cell without searching for atomic regions or analyzing the electron density in any other way. The basic algorithms of positivity, histogram matching and low-density elimination were tested by their solution statistics. It is concluded that, while all these algorithms based on weak constraints are practically useless in their pure forms, appropriate volumic omit maps can transform them to practically useful methods. In addition, the efficiency of the already useful reflector-type charge-flipping algorithm can be further improved. It is important that these results are obtained by using non-sharpened structure factors and without any weighting scheme of reciprocal-space perturbation.

Grants

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Saarland University (Saarbrücken, Germany), Nonequilibrium quench dynamics of quantum systems (F. Iglói, G. Roósz)

Institute Néel (Grenoble, France), Phase transitions of systems with long-range interactions (F. Iglói)

National Chengchi University (Taipei, Taiwan), Critical quench dynamics of random spin chains (F. Iglói, G. Roósz)

Kuwait University (Safat, Kuwait), Entanglement entropy at first-order transitions (F. Iglói)

Publications

Articles

1. Anglès D'Auriac J-C, Iglói F: Phase transitions of the random-bond Potts chain with long-range interactions. ***PHYS REV E*** 94:(6) 062126-1-9 (2016)

2. Kovács IA, Juhász R, Iglói F: Long-range random transverse-field Ising model in three dimensions. ***PHYS REV B*** 93:(18) 184203/1-8 (2016)

3. Roósz G, Juhász R, Iglói F: Nonequilibrium dynamics of the Ising chain in a fluctuating transverse field. ***PHYS REV B*** 93:(13) 134305/1-11 (2016)

Others

4. Szépfalusy P, Csordás A: A Bose-Einstein-kondenzációtól az atomlézerig (From Bose-Einstein condensation to atomic lasers, in Hungarian) ***FIZIKAI SZEMLE*** 66:(1) 17-24 (2016)

See also S-F.6., S-T.(Asbóth)

S-C. Long-range order in condensed systems

Wigner research group

Balázs Újfalussy, Péter Balla#, Gábor Csire#, Annamária Kiss, Zsolt Maksa#, Balázs Nagyfalusi#, Karlo Penc, István TüttőA, Lajos Károly VargaA, Ádám Vida#, Levente Vitos

Superconductivity in layered heterostructures. — The physics of superconductor/normal metal heterostructures has become a very intensively studied research field since modern deposition techniques allow to create very high-quality thin films and overlayers. In such systems, superconducting correlations are introduced in the normal metal by the so-called Andreev scattering, when an electron, with energy lying in the superconducting gap, arriving from the normal metal to the superconductor/normal metal (S/N) interface is retro-reflected as a hole and a Cooper pair is formed in the superconductor. This effect controls the transport properties of such systems and allows the understanding of the proximity-effect on a microscopic scale. It is also known that the Andreev reflection is the key effect behind the formation of Andreev bound states. While a great many theoretical works were dedicated to study the Andreev reflection and the Andreev bound states, it was done on model systems only, their material specific dispersion, their ``band structure'' has never been calculated (nor observed experimentally) to date. While the theory of Bardeen, Cooper, and Schrieffer (BCS) successfully describes the universal properties of conventional (s-wave) superconductors, it can not be applied easily to inhomogeneous systems where the wave number is not a good quantum number.

We developed a new method, which allows the quantitative and material-specific description of superconductivity-related phenomena. Density functional theory (DFT) has already been generalized for the superconducting state (Kohn-Sham-Bogoliubov-de Gennes, KSBdG, equations) and applied successfully in bulk superconducting systems. At present, this is the most accurate theory which allows the first-principles calculation of the superconducting transition temperature.

The superconductor/normal metal hetereostructures can also be well described by these equations. By the generalization of the screened Korringa-Kohn-Rostoker (Green function) method to the superconducting state via the KSBdG equations, it is possible to calculate the dispersion relation, charge densities, density of states, bound-state energies, the superconducting order parameter and many other physical properties of the superconducting system with arbitrary (e.g., semi-infinite) geometry. A fully ab-initio approach can also be constructed by taking into account the electron-phonon coupling within a simple approximation for the exchange functional.

The new KSBdG-SKKR method was applied to Nb/Au heterostructures where the superconductor's thickness is in the range of the coherence length, i.e., thick superconductor.

Ph.D. student

Simplified treatment of the electron-phonon interaction. — To calculate the superconducting properties at the interface, a simple step function was used to model the changes of the pairing potential at the interface (assuming the experimental value of the bulk gap in the superconductor). We showed that the quantum-well states, which we found to exist in the normal-state band structure, become bound Andreev states due to Andreev scattering. We found that the proximity of a superconductor in the studied heterostructures induces the mirroring of the electronic bands, and opens up a gap at each band crossing. For those materials where no quantum-well states are present, this simple picture is not applicable for the quasiparticle spectrum. It was obtained that the induced gap observed in the normal metal remains constant for each layer for a given Au thickness; however, the size of the gap decays as a function of the Au thickness, and the superconducting order parameter extends well into the normal metal and, interestingly, follows a 1/L decay. Nevertheless, the anomalous charge per layer (which is related to the superconducting order parameter) shows the usual layer-dependent property of the proximity effect as it follows a 1/L decay in the normal metal, which agrees with one-dimensional model calculations in the literature.

Based on the properties of the Andreev spectrum, a simple phenomenological method was developed to predict the transition temperature of such heterostructures which give very good agreements with the experiments (see Figure 1) in the case of the Nb/Au system. The theory was also applied to several different metal overlayers on a Nb host to predict the superconducting transition temperature.

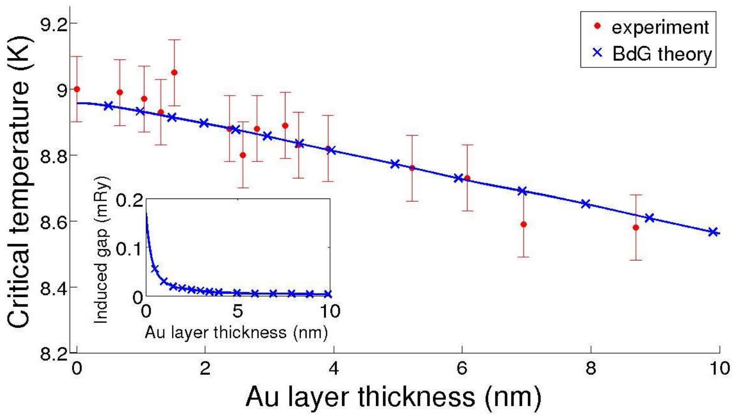

Figure 1. *Dependence of the superconducting transition temperature on the overlayer thickness in a Au/Nb(110) sample. The red dots with errorbars are taken from experiments of Yamazaki et al., Phys. Rev. B 81, 094503 (2010). The inset shows the induced gap in the Andreev spectrum*

If the superconductor is also ultrathin, the calculation of the electron-phonon coupling is necessary, which makes the theory fully first-principles.Therefore, the McMillan-Gaspari-Győrffy theory was extended to slabs and heterostructures and then it was connected to the exchange functional. The McMillan-Hopfield parameter was obtained from the Gaspari-Győrffy formula (using the SKKR method). KSBdG equations were solved self-consistently and the critical temperatue was obtained. This method was applied to Nb/Au thin films where the inverse proximity could be observed. The critical temperature grows if we add only one gold layer to the ultrathin niobium. It was shown that this effect is a consequence of the induced changes in the effective electron-phonon coupling.

High-Entropy Alloys. — The equimolar NiCoFeCr is a face-centered cubic single-phase high-entropy alloy (HEA). Four different sp elements were added in equimolar ratios: NiCoFeCrAl, NiCoFeCrGa, NiCoFeCrGe and NiCoFeCrSn. The initially non-magnetic and single-phase structure turned into multiphase magnetic alloys. Investigations done using first-principles calculations and key experimental measurements revealed that the equimolar FeCrCoNiGe system is decomposed into a mixture of face-centered cubic and body-centered cubic solid solution phases. The increased stability of the ferromagnetic order in the as-cast FeCrCoNiGe composite, with measured Curie temperature of 640 K, is explained using the exchange interactions.

Continuing the structural investigations of these sp-element doped HEAs, X-ray diffraction and scanning electron microscopy (SEM) measurements were performed. The nanoindentation test revealed a 'fingerprint" of the two-phase structure. The Young's and shear moduli of the investigated HEAs were also determined using ultrasound methods. The correlation between these two moduli suggests a general relationship for metallic alloys.

Chiral spin liquids in triangular-lattice SU(N) fermionic Mott insulators with artificial gauge fields — The competition of different interactions in frustrated spin systems may lead to entangled quantum mechanical states, where some kind of local order parameter is formed. Correlated phases without local order are more exciting, such as the chiral spin liquid, proposed by Kalmeyer and Laughlin in 1987 as a variational ground state for spin-1/2 Mott insulators. It can be viewed as a bosonic analogue of the fractional quantum Hall effect, with universal properties such as ground-state degeneracy which depends on the boundary conditions and topologically protected edge excitations. Most interestingly, its excitations are believed to be anyons - excitations that are neither fermionic nor bosonic in nature. These anyonic particles can be braided, allowing for a topological quantum computers, making them relevant also for technological applications. The chiral spin liquid state appears to be fragile, it was found only recently in some spin-1/2 models.

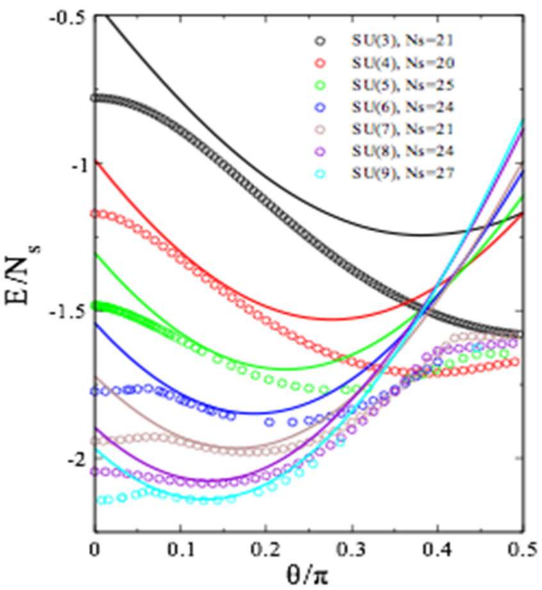

Figure 2. *Comparison of the ground-state energy per site between the exact diagonalization of NS-site clusters (open circles) and the variational energy (full lines) based on Gutzwiller-projected fermionic wave functions with flux π/N per triangular plaquette. The ϑ measures the strength of the 3-site ring exchange. The chiral spin liquid is realised for intermediate values of ϑ/π, approximately between 0.1 and 0.2, where the two energies agree.*

Mott insulating states of ultracold atomic gases in optical lattices promise an alternative way to study quantum states of matter. Alkaline rare earths allow one to realize SU(N) symmetric Mott phases with N as large as 10, in contrast to the SU(2) symmetry of the spin-1/2 models. In this case the quantum fluctuations are enhanced due to increased number N of local degrees of freedom.

Using a variety of numerical probes, including exact diagonalization and variational Monte Carlo calculations, we have shown that, in the presence of an artificial gauge field leading to ring exchange, Mott insulating phases of ultracold fermions with one particle per site generically possess an extended chiral phase with intrinsic topological order characterized by a ground space of N low-lying singlets for periodic boundary conditions, and by chiral edge states described by the $SU(N)_1$ Wess-Zumino-Novikov-Witten conformal field theory for open boundary conditions. (Fig. 2)

Skyrmions in multilayer systems — Skyrmions are non-collinear magnetic structures which are stabilised by interactions that are beyond the reach of a Heisenberg model. The most important of these is the Dzyaloshinsky–Moriya (DM) interaction. We were able to show that frustration in the isotropic exchange interaction also lead to the formation of skyrmions; however, these have very different properties compared to skyrmions stabilised by the DM interaction. Using first-principles calculations, we showed that in $(Pt_{1-x}Ir_x)$/Fe/Pd(111) ultrathin magnetic layers both frustrated Heisenberg couplings and DM interactions are present, and the properties of the skyrmions are primarily determined by the former interaction. As a consequence, it became possible to arrange skyrmions in regular patterns, which is usually prohibited by the repulsive interaction between them. We have also shown that beside skyrmion formation, the frustrated interaction may also lead to the formation of other localised magnetic structures, with non-cylindrical symmetry (Fig. 3). This result has been recently verified by STM experiments in the literature.

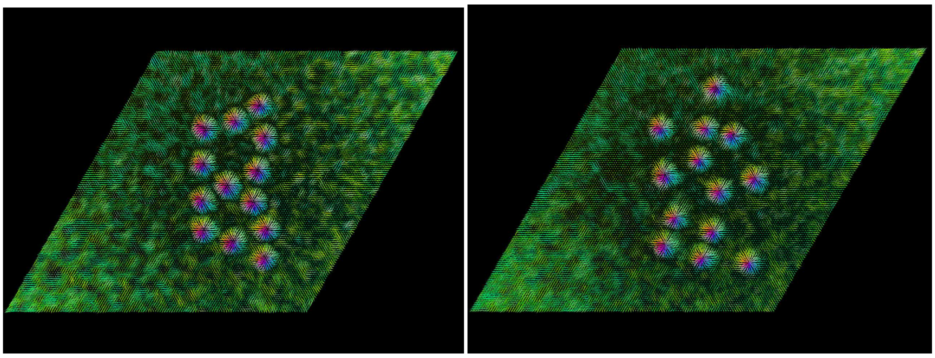

Figure 3 *Attractive (left) and repulsive (right) skyrmions at T = 4.7K*

Grants and international cooperation

OTKA K115632: Magnetism and superconductivity in intermetallic nanocomposites (B. Újfalussy, 2015-2019) in consortium with BME

OTKA K106047: Correlated states and excitations in d- and f-electron systems and ultracold Fermi gases (K.Penc, 2013-2016)

OTKA 109570: Fundamentals of complex, multicpomponent metallic alloys (L. Vitos, 2013-2016)

MTA Mobility program: Infrared, ESR and NMR spectroscopy of functional insulators in magnetic fields, SNK-64/2013 (K. Penc)

Oak Ridge National Laboratory, Magnetic interactions in distorted systems, (B. Újfalussy, 2016)

TÉT_13_DST-1-2013-0004 Production of zero-valence iron nanoparticles, and their application for water treatments and shielding electromagnetic radiation (L. Varga)

GINOP-2.2.1: Research & development of technologies and semi-industrial equipments suitable for producing novel full scale metallic glass-based soft magnetic matrerials (L. Varga)

Publications

Articles

1. Li C-M, Yang R, Johansson B, Vitos L: Anomalous thermodynamic properties and phase stability of δ-$Pu_{1-x}M_x$ (M= Ga and Al) alloys from first-principles calculations. ***PHYS REV B*** 94:(21) 214108/1-8 (2016)

2. Csire G, Cserti J, Ujfalussy B: First principles based proximity effect of superconductor-normal metal heterostructures. ***J PHYS-CONDENS MAT*** 28:(49) 495701/1-7 (2016)

3. Csire G, Schönecker S, Újfalussy B: First-principles approach to thin superconducting slabs and heterostructures. ***PHYS REV B*** 94:(14) 140502/1-5 (2016)

4. Csire G, Cserti J, Tutto I, Ujfalussy B: Prediction of superconducting transition temperatures of heterostructures based on the quasiparticle spectrum. ***PHYS REV B*** 94:(10) 104511/1-4 (2016)

5. Dong Z, Chen D, Long M, Li W, Chen H, Vitos L: Computation of phase fractions in austenite transformation with the dilation curve for various cooling regimens in continuous casting. ***METAL MATER TRANS B*** 47:(3) 1553-1564 (2016)

6. Huang S, Li W, Li X, Schönecker S, Bergqvist L, Holmström E, Varga LK, Vitos L: Mechanism of magnetic transition in FeCrCoNi-based high entropy alloys. ***MATER DESIGN*** 103: 71-74 (2016)

7. Kim D, Vitos L: Tuned magnetic properties of $L1_0$-MnGa/Co(001) films by epitaxial strain. ***SCI REP-UK*** 6: 19508/1-8 (2016)

8. Kiss A, Szolnoki L, Simon F: The Elliott-Yafet theory of spin relaxation generalized for large spin-orbit coupling. ***SCI REP-UK*** 6: 22706/1-10 (2016)

9. Li G, Eriksson O, Johansson B, Vitos L: Ab initio investigation of competing antiferromagnetic structures in low Si-content FeMn(PSi) alloy. ***J PHYS-CONDENS MAT*** 28:(21) 216002/1-6 (2016)

10. Li R, Lu S, Kim D, Schönecker S, Zhao J, Kwon SK, Vitos L: Stacking fault energy of face-centered cubic metals: Thermodynamic and ab initio approaches. ***J PHYS-CONDENS MAT*** 28:(39) 395001/1-10 (2016)

11. Li W, Lu S, Kim D, Kokko K, Hertzman S, Kwon SK, Vitos L: First-principles prediction of the deformation modes in austenitic Fe-Cr-Ni alloys. ***APPL PHYS LETT*** 108:(8) 081903/1-4 (2016)

12. Li W, Lu S, Hu Q-M, Johansson B, Kwon SK, Grehk M, Johnsson JY, Vitos L: Generalized stacking fault energy of γ-Fe. ***PHILOS MAG*** 96:(6) 524-541 (2016)

13. Li X, Schönecker S, Li R, Li X, Wang Y, Zhao J, Johansson B, Vitos L: Ab initio

calculations of mechanical properties of bcc W-Re-Os random alloys: Effects of transmutation of W. ***J PHYS-CONDENS MAT*** 28:(29) Paper 295501. 11 p. (2016)

14. Li X, Schönecker S, Zhao J, Johansson B, Vitos L: Alloying effect on the ideal tensile strength of ferromagnetic and paramagnetic bcc iron. ***J ALLOY COMPD*** 676: 565-574 (2016)

15. Nataf P, Lajkó M, Wietek A, Penc K, Mila F, Läuchli AM: Chiral spin liquids in triangular-lattice SU (N) fermionic Mott Insulators with artificial gauge fields. ***PHYS REV LETT*** 117:(16) 167202/1-6 (2016)

16. Nataf P, Lajkó M, Corboz P, Läuchli AM, Penc K, Mila F: Plaquette order in the SU(6) Heisenberg model on the honeycomb lattice. ***PHYS REV B*** 93:(20) 201113/1-6 (2016)

17. Nurmi E, Wang G, Kokko K, Vitos L: Assessing the elastic properties and ductility of Fe–Cr–Al alloys from ab initio calculations. ***PHILOS MAG*** 96:(2) 122-133 (2016)

18. Nurmi E, Tuuli E, Levämäki H, Kokko K, Leiro J, Vitos L: Directional Young's modulus of single-crystal and cold-rolled titanium from ab initio calculations: Preferred crystal orientation due to cold rolling. ***PHILOS MAG*** 96:(26) 2736-2751 (2016)

19. Oshtrakh MI, Klencsár Z, Semionkin VA, Kuzmann E, Homonnay Z, Varga LK: Annealed FINEMET ribbons: Structure and magnetic anisotropy as revealed by the high velocity resolution Mössbauer spectroscopy. ***MATER CHEM PHYS*** 180: 66-74 (2016)

20. Östlin A, Appelt WH, Di Marco I, Sun W, Radonjić M, Sekania M, Vitos L, Tjernberg O, Chioncel L: Electronic structure of palladium in the presence of many-body effects. ***PHYS REV B*** 93:(15) 155152/1-11 (2016)

21. Östlin A, Di Marco I, Locht ILM, Lashley JC, Vitos L: Stacking fault energetics of α- and γ-cerium investigated with ab initio calculations. ***PHYS REV B*** 93:(9) 094103/1-8 (2016)

22. Hu Q-M, Yang R, Johansson B, Vitos L: Composition dependent hardness of covalent solid solutions and its electronic structure origin. ***CERAM ENG SCI PROC*** 36:(8) 143-151 (2016) (Developments in Strategic Ceramic Materials - 39th International Conference on Advanced Ceramics and Composites, ICACC 2015. 2015.01.25 - 2015.01.30. (ISBN 9781119040439)

23. Rózsa L, Simon E, Palotás K, Udvardi L, Szunyogh L: Complex magnetic phase diagram and skyrmion lifetime in an ultrathin film from atomistic simulations. ***PHYS REV B*** 93:(2) 024417/1-10 (2016)

24. Rózsa L, Deák A, Simon E, Yanes R, Udvardi L, Szunyogh L, Nowak U: Skyrmions with attractive interactions in an ultrathin magnetic film. ***PHYS REV LETT*** 117:(15) 157205/1-6 (2016)

25. Seredina M, Lyange M, Khovaylo V, Taskaev S, Miki H, Takagi T, Singh R, Chatterjee R, Varga LK: Electric resistivity and hall effect of ni(Co)-mn-al melt spun ribbons. ***MATER SCI FORUM*** 845: 65-68 (2016)

26. Streltsov DR, Buzin AI, Dmitryakov PV, Kamasa P, Ivanov DA, Chvalun SN: A study of p-xylylene polymerization kinetics using high-vacuum in-situ differential scanning calorimetry. ***THERMOCHIM ACTA*** 643: 65-72 (2016)

27. Tian F, Varga LK, Shen J, Vitos L: Calculating elastic constants in high-entropy alloys using the coherent potential approximation: Current issues and errors. ***COMP MATER SCI*** 111: 350-358 (2016)

28. Tian L-Y, Levämäki H, Ropo M, Kokko K, Nagy Á, Vitos L: Exchange-correlation catastrophe in Cu-Au: A challenge for semilocal density functional approximations. ***PHYS REV LETTER*** 117:(6) 066401/1-5 (2016)

29. Uusitalo R-R, Lahti A, Levämäki H, Punkkinen MPJ, Vilja I, Kokko K, Vitos L: Order–disorder transition of alloys. ***PHILOS MAG*** 96:(36) 3697-3710 (2016)

30. Vida A, Varga LK, Chinh NQ, Molnar D, Huang S, Vitos L: Effects of the *sp* element additions on the microstructure and mechanical properties of NiCoFeCr based high entropy alloys. ***MAT SCI ENG A-STRUCT*** 669: 14-19 (2016)

31. Vida GyJ, Simon E, Rózsa L, Palotás K, Szunyogh L: Domain-wall profiles in Co/Ir_n /Pt(111) ultrathin films: Influence of the Dzyaloshinskii-Moriya interaction. ***PHYS REV B*** 94:(21) 214422/1-9 (2016)

32. Zhang S-Z, Cui H, Li M-M, Yu H, Vitos L, Yang R, Hu Q-M: First-principles study of phase stability and elastic properties of binary Ti-*x*TM (TM = V,Cr,Nb,Mo) and ternary Ti-15TM-*y*Al alloys. ***MATER DESIGN*** 110: 80-89 (2016)

Book chapter

33. Tian F, Wang Y, Irving DL, Vitos L: Applications of coherent potential approximation to HEAs. In: High-Entropy Alloys: Fundamentals and Applications (Eds.: Gao M C, Yeh J - W, Liaw P K, Zhang Y, Springer International Publishing, 2016) pp. 299-332.

See also S-G.2, S-P.8, S-S.1

S-D. Semiconductor nanostructures

"Momentum" research team

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Design and fabrication of semiconductor nanostructures for bioimaging, quantum computing and 3rd generation photovoltaics

The research team is active in three main different fields, developing new type of i) biomarkers, ii) quantum bits for quantum computation, and iii) 3rd generation solar cells.

Diamond is a known host of solid state qubits and single-photon emitters. Our group seeks for novel potential qubit candidates in diamond, and carries out in-depth characterization by means of *ab initio* atomistic simulations. The properties of oxygen impurity in diamond is largely unexplored, however, they may form defects that can be useful for quantum computation. Oxygen can be introduced by implantation or during chemical vapor deposition. In the latter case, hydrogen can also enter diamond, thus complex formation of oxygen, vacancy and hydrogen could be expected. We examined theoretically several such complexes, some of which have already been observed, others which could potentially form (see Figure 1). Using hybrid density functional theory for the treatment of highly correlated orbitals, many measurable quantities are calculated. We highlight a result from this study: we showed that the neutral oxygen-vacancy complex isovalent with the negatively charged nitrogen-vacancy qubit (NV center) in diamond is not a good candidate for qubit because of the rapid non-radiative decay rate of its excited state.

We implemented and applied theories to study the coupled electron-phonon systems that can be very important in understanding the photoexcitation spectrum of qubits and nanostructures. We showed that the phonon sideband of the photoluminescence spectrum for the silicon-vacancy qubit in diamond can only be interpreted by inclusion of the so-called Herzberg-Teller effect. This result was published in *Physical Review B*. We used methods that go beyond the Born-Oppenheimer approximation and involve many-body perturbation theory in the electron-phonon interaction. We showed that photoemission spectrum of diamondoids can only be understood by strongly coupled electron-phonon interaction (see Figure 2). In conjunction to defect qubits in diamond, we analyzed the optically detected magnetic resonance spectrum of the NV center in ^{13}C-enriched diamond. We developed an effective spin-Hamiltonian model for this system that described well the observed spectra.

Ph.D student

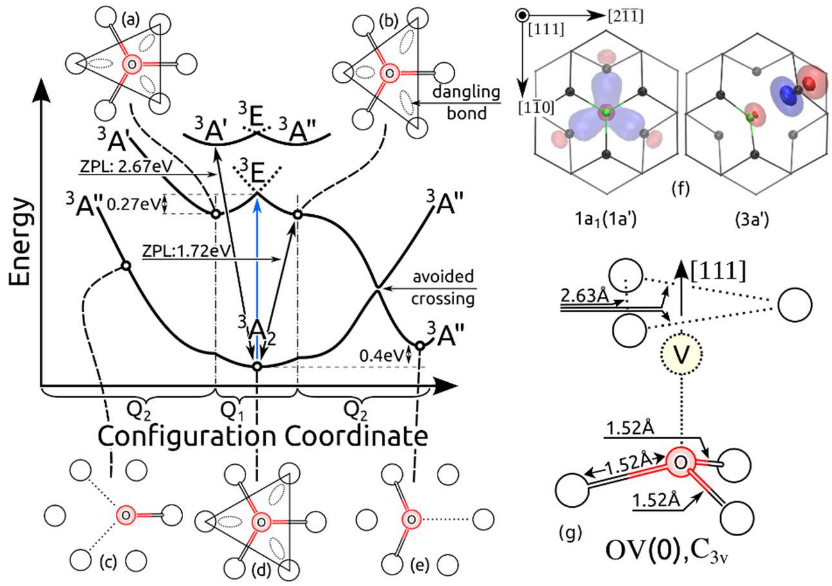

Figure 1. *Potential energy surface of the ground and excited states of OV(0). The different configurations of the defect are depicted in **(a-e)**. **(f)** depicts the one-electron orbitals participating in this excitation process. An electron is promoted from the 1a' level to 3a'. **(g)** shows the ground state geometry in a different orientation. If the defect is excited at the 1.72 eV resonance, the system non-radiatively relaxes back through an intersystem crossing to its ground state without an emission of a photon. While the ground state of OV(0) is very similar to that of the well-known NV(-) system, the excitation process above is very different from that of NV(-) according to our results.*

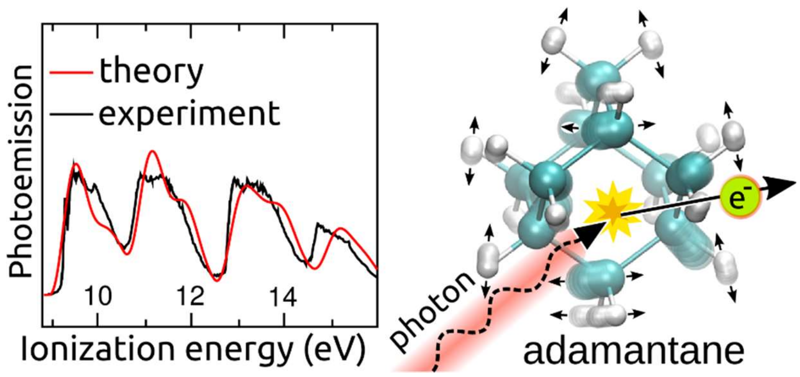

Figure 2. *Photoemission spectrum (PES) of adamantane: theory and experiment. Our theoretical method includes the electron-electron correlation with the so-called GW calculation. In the ionization process, we also include electron-phonon interaction in order to properly describe the dynamic Jahn-Teller or polaronic nature of an ionized adamantane molecule. This effect is depicted on the left, if an electron is removed from the system, the atoms start vibrating. We could reproduce the ionization threshold at 9 eV, as well as the overall lineshape is fully ab initio - no empirical factors from experiments are used. The right panel depicts the structure of the adamantane molecule for which the PES was calculated.*

Significant results have been achieved in the research of solid-state quantum bits, which are the building blocks of a future implementation of the quantum computer. A prominent candidate is the so-called divacancy defect in silicon carbide which has a high-spin ground state. This electron spin may interact with the nearby nuclear spins in the lattice that can naturally occur in SiC. We developed a detailed theory on the optical dynamic spin polarization of the nuclear spins driven by the coherent control of the electron spins of the point defect. Our simulations unraveled that certain nuclear spins can be optically spin-polarized at a given direction depending on the magnitude of a small external magnetic field, thus a bidirectional spin-polarization can be achieved without the need of radiofrequency excitation of the nuclear spins. The proof-of-principle measurement was carried out for proximate nuclear spins by Awschalom group at Chicago University for which theory predicted 25% spin inversion probability at a certain magnitude of the external magnetic field (see Figure 3). These results suggest the incorporation of optical dynamic spin polarization techniques into future quantum information processing and quantum sensing protocols. We contributed to the characterization of nitrogen-vacancy defect in hexagonal SiC, that might be a near-infrared (NIR) counterpart of the famous nitrogen-vacancy center in diamond that operates rather in the visible region.

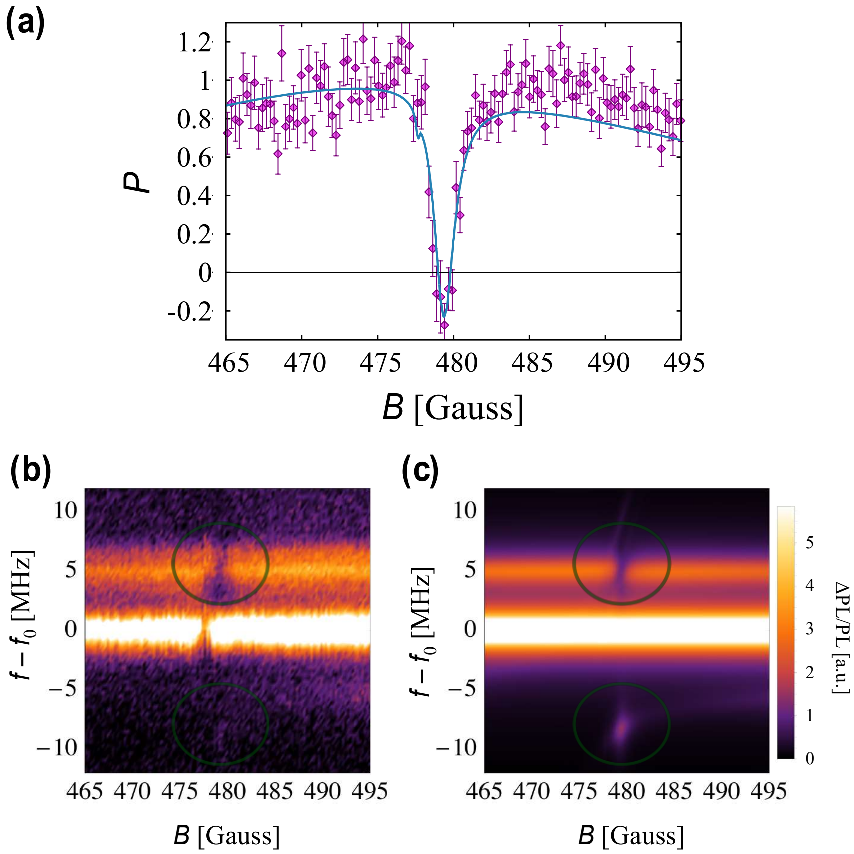

Figure 3. *Experimental and theoretical ^{29}Si nuclear spin polarization and ODMR spectrum of the m_S = 0 to m_S = +1 spin transition of PL6 qubits in 4H-SiC at the GSLAC region.* ***(a)*** *The measured (points) and calculated (thick line) magnetic field dependence of the nuclear spin polarization of a ^{29}Si nucleus at the Si_{IIb} site. DNP is highly efficient up until the LAC-c, at which point it exhibits a sharp drop and reversal. Measurements are carried out at room temperature.* ***(b)*** *The experimental low-microwave-power ODMR spectrum. The measurements are carried out on an ensemble of PL6 divacancy-related qubits in 4H-SiC at room temperature. f_0 = $f_0(B)$ describes the zero-field-splitting and Zeeman shift of the m_S = +1 spin state.* ***(c)*** *Theoretical simulation of the ODMR spectrum which takes into account the DNP of the ^{29}Si nucleus at the Si_{IIb} site and the microwave transition strength in the m_S = |0,+1> manifold. The green ellipsoids on* ***(b)*** *and* ***(c)*** *highlight the signs of the nuclear spin polarization reversal.*

Biologists urgently need biomarker systems which trace, e.g., cancer cells in the blood stream or provide fluorescent signals depending on the activity of neurons in brain. Such systems have been developed so far, but most of them are either unstable or toxic, thus they are not suitable for therapy. Our Momentum Semiconductor Nanostructures Research Group is, however, seeking such solutions that can be applied *in vivo*. Molecular-sized colloid SiC nanoparticles (NP) are very promising candidates to realize bioinert nonperturbative fluorescent nanoparticles for *in vivo* bioimaging. Fluorescent water-soluble silicon carbide (SiC) nanocrystals have been previously identified as complex molecular systems of silicon, carbon, oxygen, and hydrogen held together by covalent bonds that made the identification of their luminescence centers unambiguous. Understanding the fluorescence of this complex system with various surface terminations in solution is still a scientific challenge. We showed that the combination of advanced time-resolved spectroscopy and ab initio simulations, aided by surface engineering, is able to identify the luminescence centers of such complex systems. We identified two emission centers of this complex system: surface groups involving carbon–oxygen bonds and a defect consisting of silicon–oxygen bonds that becomes the dominant pathway for radiative decay after total reduction of the surface (see Figure 4). The identification of these luminescent centers reconciles previous experimental results on the surface- and pH-dependent emission of SiC nanocrystals and helps design optimized fluorophores and nanosensors for in vivo bioimaging.

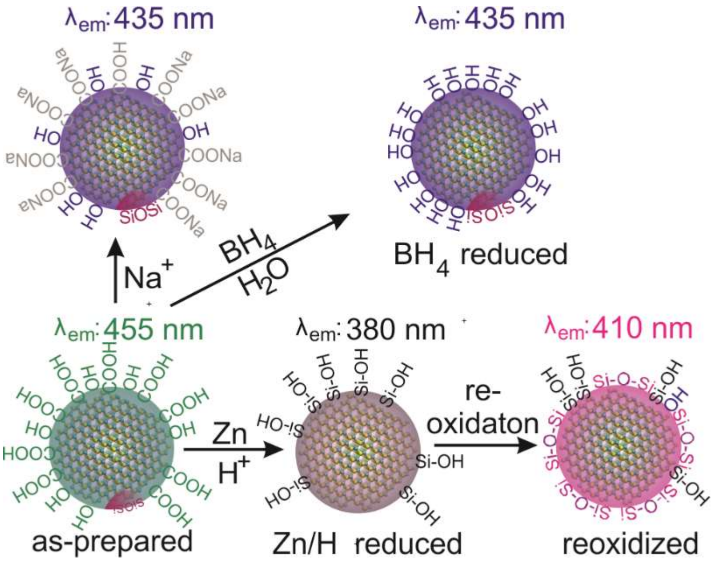

Figure 4. *Surface- and environment-dependent luminescence of SiC NPs. The combination of advanced time-resolved spectroscopy and ab initio simulations, aided by surface engineering, is able to identify the luminescence centers of complex systems. Using such a method, SiOx-defect-related color centers (pink regions on NPs) at the surface of SiC NPs have been identified. From the experimental data, it is possible to build a framework for the surface-related luminescence which can describe the connection between luminescence and surface chemistry.*

Grants

OTKA No. K101819: Design, fabrication and analysis of luminescent silicon carbide nanocrystals for in vivo biomarker applications (Adam Gali, 2012-2016)

OTKA No. K106114: Development of novel silicon carbide nanomarkers and more effective glutamate and GABA uncaging materials for measurement of neuronal network activity and dendritic integration with three-dimensional real-time two-photon microscopy (Adam Gali, 2012-2016)

EU FP7 No. 611143: DIADEMS-Diamond devices enabled metrology and sensing (Adam Gali, 2013-2017)

Visegrad Group (V4) + Japan Joint Research Project on Advanced Materials: Nanophotonics with metal - group IV-semiconductor nanocomposites: From single nanoobjects to functional ensembles (NaMSeN), 2016-2018

International cooperation

Pontificia Universidad Católica de Chile (Santiago de Chile, Chile), Biophysics with color centers in diamond and related materials (J. R. Maze)

RMIT (Melbourne, Australia), Color centers in SiC nanoparticles for bioimaging (S. Castalletto)

University of Melbourne (Melbourne, Australia), Single photon emitters in SiC devices (B.C. Johnson)

University of Pittsburgh (USA), Prof. W. J. Choyke experimental group, SiC (nano)particles

University of Linköping (Sweden), Prof. Erik Janzén experimental group, point defects in SiC

Harvard University (USA), Prof. Michael Lukin experimental group, defects for quantum computing

University of Chicago (USA), Prof. David D. Awschalom experimental group, SiC defects for quantum computing

University of Stuttgart (Germany), Prof. Jörg Wrachtrup experimental group, defects for quantum computing

University of Ulm (Germany), Prof. Fedor Jelezko experimental group, defects for quantum computing

Hasselt University (Belgium), Prof. Milos Nesladek experimental group, defects in diamond

Kaunas University of Technology (Lithuania), Dr. Audrius Alkauskas theoretician group, defects in diamond and SiC

University of Erlangen-Nürnberg (Germany), Dr. Michel Bockstedte theoretician group, defects in diamond and SiC

University of Kobe (Japan), Prof. Minoru Fujii experimental group, Si nanoparticles

Charles University (Czechia), Prof. Jan Valenta experimental group, Si nanoparticles

Slovakian Academy of Sciences (Slovakia), Prof. Ivan Stich theoretician group, quantum Monte Carlo methods in Si nanoparticles

Warsaw University of Technology (Poland), Prof. Romuald B. Beck experimental group, Si layers and devices

University of Mainz (Germany), Prof. Dmitrii Budker experimental group, diamond defects

University of Saarland (Germany), Prof. Christoph Becher experimental group, diamond defects

Publications

Articles

1. Beke D, Jánosi TZ, Somogyi B, Major DÁ, Szekrényes Zs, Erostyák J, Kamarás K, Gali A: Identification of luminescence centers in molecular-sized silicon carbide nanocrystals. ***J PHYS CHEM C*** 120:(1) 685-691 (2016)

2. Csóré A, Gällström A, Janzén E, Gali A: Investigation of Mo defects in 4H-SiC by means

of density functional theory. ***MATER SCI FORUM*** 858: 261-264 (2016)

3. Gali A, Demján T, Vörös M, Thiering G, Cannuccia E, Marini A: Electron-vibration coupling induced renormalization in the photoemission spectrum of diamondoids. ***NAT COMMUN*** 7: 11327/1-9 (2016)

4. Gruznev DV, Bondarenko LV, Matetskiy AV, Mihalyuk AN, Tupchaya AY, Utas OA, Eremeev SV, Hsing C-R, Chou J-P, Wei C-M, Zotov AV, Saranin AA: Synthesis of two-dimensional Tl_x Bi_{1-x} compounds and Archimedean encoding of their atomic structure. ***SCI REP-UK*** 6: 19446/1-9 (2016)

5. Ivády V, Szász K, Falk AL, Klimov PV, Janzén E, Abrikosov IA, Awschalom DD, Gali A: First principles identification of divacancy related photoluminescence lines in 4H and 6H-SiC. ***MATER SCI FORUM*** 858: 322-325 (2016)

6. Ivády V, Klimov PV, Miao KC, Falk AL, Christle DJ, Szász K, Abrikosov IA, Awschalom DD, Gali A: High-fidelity bidirectional nuclear qubit initialization in SiC. ***PHYS REV LETT*** 117:(22) 220503/1-6 (2016)

7. Ivády V, Szász K, Falk AL, Klimov PV, Christle DJ, Koehl WF, Janzén E, Abrikosov IA, Awschalom DD, Gali A: Optical nuclear spin polarization of divacancies in SiC. ***MATER SCI FORUM*** 858: 287-290 (2016)

8. Jarmola A, Bodrog Z, Kehayias P, Markham M, Hall J, Twitchen DJ, Acosta VM, Gali A, Budker D: Optically detected magnetic resonances of nitrogen-vacancy ensembles in ^{13}C-enriched diamond. ***PHYS REV B*** 94:(9) 094108/1-5 (2016)

9. Lohrmann A, Johnson BC, Almutairi AFM, Lau DWM, Negri M, Bosi M, Gibson BC, McCallum JC, Gali A, Ohshima T, Castelletto S: Engineering single defects in silicon carbide bulk, nanostructures and devices. ***MATER SCI FORUM*** 858: 312-317 (2016) Proc. Conf. Silicon Carbide and Related Materials 2015.

10. Norambuena A, Reyes SA, Mejía-Lopéz J, Gali A, Maze JR: Microscopic modeling of the effect of phonons on the optical properties of solid-state emitters. ***PHYS REV B*** 94:(13) 134305/1-8 (2016)

11. Thiering G, Gali A: Characterization of oxygen defects in diamond by means of density functional theory calculations. ***PHYS REVB*** 94:(12) 125202/1-15 (2016)

12. von Bardeleben H J, Cantin J L, Csóré A, Gali A, Rauls E, Gerstmann U: NV centers in 3*C*,4*H*, and 6*H* silicon carbide: A variable platform for solid-state qubits and nanosensors. ***PHYS REV B*** 94:(12) 121202/1-6 (2016)

See also: S-Q.1

S-P. Ultrafast, high intensity light-matter interactions

"Momentum" research team

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Strong-field interactions and nano-optics experiments. — Probing nanooptical near-fields is a major challenge in plasmonics. Here, we demonstrate an experimental method based on utilizing ultrafast photoemission from plasmonic nanostructures that is capable of probing the maximum nanoplasmonic field enhancement in any metallic surface environment. Directly measured maximum field enhancement values for various samples are in good agreement with detailed finite-difference time-domain simulations. These results establish ultrafast plasmonic photoelectrons as versatile probes for nanoplasmonic near-fields. Fig. 1 shows the measurement scheme and spectral cutoffs according to which maximum field enhancement values are determined.

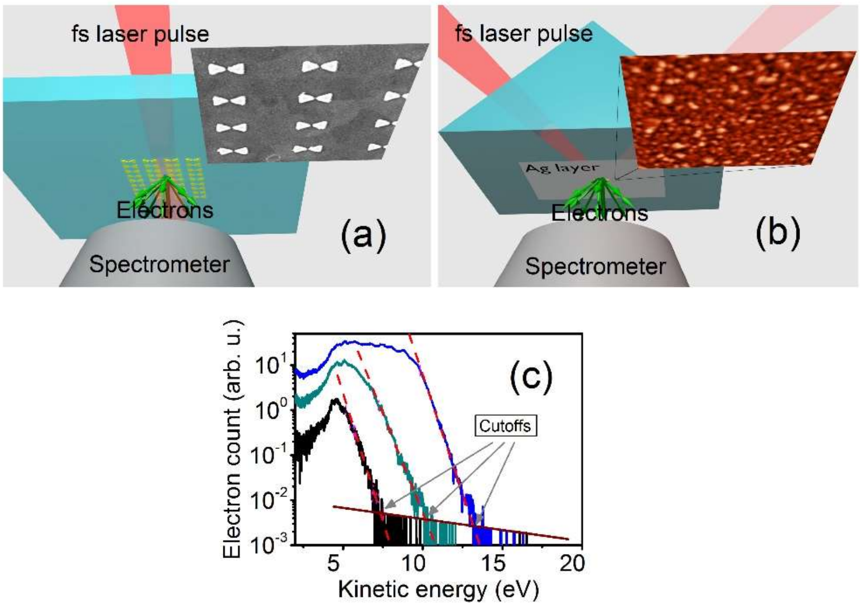

Figure 1. *(a) Experimental scheme for measuring photoemission spectra induced by localized plasmon fields at gold nanoparticle arrays. The sample is in vacuum and the substrate is illuminated from the back side through the transparent substrate, so that photoelectrons emitted from the nanoparticles can directly enter a time-of-flight electron spectrometer. (b) Experimental scheme for measurement of plasmonic photoelectrons from silver layers of some 50 nm thickness exhibiting different surface roughnesses. (c) Typical plasmonic photoelectron spectra. Intersection of the red line fitted to the decaying section of the spectrum and that fitted to the baseline define the maximum electron kinetic energy (cutoff) based on which we determine maximum field enhancement factors between 17 and 52.*

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We also developed an efficient, tailored optimization method for attopulse generation using a light-field-synthesizer which was demonstrated by M. Hassan et al. at the Max Planck Institute of Quantum Optics (Nature 530, 66 (2016)). We adapted genetic optimization of single-cycle and sub-cycle waveforms to attosecond pulse generation and achieved significantly improved convergence to several targeted attosecond pulse shapes. Importantly, we show that the single-atom approach based on strong-field approximation gives similar results to the more complex and numerically intensive 3D model of the attopulse generation process and that spectrally tunable attosecond pulses can be produced with a light-field synthesizer.

Femtosecond photonics. — Improving the laser-induced damage threshold of optical components is a basic endeavor in femtosecond technology. By testing more than 30 different femtosecond mirrors with 42 fs laser pulses at 1 kHz repetition rate, we found that a combination of high-bandgap dielectric materials and improved design and coating techniques enable femtosecond multilayer damage thresholds exceeding 2 J/cm^2 in some cases. A significant improvement by a factor of 2.5 in damage resistance can also be achieved for hybrid Ag-multilayer mirrors exhibiting more than 1 J/cm^2 threshold with a clear anticorrelation between damage resistance and peak field strength in the stack. Slight dependence on femtosecond pulse length and substantial decrease for high (MHz) repetition rates are also observed.

Surface plasmon studies. — In 2016, like in earlier years, we studied the properties of surface plasmon polaron (SPP)-assisted electron and photon emission in gold films. The surface plasmons were excited by femtosecond pulses of a Ti:sapphire laser in the 10 – 200 GW/cm^2 intensity range. We have found oscillatory electromagnetic field dependence of the SPP dispersion curve and concluded, that the effect is due to the dynamical screening of electrons by the plasmonic/photonic field. A simple theoretical model agrees well with the experimental data if we suppose that the effective mass of the screened electrons is smaller, than the free electron mass and decreases with increasing laser intensity. We have also found strong evidence that in a laser intensity range around 80 GW/cm^2, the gold film turns into ideal diamagnetism.

In some further experiments, the 45 nm thick gold film was evaporated on an ordered surface of 100 nm glass spheres. The qualitative results of SPP-assisted electron and photon emission agree quite well with those of irregular surfaces, but with some modifications, indicating some interference of the emitted electrons and photons. To explain these experimental findings, further experiments are needed.

Theoretical quantum optics. — Recently, we have introduced a new regular phase operator, coherent-phase states (a special type of SU(1,1) coherent states), and the associated quantum phase probability distributions of electromagnetic radiation modes. This general formalism is expected to apply in quantifying the quantum phase uncertainties of extreme optical fields like high harmonics of strong laser fields, which we have been studying in various cases. In the meantime, by analyzing the time evolution of the regular phase operator, we have proved that in addition to the deterministic (linear) phase variation, there exists a second quantum term, which is in fact an invariant Haar integral of a positive operator-valued measure on the Blaschke group (which is another parametrization of the SU(1,1) group). In Figure 2 we illustrate this result by plotting the time-evolution of the expectation value of these two term and their sum. The above result may be considered as a proof of the periodicity of the complete physical phase. We also note that the matrix elements between photon number eigenstates of a certain unitary representation of the Blaschke group, appearing in our formalism, are directly expressed by the Zernike polynomials, which play an important role in optical wavefront analysis.

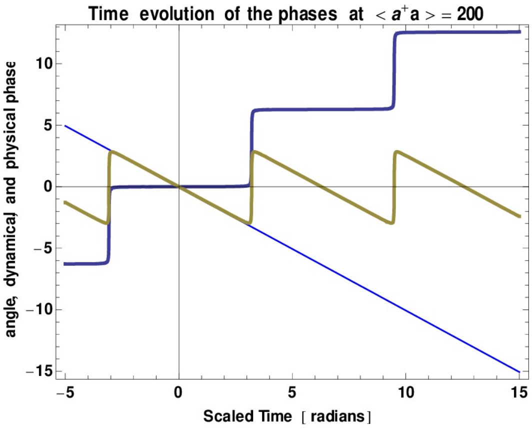

Figure 2. *Time evolution of the expectation value in a regular coherent phase state (with a mean photon number of 200) of the components of the regular phase operator. The straight line with tangent -1 is the usual classical time dependence of a harmonic oscillator in phase space (clock-wise rotation in the q-p complex amplitude plane), which has a sharp value, also for all quantum states of the oscillator. The step-like curve (with 2π jumps) illustrates the increase of the quantum angle, which we call the Blaschke contribution. The 2π accumulations come from the invariant Haar integral of the positive operator-valued measure on the Blaschke group. The sum of these two contributions (i.e., the complete physical phase) appears as a periodic saw-tooth-like function. For increasing excitation amplitudes this curve gets sharper, and approaches the ideal saw-tooth function.*

Grants

"Momentum" Program of the HAS (P. Dombi, 2014-2019)

Ma x Planck Society Partner Group Grant: Ultrafast strong-field nanoplasmonics (P. Dombi, 2014-2019)

OTKA 109257: Time-resolved investigations of functional molecules and metal nanoparticles (P. Dombi, 2014-2018)

OTKA 109472: Ultrafast processes in nanolocalized electromagnetic fields (P. Rácz, 2014-2017)

International cooperations

Max Planck Institute of Quantum Optics (Garching, Germany) with P. Dombi.

Carl von Ossietzky University (Oldenburg, Germany) with P. Dombi and B. Nagy.

Texas A&M University (College Station, USA) with N. Kroó.

University of Ulm (Germany) with N. Kroó and S. Varró.

University of Graz (Austria) with P. Dombi.

Publications

Articles

1. Hack Sz, Varró S, Czirják A: Interaction of relativistic electrons with an intense laser

pulse: High-order harmonic generation based on Thomson scattering. ***NUCL INSTRUM METH B*** 369: 45-49 (2016) Proc. of Photon and fast Ion induced Processes in Atoms, Molecules and Nanostructures (PIPAMON).

2. Kroó N, Rácz P, Varró S: Bright new world. ***NUCL INSTRUM METH B*** 369: 55-59 (2016) Proc. of International Workshop on Photon and fast Ion induced Processes in Atoms, Molecules and Nanostructures (PIPAMON) Debrecen, Hungary, .24-03-2015 – 26-03-2015

3. Varro S, Szabo LZ, Czirjak A: Laser-assisted electron scattering on a nano-sphere. ***NUCL INSTRUM METH B*** 369: 29-33 (2016) Proc. of International Workshop on Photon and Fast Ion induced Processes inAtoms, Molecules and Nanostructures (PIPAMON). Debrecen, Magyarország: 2015.03.24 -2015.03.26.

4. Ayadi V, Benedict MG, Dombi P, Földi P: Atomic coherence effects in few-cycle pulse induced ionization. ***EUR PHYS J D*** 70:(12) 266/1-8 (2016)

5. Bódi B, Balogh E, Tosa V, Goulielmakis E, Varjú K, Dombi P: Attosecond pulse generation with an optimization loop in a light-field-synthesizer. ***OPT EXPRESS*** 24:(19) 21957-21962 (2016)

6. Csajbók V, Szikszai L, Nagy BJ, Dombi P: Femtosecond damage resistance of femtosecond multilayer and hybrid mirrors. ***OPT LETT*** 41:(15) 3527-3530 (2016)

7. Gombkötő Á, Czirják A, Varró S, Földi P: Quantum-optical model for the dynamics of high-order-harmonic generation. ***PHYS REV A*** 94:(1) 013853/1-8 (2016)

8. Kroó N, Rácz P, Tüttő I: Plasmonic dynamic screening in a gold film by intense femtosecond laser light. ***EUROPHYS LETT*** 115:(2) 27010/1-4 (2016)

9. Kroó N, Rácz P: Plasmonics - The interaction of light with metal surface electrons. ***LASER PHYS*** 26:(8) 084011/1-5 (2016)

10. Kroo N, Varro S, Racz P, Dombi P: Surface plasmons: a strong alliance of electrons and light. ***PHYS SCRIPTA*** 91:(5) 053010/1-13 (2016)

11. Márton I, Ayadi V, Rácz P, Stefaniuk T, Wróbel P, Földi P, Dombi P: Ultrafast plasmonic electron emission from Ag nanolayers with different roughness. ***PLASMONICS*** 11:(3) 811-816 (2016)

12. Tsatrafyllis N, Bergues B, Schröder H, Veisz L, Skantzakis E, Gray D, Bodi B, Kuhn S, Tsakiris GD, Charalambidis D, Tzallas P: The ion microscope as a tool for quantitative measurements in the extreme ultraviolet. ***SCI REP-UK*** 6: 21556 (2016)

Conference proceedings

13. Vogelsang J, Robin J, Nagy BJ, Dombi P, Rosenkranz D, Schiek M, Gross P, Lienau C: Remotely driven electron emission for ultrafast electron microscopy. *In: Proc. of Conference on Lasers and Electro-Optics (CLEO). San Jose, USA, 05-06-2016 - 10-06-2016*. (ISBN 978-1-9435-8011-8) Paper 7787747. 4 p. (2016)

14. Robin J, Vogelsang J, Nagy BJ, Dombi P, Groß P, Lienau C: Strong field above threshold ionization of rydberg electrons localized to a gold nanotip. *In: Proc. Conference on Lasers and Electro-Optics (CLEO). San Jose, USA, 05-06-2016 – 10-06-2016.* OSA, Washington. (ISBN 978-1-9435-8011-8) Paper 7787745 4 p. (2016)

15. Rácz P, Teichmann SM, Ciappina MF, Perez-Hernandez JA, Thai A, Fekete J, Elezzabi AY, Veisz L, Biegert J, Dombi P: Strong field nanoplasmonic photoemission in the mid-IR at <1 GW/cm2 intensity. *In: Proc. of the 11th Conference on Lasers and Electro-Optics Pacific Rim, CLEO-PR 2015, Busan, South-Korea, 24-08-2015 – 28-08-2015.* IEEE, Seattle, (ISBN:9781467371094) Paper 7376398 2 p. (2016)

16. Robin J, Vogelsang J, Nagy BJ, Dombi P, Lienau C, Groß P: A road toward attosecond physics in solids-atomic-like rydberg states localized at a nanotip. *In: Proc. of International Conference on Ultrafast Phenomena 2016 Santa Fe, USA, 17-07-2016 – 22-07-2016.* Optical Society of America (OSA) Washington. (ISBN:978-1-943580-18-7) Paper Utu5A.3 (2016)

17. Vogelsang J, Robin J, Nagy BJ, Dombi P, Groß P, Lienau C: Efficient emission of ultrafast electron bursts by plasmonic nanofocusing of light. *In: Proc. Conference on Lasers and Electro-Optics (CLEO). San Jose, USA, 05-06-2016 – 10-06-2016.* OSA, Washington. (ISBN 978-1-9435-8011-8) Paper UW1A.6. (ISBN:978-1-943580-18-7) (2016)

See also R-P.1, R-P.2, R-P.6

S-R. Nanostructures and applied spectroscopy

Wigner research group

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Silicon-vacancy center in nanodiamonds. – Due to their excellent light emission properties, the investigation of the negatively charged silicon–vacancy (SiV^-) centers in diamond nanostructures has attracted much interest during last decades. The SiV^- center consisting of one interstitial silicon atom in a split–vacancy configuration with D_{3d} symmetry has a bright, stable and narrow zero-phonon line (ZPL) at 1.681 eV. It has a weak phonon sideband since more than 70% of the emitted light is concentrated into the ZPL even at room temperature. These advantageous properties of the optical transition make the SiV^- center a promising candidate for solid-state single-photon emitter that can be used to realize numerous novel applications in quantum computing and cryptography or nanoscopy and cell biology, etc. For quantum information and quantum processing purposes, indistinguishable single photons from distinct SiV^- center emitters are required. Variation of spectral parameters of the mentioned center observed by different groups strongly restricts its implementation to real applications. Novel methods have to be developed for the creation of uniformly emitting silicon–vacancy centers in diamond nanostructures on large scale, and the origin of the processes responsible for the variation of the ZPL of the SiV^- centers has to be resolved.

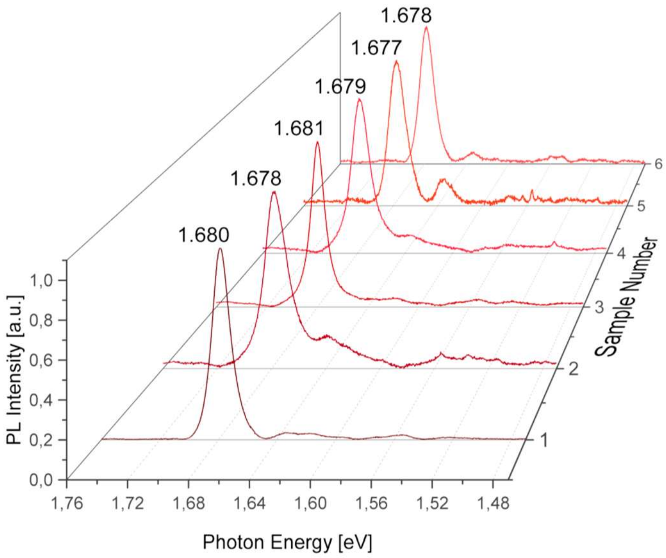

Figure 1. *Spectral distribution of SiV^- center emission line in photo-luminescence spectra measured at room temperature in nanocrystalline diamond layers grown at substrate temperatures and methane concentrations in the precursor Ar + CH_4 mixture of (1) T=700 °C and 2.0% CH_4 (2) T=750 °C and 0.2% CH_4 (3) T=750 °C and 3.0% CH_4 (4) T=800 °C and 1.0% CH_4 (5) T=850 °C and 0.2% CH_4 (6) T=850 °C and 3.0% CH_4. The emission was excited by the 2.54 eV line of an Ar-ion laser.*

In order to have detailed overview on the spectral properties, SiV^- center ensembles were investigated in a large number of nanodiamond films by fluorescence spectroscopy (Fig. 1). Conditions of SiV^- center formation were varied systematically in microwave plasma-assisted chemical vapor deposition (MW CVD) process and spectral parameters of the zero-

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phonon line (ZPL) were obtained by fitting procedure from experimentally measured spectra. The average size of nanodiamond grains determined from scanning electron microscopic (SEM) micrographs and residual stress of diamond layer calculated from diamond Raman peak position were used as sample parameters. The SiV^- centers ZPL peak positions were found to vary from 1.677 to 1.681 eV, while their line broadening between 6.5 and 18.1 meV. The smallest linewidth was observed in a diamond layer of 30 nm average grain size and it was comparable with line broadening values reported for individual SiV^- centers.

A significant blue shift and line narrowing of the ZPL peak position was observed with decreasing average grain size of the SiV^- containing diamond thin films. The residual stress, being dependent on the grain size, was identified as the major cause of the variation of the ZPL parameters. It was found that the increase of the residual stress from 0.64 GPa tensile to 2.25 GPa compressive one correlates well with the changes in ZPL peak parameters. The blue shift and line narrowing of SiV^- centers were explained by the suppression of the orbital relaxation processes, involving ground and excited electronic levels, initiated by the different local strain fields in the vicinity of the SiV^- centers. Acoustic phonon mode confinement due to small diamond grain size also contributes to the suppression of relaxation process by electron–phonon transitions. Our results indicate decisive influence of the diamond grain size and internal residual stress of the layer on the spectral parameters of the zero phonon line of the SiV^- centers.

Nickel-silicon (Ni-Si) related complex color center in nanodiamond. — Ni-Si related complex color center was successfully created in nanocrystalline diamond grains through CVD deposition process, which emits highly intensive narrow-bandwidth ZPL at 865 nm (1.433 eV) with 2 nm (3 meV) full width at half maximum. This color center is highly significant in the field of biological and medical applications since its excitation and emission wavelength range is lying in the near-infrared window of biological tissues. Variation of ZPL peak position and line width have been detected in nanodiamond grains prepared under different conditions (Fig. 2). Experimental results on the residual stress determined from the position of diamond Raman peak measured on different nanodiamond grains exhibit different values in the range of -0.963 to +0.284 GPa, and can be of compressive or tensile type. In contrast to the SiV^- color center, direct relation between the ZPL position and local stress has not been established until now. The relatively large size of the complex center and the lack of vacancy in the center could be the possible reasons of this behavior. (Fig. 2)

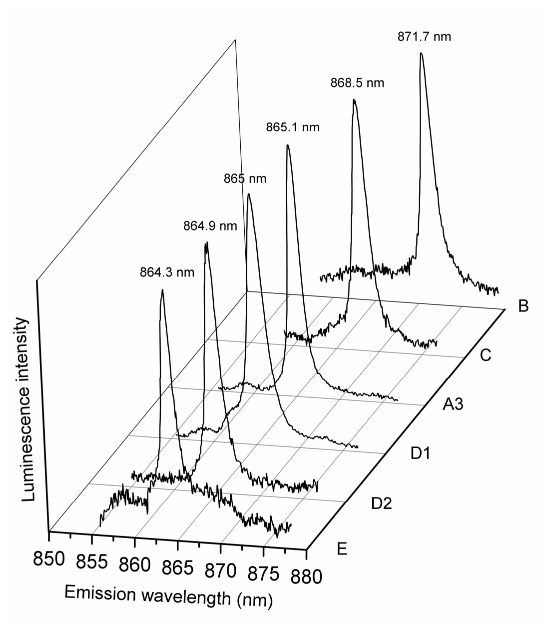

Figure 2. *Dependence of the ZPL spectral shape of Ni-Si related complex impurity center in diamond nanograins on deposition conditions. The spectra were recorded by 488 nm laser excitation at room temperature.*

Preparation of nanocrystalline diamond and nanocrystalline silicon carbide by ultrashort laser pulses

Favorable properties of color centers formed in nanodiamond for various applications in quantum informatics, medical imaging and biolabeling generate a need to develop fast, reliable and widespread technology for their fabrication. Therefore a new concept was introduced for the creation of one-photon emitter centers in nanodiamond by using ultrashort laser pulses (800 nm center wavelength with 1 kHz repetition rate and 42 fs pulse duration). Nanodiamond crystals were produced with ultrashort laser pulses by using different carbon- and silicon-based materials as source material. Surface-enhanced Raman spectroscopy measurements were performed to prove the presence of diamond nanocrystals (Fig. 3, left). The incorporation of silicon foreign atoms into the nanodiamond structure under laser irradiation was also demonstrated.

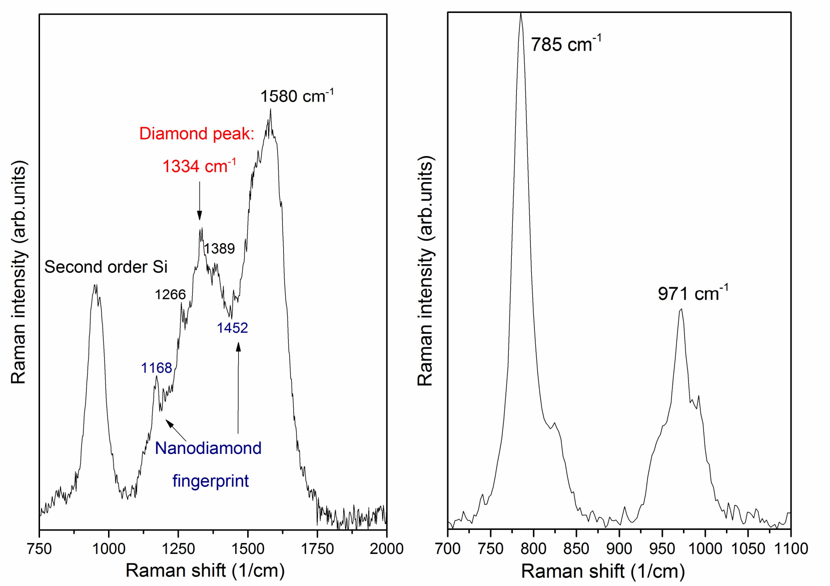

Figure 3. *(Left) Surface-enhanced Raman scattering spectrum of nanocrystalline diamond grains. (Right) Micro-Raman spectrum of the silicon carbide agglomerate excited by 514 nm probing wavelength.*

Silicon carbide (SiC) nanocrystals were created successfully by the irradiation of carbon- and silicon-based materials with femtosecond laser pulses (800 nm center wavelength with 1 kHz repetition rate and 42 fs pulse duration) in air at room temperature. Micro-Raman spectroscopic and scanning electron microscopy measurements were carried out to prove the presence of SiC nanocrystals and to analyze the bonding structure of formed nanostructures. Detailed analysis of the transversal (TO) and longitudinal (LO) optical modes support the formation of cubic and hexagonal SiC nanocrystals (3C, 4H and 6H) with average grain size of 100-500 nm (Fig. 3, right).

Grants

Bolyai János Scholarship of the H.A.S.: Creation of light emitting color centers using novel techniques in diamond nanocrystals (S. Tóth, 2016-2019)

Bolyai János Scholarship of the H.A.S.: Detection of disease-marker molecules in the exhaled breath using surface enhanced Raman spectroscopy (M. Veres, 2014-2017)

Academic Excellence Program, EXMET: Development of combined LIBS-Raman equipment (M. Veres, 2015-2017)

EU H2020 FET-Open: Visual genetics: establishment of a new discipline to visualize neuronal nuclear functions in real-time in intact nervous system by 4D Raman spectroscopy (M. Veres, 2016-2019)

COST MP1401: Advanced fibre laser and coherent source as tools for society, manufacturing and lifescience (M. Veres, 2016-2018)

H2020-MSCA-RISE-2016 VISGEN -Transcribing the processes of life: Visual Genetics (M. Veres, 2017-2021)

International cooperation

Saint Petersburg National Research University of Information Technologies (St. Petersburg, Russia), Light emission properties of polymers with plasmonic nanoparticles (S. Tóth)

Universität Kassel (Kassel, Germany) Surface functionalization of nanodiamond (M. Veres)

Uzhhorod National University (Uzhhorod, Ukraine), Structural transformations in chalcogenides (M. Veres)

V. Lashkaryov Institute of Semiconductor Physics (Kiev, Ukraine), Structural properties of gyrotropic cadmium diphosphide crystals (M. Veres)

A.M. Prokhorov General Physics Institute of RAS (Moscow, Russia), Nanodiamond characterization (M Veres)

University of Birmingham (Birmingham, United Kingdom), Stimulated Raman scattering of alkyne tagged DNA and other biomolecules (M. Veres)

Max Planck Institute for Neurobiology (Martinsried, Germany), Stimulated Raman scattering techniques for zebrafish studies (M. Veres)

Publications

Articles

1. Ignatovych M, Borysenko M, Davydenko L, Borysenko L, Veres M, Himics L, Koós M: Cerium and europium nanospecies in quartz glass: Synthesis and spectral study (Cer- und Europium-haltige Nanopartikel in Quarzglas: Synthese und spektroskopische Eigenschaften, in German) ***MATERIALWISS WERKST*** 47:(2-3) 193-197 (2016) doi: 10.1002/mawe.201600475

2. Tóth S, Himics L, Koós M: Creation of near-infrared emitting optical center related to nickel–silicon impurity complex in nanodiamond grains. ***J LUMIN*** 176: 367-371 (2016) doi: 10.1016/j.jlumin.2016.04.015

3. Himics L, Tóth S, Veres M, Koós M: Spectral properties of the zero-phonon line from ensemble of silicon–vacancy center in nanodiamond. ***OPT QUANT ELECTRON*** 48:(8) 394/1-11 (2016) doi: 10.1007/s11082-016-0663-2

4. Mitsa V, Holomb R, Marton A, Veres M, Tóth S, Himics L, Lorinczi A, Popescu M: Investigation of atmospheric corrosion by photon energy dependent luminescence and Raman spectroscopy in aged and freshly fractured g-,c-As2S3 with photosensitive realgar inclusions. ***J NON-CRYST SOLIDS*** 453: 23-27 (2016) doi: 10.1016/j.jnoncrysol.2016.09.022

5. Csarnovics I, Cserhati C, Kokenyesi S, Latif MR, Mitkova M, Nemec P, Hawlova P, Nichol T, Veres M: Light and electron beam induced surface patterning in Ge-Se system. ***J OPTOELECTRON ADV M*** 18:(9-10) 793-797 (2016)

6. Rigó I, Veres M, Himics L, Tóth S, Czitrovszky A, Nagy A, Fürjes P: Comparative analysis of SERS substrates of different morphology. ***PROCEDIA ENGINEERING*** 168: 371-374 (2016) doi: 10.1016/j.proeng.2016.11.131

7. Bonyár A, Csarnovics I, Veres M, Himics L, Csík A, Kámán J, Balázs L, Kökényesi S: Investigation of the performance of thermally generated Au/Ag nanoislands for SERS and LSPR applications. ***PROCEDIA ENGINEERING*** 168: 1152-1155 (2016) doi: 10.1016/j.proeng.2016.11.384

See also: R- M. (Bányász), R-M. (Bányász), S-N.2, S-N.4

S-S. Quantum optics

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Cavity Quantum Electrodynamics, quantum critical phenomena. — Quantum phase transitions in driven-dissipative systems opened up a novel research area in the field of critical phenomena. These transitions lie beyond the standard classification of dynamical or equilibrium phase transitions, and define completely new universality classes. In an open quantum system, the critical behaviour appears in the state formed by the dynamical equilibrium of the external driving and dissipation processes. The abrupt symmetry breaking change of such a steady state takes place when the external control parameters are continuously tuned across the critical point. The correlation functions at the critical point are determined by non-equilibrium noise rather than thermal or ground-state quantum fluctuations. We demonstrated that criticality in a driven-dissipative system is strongly influenced by the spectral properties of the bath. We studied the open-system realization of the Dicke model, where a bosonic cavity mode couples to a fictious large spin formed by two motional modes of an atomic Bose-Einstein condensate. The cavity mode is driven by a high-frequency laser and it decays to a Markovian bath, while the atomic mode interacts with a colored bath. We revealed that the soft mode fails to describe the characteristics of the criticality. We calculated the critical exponent of the superradiant phase transition and identified an inherent relation to the low-frequency spectral density function of the colored bath. We showed that a finite temperature of the colored bath does not modify qualitatively this dependence on the spectral density function.

We investigated the possibility of the Dicke-type superradiant phase transition of an atomic gas. We described the ultrastrong coupling limit of the interaction between light and atoms within the regularized electric dipole gauge, in which we can take into account the short-range depolarizing interactions between atoms that approach each other as close as the atomic size scale. By using a mean field model, we find that a critical point does indeed exist, though the atom-atom contact interaction shifts it to a higher value than what can be obtained from the bare Dicke-model. We pointed out the proximity of the critical density to that of solidification, which leads to the conjecture that the system, at the critical density, goes over to the condensed rather than to the "superradiant" phase.

Ultracold gases, Bose-Einstein condensates. — Bose-Einstein condensates of ultracold atoms can be used to sense fluctuations of the magnetic field by means of transitions into untrapped hyperfine states. It has been shown recently that counting the outcoupled atoms can yield the power spectrum of the magnetic noise. As a continuation of our previous investigations, we calculated the spectral resolution function, which characterizes the condensate as a noise measurement device in this scheme. We used the description of the

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radio-frequency outcoupling scheme of an atom laser, which takes into account the gravitational acceleration. Employing both an intuitive and the exact three-dimensional and fully quantum mechanical approach, we derived the position-dependent spectral resolution function for condensates of different size and shape.

We investigated the magnetic properties of strongly interacting four-component spin-3/2 ultracold fermionic atoms in the Mott insulator limit with one particle per site in an optical lattice with honeycomb symmetry. In this limit, atomic tunneling is virtual, and only the atomic spins can exchange. We found a competition between symmetry-breaking and liquid-like disordered phases. Particularly interesting are the non-singlet valence bond states (where the valence bonds have non-zero magnetization) which are situated between the ferromagnetic and conventional valence bond phases. In the framework of a mean-field theory, we calculated the phase diagram and identified an experimentally relevant parameter region where a homogeneous SU(4) symmetric Affleck-Kennedy-Lieb-Tasaki–like valence bond state is present.

The classical ground states of the SU(4) Heisenberg model on the face-centered-cubic lattice constitute a highly degenerate manifold. We explicitly constructed all the classical ground states of the model. To describe quantum fluctuations above these classical states, we applied linear flavor-wave theory. At zero temperature, the bosonic flavor waves select the simplest of these SU(4) symmetry-breaking states, the four-sublattice-ordered state defined by the cubic unit cell of the fcc lattice. Due to geometrical constraints, flavor waves interact along specific planes only, thus rendering the system effectively two dimensional and forbidding ordering at finite temperatures. We showed that longer-range interactions generated by quantum fluctuations can shift the transition to finite temperatures.

Grants

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MTA INFRA Infrastructural development fund, Wigner Atomlaser Lab (P. Domokos)

MTA Visiting Professor Fellowship, (Prof. Fortágh József)

Publications

Articles

1. Sinkovicz P, Szirmai G, Penc K: Order by disorder in a four-flavor Mott insulator on the fcc lattice. ***PHYS REV B*** 93:(7) 075137/1-11 (2016) doi: 10.1103/PhysRevB.93.075137

2. Jakab D, Szirmai E, Lewenstein M, Szirmai G: Competing valence bond and symmetry-breaking Mott states of spin- 32 fermions on a honeycomb lattice. ***PHYS REV B*** 93:(6) 064434/1-10 (2016) doi: 10.1103/PhysRevB.93.064434

3. Sinkovicz P, Kiss T, Asbóth JK: Generalized Kac lemma for recurrence time in iterated open quantum systems. ***PHYS REV A*** 93:(5) 050101/1-5 (2016) doi: 10.1103/PhysRevA.93.050101

4. Griesser T, Vukics A, Domokos P: Depolarization shift of the superradiant phase transition. PHYS REV A 94:(3) 033815/1-7 (2016) doi: 10.1103/PhysRevA.94.033815

5. Altenburg S, Wölk S, Tóth G, Gühne O: Optimized parameter estimation in the presence of collective phase noise. ***PHYS REV A*** 94:(5) 052306/1-15 (2016) doi: 10.1103/PhysRevA.94.052306

6. Nagy D, Domokos P: Critical exponent of quantum phase transitions driven by colored noise. ***PHYS REV A*** 94:(6) 063862/1-11 (2016) doi: 10.1103/PhysRevA.94.063862

See also: S-T.4

S-T. Quantum information and foundations of quantum mechanics

Wigner research group

Tamás Kiss, János Asbóth, Péter Ádám, Zoltán Darázs, Aurél Gábris[A], András Gilyén[#], Orsolya Kálmán, Zsolt Kis, Miklós Kornyik[#], Viktor Szalay, Géza Tóth[A]

Quantum information processing, quantum walks. — State-selective protocols, like entanglement purification, lead to an essentially non-linear quantum evolution, unusual in naturally occurring quantum processes. Sensitivity to initial states in quantum systems, stemming from such non-linear dynamics, is a promising perspective for applications. Here, we demonstrate that chaotic behaviour is a rather generic feature in state-selective protocols: exponential sensitivity can exist for all initial states in an experimentally realisable optical scheme. Moreover, any complex rational polynomial map including the example of the Mandelbrot set can be directly realised. In state-selective protocols, one needs an ensemble of initial states, the size of which decreases with each iteration. We prove that exponential sensitivity to initial states in any quantum system has to be related to downsizing the initial ensemble also exponentially. Our results show that magnifying initial differences of quantum states (a Schrödinger microscope) is possible, see Fig. 1; however, there is a strict bound on the number of copies needed.

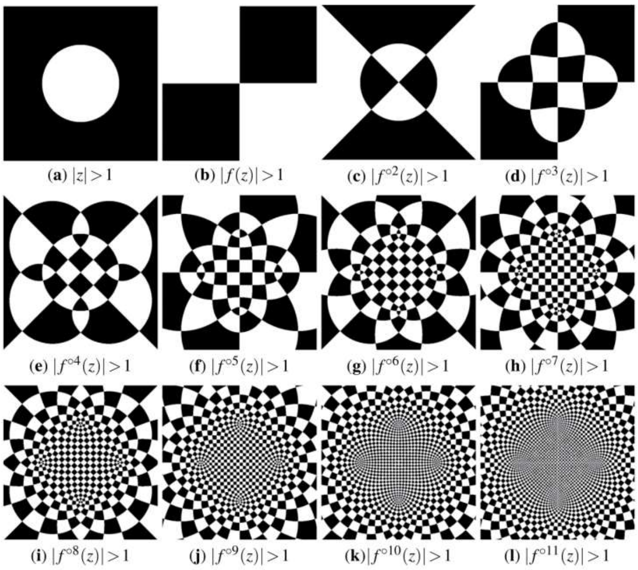

Figure 1. *Iterations of an exponentially mixing map. (a–l) Visualisation of the iteratives of f, the complex function defining the dynamics on the Bloch spere. The domains are coloured according to whether $|f^{\circ n}|>1$ (black) or ≤ 1 (white), distinguishing the northern and southern half of the Bloch sphere. After a few iterations, even very close states get mapped to different halves of the Bloch sphere as indicated by the rapid alternation of black and white domains.*

We considered recurrence to the initial state after repeated actions of a quantum channel. After each iteration, a projective measurement is applied to check recurrence. The corresponding return time is known to be an integer for the special case of unital channels, including unitary channels. We prove that for a more general class of quantum channels, the expected return time can be given as the inverse of the weight of the initial state in the

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steady state. This statement is a generalization of the Kac lemma for classical Markov chains.

Topological phases. — In a collaboration with an experimental group at Bonn University, we studied the expected effect of decoherence on edge states in topologically non-trivial quantum walks, realized on trapped atoms in optical lattices. This is an important issue when quantum walks are used as simulators for model Hamiltonians from solid state physics since the sources of decoherence in these experiments are quite different from those in solid state. We used models for decoherence previously introduced and tested in one-dimensional quantum walk experiments, and studied their effects on edge states in one- and two-dimensional topologically non-trivial quantum walks. We developed a simple analytical model quantifying the robustness of these edge states against either spin or spatial dephasing, predicting an exponential decay of their population. Moreover, we presented a realistic experimental proposal to realize spatial boundaries between distinct topological phases, relying on a new scheme to implement spin-dependent discrete shift operations. This is part of a preparation for the first experimental demonstration of two-dimensional quantum walks in such setups.

Ultracold gases, Bose-Einstein condensates. — Bose-Einstein condensates of ultracold atoms can be used to sense fluctuations of the magnetic field by means of transitions into untrapped hyperfine states. It has been shown recently that counting the outcoupled atoms can yield the power spectrum of the magnetic noise. In our work, we calculated the spectral resolution function which characterizes the condensate as a noise measurement device in this scheme. We used the description of the radio-frequency outcoupling scheme of an atom laser which takes into account the gravitational acceleration. Employing both an intuitive and the exact three-dimensional and fully quantum mechanical approach, we derived the position-dependent spectral resolution function for condensates of different size and shape.

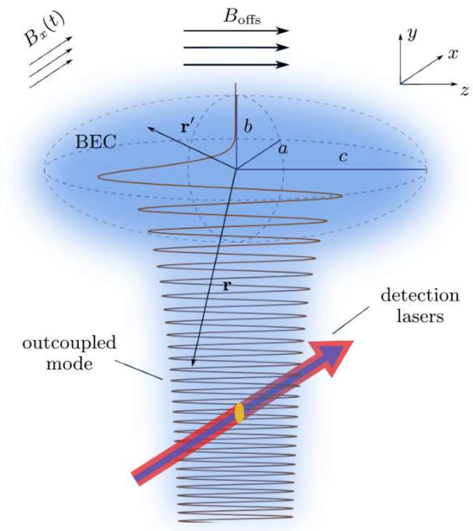

***Figure 2.** Sketch of the system and the outcoupled mode for a monochromatic outcoupling field.*

Single-photon sources. —We consider periodic single-photon sources with combined multiplexing in which the outputs of several time-multiplexed sources are spatially multiplexed. We give a full statistical description of such systems in order to optimize them with respect to maximal single-photon probability. We carry out the optimization for a particular scenario which can be realized in bulk optics and its expected performance is extremely good at the present state of the art. We find that combined multiplexing outperforms purely spatially or time-multiplexed sources for certain parameters only, and we characterize these cases. Combined multiplexing can have the advantages of possibly using less non-linear sources, achieving higher repetition rates, and the potential applicability for continuous pumping. We estimate an achievable single-photon probability between 85 % and 89 %.

Nanophotonics. —A detailed analysis of the optical reflectivity of a monolithic, T-shaped surface relief grating structure is carried out. It is shown that by changing the groove depths and widths, the frequency-dependent reflectivity of the diffraction grating can be greatly modified to obtain various specific optical elements. The basic T-shaped grating structure is optimized for three specific applications: a perfect mirror with a wide maximal reflection plateau, a bandpass filter, and a dichroic beam splitter. These specific mirrors could be used to steer the propagation of bichromatic laser fields in situations where multilayer dielectric mirrors cannot be applied due to their worse thermomechanical properties. Colored maps are presented to show the reflection dependency on the variation of several critical structure parameters. To check the accuracy of the numerical results, four independent methods are used: finite-difference time-domain, finite-difference frequency-domain, method of lines, and rigorous coupled-wave analysis. The results of the independent numerical methods agree very well with each other indicating their correctness.

Grants

OTKA NN109651: Iterative dynamics of quantum systems: non-classical properties, applications for modelling physical systems and optical realizations (T. Kiss, 2013-2017)

NKFI PD 120975 Dynamics of hybrid quantum systems (O. Kálmán, 2016-2019)

ERC Starting Grant GEDENTQOPT (G. Tóth, 2011-2017)

International cooperation

Technical University, Darmstadt (Gernot Alber) – Dynamics and Control of Quantum Networks (T. Kiss)

Czech Technical University in Prague (Igor Jex) – Iterative dynamics of quantum systems (T. Kiss)

University of Osnabrück – Small polarons in luminescent LiNbO3: From bulk crystals to nanocrystals (Z. Kis)

Publications

Articles

1. Ádám P, Andreev VA, Isar A, Man'ko VI, Man'ko MA: Star product, discrete Wigner functions, and spin-system tomograms. ***THEOR MATH PHYS+*** 186:(3) 346-364 (2016) doi: 10.1134/S0040577916030041

2. Bodog F, Ádám P, Mechler M, Santa I, Koniorczyk M: Optimization of periodic single-photon sources based on combined multiplexing. ***PHYS REV A*** 94:(3) 033853/1-10 (2016) doi: 10.1103/PhysRevA.94.033853

3. Ádám P, Andreev VA, Isar A, Man'ko MA, Man'ko VI: Continuous sets of dequantizers and quantizers for one-qubit states. ***J RUSS LASER RES*** 37:(6) 544-555 (2016) doi: 10.1007/s10946-016-9606-4

4. Kálmán O, Darázs Z, Brennecke F, Domokos P: Magnetic-noise-spectrum measurement by an atom laser in gravity. ***PHYS REV A*** 94:(3) 033626/1-8 (2016) doi:

10.1103/PhysRevA.94.033626

5. Szarvas T, Kis Z: Optimization of a T-shaped optical grating for specific applications. ***OPT ENG*** 55:(7) 077103/1-8 (2016) doi: 10.1117/1.OE.55.7.077103

6. Groh T, Brakhane S, Alt W, Meschede D, Asbóth JK, Alberti A: Robustness of topologically protected edge states in quantum walk experiments with neutral atoms. ***PHYS REV A*** 94:(1) 013620/1-15 (2016) doi: 10.1103/PhysRevA.94.013620

7. Mugel S, Celi A, Massignan P, Asbóth JK, Lewenstein M, Lobo C: Topological bound states of a quantum walk with cold atoms. ***PHYS REV A*** 94:(2) 023631/1-16 (2016) doi: 10.1103/PhysRevA.94.023631

8. Gilyén A, Kiss T, Jex I: Exponential sensitivity and its cost in quantum physics. ***SCI REP*** 6: 20076/1-10 (2016) doi: 10.1038/srep20076

Conference proceedings

9. Bacsardi L, Kis Zs, Imre S: Second generation QKD system over commercial fibers. In: *24th European Signal Processing Conference, EUSIPCO 2016, 29 August-2 September 2016, Budapest, Hungary*. IEEE New York, pp. 488-492 (2016) doi: 10.1109/EUSIPCO.2016.7760296

10. Schranz Á, Udvary E, Kis Zs: Photon statistics determination for single photon based quantum key distribution. In: *Proc. 18th International Conference on Transparent Optical Networks (ICTON), Trento, Italy, 10-07-2016 – 14-07-2016*. Eds.: Ferrari M, Dorosz D, Marciniak M, Tu.P.12 (4 pages) (2016) doi: 10.1109/ICTON.2016.7550483

Book

11. Asbóth JK, Oroszlány L, Pályi A: A short course on topological insulators: Band-structure topology and edge states in one and two dimensions. Springer Verlag, Berlin; Heidelberg, pp. 1-180 (2016) doi: 10.1007/978-3-319-25607-8

Other

12. Asbóth J, Iglói F: A 2016. évi Fizikai Nobel-díj (The 2016 Nobel Prize in Physics, in Hungarian). ***FIZIKAI SZEMLE*** 66:(11) 358-364 (2016)

See also: R-I.8, S-Q.4, S-S.3

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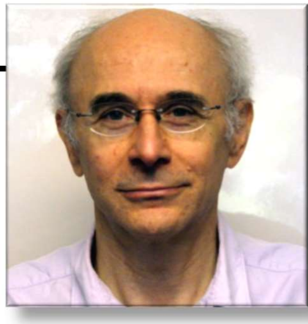
R-A. Field theory



Péter Forgács, Gabriella Böhm, Viktor Czinner, László Fehér, Gyula Fodor, Andor Frenkel[A], Gyula Kluge, Zoltán Kunszt[A], Árpád Lukács, Balázs Mikóczi, Júlia Nyíri[A], László B. Szabados, Kornél Szlachányi, Kálmán Tóth[A], Péter Vecsernyés, Z. Zimborás

Although Hopf algebras successfully generalize groups in many situations, in several mathematical and physical applications they turned out not to be sufficiently general. Research for a suitable mathematical structure, to describe the symmetry at as a wide generality as possible, has been running worldwide for several decades. For different purposes weak Hopf algebras and multiplier Hopf algebras have been applied succesfully. In 2016, we formulated the axioms in an arbitrary braided monoidal category of the so-called "weak multiplier bialgebras" simultaneously generalizing these. It was proved that such algebras and their representation theory possess the expected properties which are important in the applications.

The Skyrme model is a QCD-motivated effective model of the low-energy behaviour of strong interactions. A variant of this model is consistent with the liquid drop model of nuclei, and has a broad range of applicability, including the derivation of an equation of state for neutron star matter. In collaboration with Thessaloniki, Greece we have demonstrated numerically that – with a modification of the potential of the model- the dynamics of this Skyrme model is well tractable, and the oscillational frequencies of the classical solutions can be obtained both numerically and with the aid of soliton perturbation theory. These frequencies are necessary for the quantisation of the theory.

We discovered a direct construction of those compact real forms of the trigonometric n-particle Ruijsenaars-Schneider systems whose completed center-of-mass phase space is the complex projective space with the Fubini-Study symplectic structure. This construction was also generalized to the case of elliptic n-particle systems, whose compactification was not studied previously in the literature.

We have published our results on vortices in two-component Ginzburg-Landau theories in two papers. The results have relevance to *high-pressure superconducting liquid metallic hydrogen*, close to the second phase transition, where the protons in the material become superconducting, in addition to electrons. It has been shown that the behaviour of flux tubes deviates from the usual ones in type-I/type-II super-conductors, even at temperatures above the transition. *Stable giant vortices* with a large number of flux quanta form. These vortices are distinguished from ordinary Abrikosov ones by the formation of the second (proton-pair) condensate in their cores, when there is no protonic condensate in the bulk of the sample.

We have investigated the motion of eccentric compact binaries taking into account the leading-order spin-orbit interaction and the dissipation due to gravitational radiation. The orbital parameters were computed in function of the spin supplementary conditions (SSC). It

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was shown that the instantenous loss of energy and of orbital angular momentum due to the radiation of gravitational waves depends on the SSC, but the SSC dependence disappears when averaging over one orbital period. We have also found that to leading order the measurable quantities do not depend on the SSC.

Grants

OTKA K108384, “Category Theoretical Investigations of Quantum symmetries”, (G. Böhm, 2013-2017)

OTKA K111697, "Group-theoretic aspects of integrable systems and theire dualities", (L. Fehér, 2014-2018)

OTKA K101709, "Nonlinear interactions of waves and particles in field theories and some of their consequences in astro-particle physics and in cosmology”, (P. Forgács 2012-2016)

OTKA PD 116892, "Large excentricity signals in gravitational wave physics", (B. Mikóczi, 2015-2018)

Publications

Articles

1. Anisovich AV, Anisovich VV, Matveev MA, Nyiri J, Sarantsev AV, Semenova AN: Propagators of resonances and rescatterings of the decay products. ***INT J MOD PHYS A*** 31:(23) 1650124/1-22 (2016)

2. Anisovich VV, Nikonov VA, Nyiri J: Asymptotic regimes for hadron diffractive scatterings and Coulomb interaction: Arguments for the black disk mode. ***INT J MOD PHYS A*** 31:(11) 1650053/1-12 (2016)

3. Böhm G, Lack S: Hopf comonads on naturally Frobenius map-monoidales. ***J PURE APPL ALGEBRA*** 220:(6) 2177-2213 (2016)

4. Czinner VG, Mena FC: Relative information entropy in cosmology: The problem of information entanglement. ***PHYS LETT B*** 758: 9-13 (2016)

5. Czinner VG, Iguchi H: Rényi entropy and the thermodynamic stability of black holes. ***PHYS LETT B*** 752:(10) 306-310 (2016)

6. Dokshitzer Y, Lévai P, Nyíri J: Preface. ***INT J MOD PHYS A*** 31:(28-29) 1602003/1-13 (2016)

7. Fehér L, Görbe TF: Trigonometric and elliptic Ruijsenaars–Schneider systems on the complex projective space. ***LETT MATH PHYS*** 106:(10) 1429-1449 (2016)

8. Forgács P, Lukács Á, Schaposnik FA: Twisted non-Abelian vortices. ***INT J MOD PHYS A*** 31:(28-29) 1645046/1-9 (2016)

9. Forgács P, Lukács Á: Vortices and magnetic bags in Abelian models with extended scalar sectors and some of their applications. ***PHYS REV D*** 94:(12) 125018/1-19 (2016)

10. Forgács P, Lukács Á: Vortices with scalar condensates in two-component Ginzburg–Landau systems. ***PHYS LETT B*** 762:(10) 271-275 (2016)

11. Hofer-Szabó G, Vecsernyés P: A generalized definition of Bell's local causality. ***SYNTHESE*** 193:(10) 3195-3207 (2016)
12. Lu DW, Biamonte JD, Li J, Li H, Johnson TH, Bergholm V, Faccin M, Zimborás Z, Laflamme R, Baugh J, Lloyd S: Chiral quantum walks. ***PHYS REV A*** 93:(4) 042302. 7 p. (2016)
13. Lukács Á: "Half a proton" in the bogomol'nyi-prasad-sommerfield skyrme model. ***J MATH PHYS*** 57:(7) 072903/1-5 (2016)
14. Szlachányi K: Skew Monoidal Monoids. ***COMMUN ALGEBRA*** 44:(6) 2368-2388 (2016)

See: R-B.5

R-B. Heavy-ion physics

Gergely Gábor Barnaföldi, Dániel Berényi#, Gábor Bíró#, Tamás Sándor Biró, Pál Doleschal[A], Vahtang Gogohia[A], Miklós Gyulassy[A], Szilveszter Miklós Harangozó#, Miklós Horváth#, Szilvia Karsai#, Péter Kovács, Róbert Kovács#, Péter Lévai, Péter Pósfay#, János Révai[A], Zs. Szendi#, Károly Ürmössy#, Péter Ván, György Wolf, Miklós Zétényi

High-energy heavy-ion physics is connected to a large variety of physics disciplines. Our researches probe fundamental concepts of classical and modern thermodynamics, hydrodynamics, and quantum theory. Therefore, we have several theoretical and practical topical research directions covering a wide spectrum, such as: thermodynamics, perturbative and non-perturbative QCD, high-energy nuclear effects, hadronization, hadron phenomenology, phenomenology of compact stars, and gravity/cosmology. Our studies are strongly motivated by the needs of several recent and planned large-scale facilities, such as collaborations at the LHC (CERN, Switzerland) and RHIC (BNL, USA), and future experiments at FAIR (GSI, Germany) and NICA (Dubna, Russia).

New developments in the effective field theory of the strong interaction — Hot superdense matter created in high-energy heavy-ion collisions, provide the opportunity to determine the equation of state and the phase diagram of the strongly interacting matter. Superdense matter created in the GSI/FAIR accelerator is described by the non-linear sigma model. We presented a new equation of state and the phase diagram, which can be applied to the planned CBM detector in the future. The model is extended by vector mesons, Polyakov loops and constituent quarks. It predicts a critical point at large chemical potential and low temperature. We developed an Effective Lagrangian model for the angular distribution of di-lepton (electron-positron pair) production in pion-nucleon collisions. We have investigated the connection between the angular distribution and the polarization of intermediate baryon resonances and vector mesons. Also, predictions were given for an anisotropy coefficient, which can be studied by the HADES experiment. We also developed a new version of the 3-flavor extended linear sigma model by including four multiplets of baryons. We reduced the model to 2-quark flavors, determined the numerical values of parameters, and identified the chiral partners of baryons.

A transport code was developed, and the di-lepton yield was calculated in heavy-ion collision at 10 AGeV at the energy can be achieved at NICA and at FAIR/CBM.

Investigations of superdense matter and extra dimensions in compact stars— Investigation of cold compact stars provide the opportunity to investigate cold superdense matter and even speculate on new states of matter. We have constructed a framework for a polytropic equation of state family using the Functional Renormalization Group (FRG) for a one-fermion and one-boson theory with Yukawa-like coupling. We compared the equation of states and the phase structure of the theory as presented on Fig 1.

Ph.D student

[A] Associate fellow

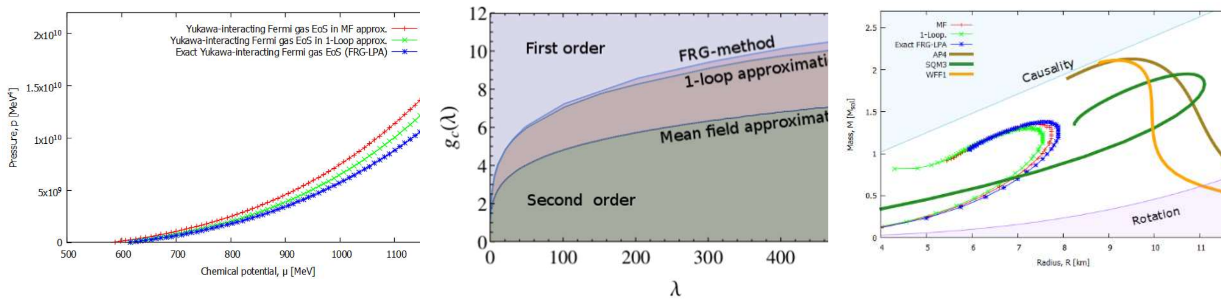


Figure 1. *Left: Comparison of equation of states of the one-fermion one boson model with Yukawa coupling, calculated in mean-field and 1-loop approximation and by the exact FRG method. Middle: the phase structure of the three calculation. Right: The effect of the quantum fluctuations as compact star observables.*

New results from the non-extensive statistical approach. — We have developed a dynamical statistical model with a special form of a master equation describing unidirectional (growth only) processes with branching possibility towards an unspecified environment. This model is capable to explain the measured negative binomial distribution of event by event fluctuations in high energy collisions and also the continuous limit of this model delivers a gamma distribution of socioeconomic systems; indeed observed frequently in taxated income distribution in modern social market economies (Fig. 2).

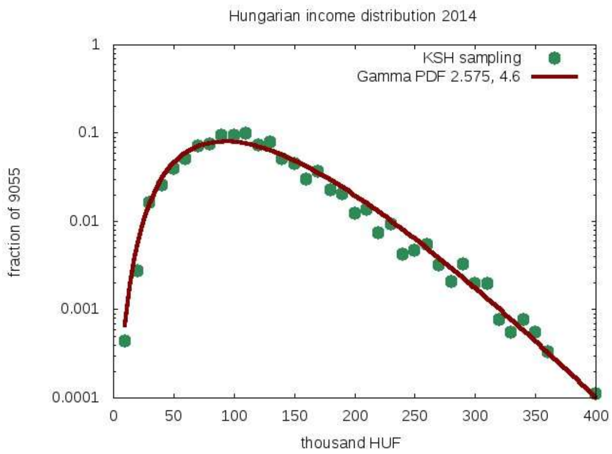


Figure 2. Gamma distributed income in Hungary on a data sample in 2014.

Phenomenology and hydrodynamics for Heavy-ion Collisions. — It is a hot and contemporary issue whether and why the seeming success of hydrodynamical description of heavy ion reactions is unreasonable. We made progress in the research of semi-classical fields, more precisely we studied radiaton patterns of two point charges. Here we have generalized the kinetic theory framework for dense systems, discussed the azimuthal asymmetry of the particle yields in a HIC and investigated the relation of the spectral density of quasi-particle states and investigated the macroscopic fluidity measure (the ratio of shear viscosity and the entropy density) and other transport properties of the system.

Our colleagues participated in the discovery of non-Fourier heat conduction at room temperature. Several artificial and natural materials proof the existence of such phenomena.

Development for heavy-ion computer simulations — In an international collaboration and also together with the GPU laboratory we developed the HIJING++ heavy-ion Monte Carlo Generator and used GPGPU techniques in a Boltzmann transport code.

Coordination of the MGGL. — Our group, together with group R-C, coordinated and organized the establishment of the Mátra Gravitational and Geophysical Laboratory of Wigner RCP.

Coordination of the CERN ALICE group. — Our group is collaborating with group R-H in this respect.

Education, PR and future. — Connected to our group we had 3 BSc and 4 MSc students. So far we have 7 young PhD fellow in the research group, too.

Group members participated in PR activities such as the Colorful Physics Bus of the Wigner RCP, the "AtomCsill" series of the ELFT and Eötvös University, Simonyi Day (Wigner RCP), Science Day (Hungarian Academy of Sciences), and CERN and Wigner Open Days. We have regularly invitation by High Schools from Hungary and abroad for PR talks. Besides these activities, we established a good media connection: we participated in several appearances of news, in radio programs, outreach films and on television.

Grants

OTKA NK 106119: Attometer physics phenomena: theoretical and experimental studies at the CERN LHC ALICE experiment (P. Lévai, 2012-2016)

OTKA K 120660: Investigation of the Identified Hadron Production in the Heavy-ion Collisions at the High-luminosity LHC by the ALICE Experiment (G.G. Barnaföldi, 2016-2020)

OTKA K104260: Particles and intense fields (Consortium leader: T.S. Biró, 2012-2016)

OTKA, K116197: Heat transport in extreme media and systems. (Consortium leader: P. Ván, 2015-2019)

OTKA K109462: Theoretical investigations of the strongly interacting matter produced at FAIR (CBM, PANDA) and NICA (Dubna) (Gy. Wolf, 2014-2017)

Bolyai fellowship of the Hungarian Academy of Sciences, (G.G. Barnaföldi, 2013-2016)

International cooperation

HIC for FAIR program participation with Frankfurt University, FIAS and GSI Darmstadt (T.S. Biró, Gy. Wolf)

UKRAINIAN – HUNGARIAN MTA-UA bilateral mobility program NKM-81/2016 (Hungarian leader: T.S. Biró, Ukrainian leader: L. Jenkovszky).

CHINESE – HUNGARIAN TéT Grant No TET_12_CN_D0524D1E (P. Lévai, 2013-2016).

CERN ALICE experiment, (G.G. Barnaföldi, group leader, and P. Lévai)

CERN ALICE TPC and O2 upgrade project, (G.G. Barnaföldi Wigner group leader, 2015-2018)

NewCompStar EU COST MP1304 action, (Hungarian Representatives: G.G. Barnaföldi – QCD Topic Leader WG2, M. Vasúth, 2013-2017)

THOR EU COST CA15213 action (Hungarian Representatives: G.G. Barnaföldi – Core member, M. Csanád, 2016-2019)

Long term visitors

Dénes Molnár, Peter Anderson, Mridula Damodaran (G.G. Barnaföldi, 2016.07.30-2016.08.31, 1 month), Miklós Gyulassy (P. Lévai, 2 months), Brian Cole (P. Lévai 2 weeks), Michal Bejger (GG Barnaföldi, M. Vasúth 1 month), Gordon Baym (GG Barnaföldi, 1 week)

Publications

Articles

1. Barnaföldi GG, Bulik T, Cieslar M, Dávid E, Dobróka M, Fenyvesi E, Gondek-Rosinska D, Gráczer Z, Hamar G, Huba G, Kis Á, Kovács R, Lemperger I, Lévai P, Molnár J, Nagy D, Novák A, Oláh L, Pázmándi P, Piri D, Starecki T, Suchenek M, Surányi G, Szalai S, Varga D, Vasúth M, Ván P, Vásárhelyi B, Wesztergom V, Wéber Z: First report of long-Term measurements of the MGGL Laboratory in the Mátra mountain range (A Mátrai Gravitációs és Geofizikai Laboratórium elso mérései és mérési programja). ***MAGYAR GEOFIZIKA*** 57:(4) 152-169 (2016)

2. Berezovski A, Ván P: Microinertia and internal variables. ***CONTINUUM MECH THERM*** 28:(4) 1027-1037 (2016)

3. Biró TS, Schram Z: Non-extensive entropic distance based on diffusion: Restrictions on parameters in entropy formulae. ***ENTROPY*** 18:(2) 42/1-9 (2016)

4. Both S, Czél B, Fülöp T, Gróf Gy, Gyenis Á, Kovács R, Ván P, Verhás J: Deviation from the Fourier law in room-temperature heat pulse experiments. ***J NON-EQUIL THERMODY*** 41:(1) 41-48. (2016)

5. Dokshitzer Y, Lévai P, Nyiri J: Preface. ***INT J MOD PHYS A*** 31:(28-29) 1602003/1-13 (2016)

6. Gogokhia V, Barnaföldi GG: General exact solutions for the full gluon propagator in QCD with the mass gap. ***INT J MOD PHYS A*** 31:(28-29) 1645027/1-16 (2016)

7. Gogokhia V, Shurgaia A, Vasúth M: The temperature-dependent Yang-Mills trace anomaly as a function of the mass gap. ***INT J MOD PHYS A*** 31:(28-29) 1645026/1-11 p. (2016)

8. Karsai S, Pósfay P, Barnaföldi GG, Lukács B: Testing a possible way of geometrization of the strong interaction by a Kaluza-Klein star. ***INT J MOD PHYS A*** 31:(28-29) 1645031/1-9 (2016)

9. Ürmössy K, Rak J: Fragmentation in the 3 theory and the LPHD hypothesis. ***INT J MOD PHYS A*** 31:(28-29) 1645045/1-6 (2016)

10. Horváth M, Jakovác A: Shear viscosity over entropy density ratio with extended quasiparticles. ***PHYS REV D*** 93:(5) 056010/1-14 (2016)

11. Kovács P, Szép Z, Wolf G: Existence of the critical endpoint in the vector meson extended linear sigma model. ***PHYS REV D*** 93:(11) 114014/1-23 (2016)

12. Kovács R, Ván P: Models of ballistic propagation of heat at low temperatures. ***INT J***

THERMOPHYS 37:(9) 95/1-13 (2016). JETC 2015: 13TH Joint European Thermodynamics Conference, Nancy, Franciaország: 20-05-2015 -22-05-2015

13. Oláh É, Ádám P, Béni N, Hamar G, Horváth Á, Horváth D, Jancsó G, Jarosievitz B, Lévai P, Péntek C, Sükösd C, Szillási Z, Trócsányi Z, Újvári B, Vámi T, Varga D: Particle physics education in Hungary. ***NUCL PART PHYS P*** 273-275: 2569-2571 (2016)

14. Oláh L, Surányi G, Barnaföldi GG, Bemmerer D, Hamar G, Melegh HG, Varga D: Cosmic background measurements at a proposed underground laboratory by the REGARD muontomograph. ***J PHYS CONF SER*** 665:(1) 012032/1-4 (2016)

15. Olbrich L, Zétényi M, Giacosa F, Rischke DH: Three-flavor chiral effective model with four baryonic multiplets within the mirror assignment. ***PHYS REV D*** 93:(3) 034021/1-16 (2016)

16. Olbrich L, Zétényi M, Giacosa F: Three-flavor chiral effective model with four baryonic multiplets within the mirror assignment. ***J PHYS CONF SER*** 742:(1) 012018/1-5 (2016) FAIRNESS 2016, Workshop for young scientists with research interests focused on physics at FAIR, 14-19 February 2016 Garmisch-Partenkirchen, Germany.

17. Révai J: Three-body calculation of the 1s level shift in kaonic deuterium with realistic $\bar{K}$ N potentials. ***PHYS REV C*** 94:(5) 054001/1-7 (2016)

18. Stoecker H, Zhou K, Schramm S, Senzel F, Greiner C, Beitel M, Gallmeister K, Gorenstein M, Mishustin I, Vasak D, Steinheimer J, Struckmeier J, Vovchenko V, Satarov L, Xu Z, Zhuang P, Csernai LP, Sinha B, Raha S, Biró TS, Panero M: Glueballs amass at the RHIC and LHC! the early quarkless first-order phase transition at T = 270 MeV - From pure Yang-Mills glue plasma to Hagedorn glueball states. ***J PHYS G-NUCL PARTIC*** 43:(1) 015105/1-11 (2016)

19. Szép Zs, Kovács P, Wolf Gy: Thermodynamics of the vector meson extended linear sigma model. ***ACTA PHYS POL B*** 9:(3) 589-595 (2016)

20. Ürmössy K, Xu Z: Three-dimensional statistical jet fragmentation. ***POS*** DIS2016: 054/1-6 (2016) 24th International Workshop on Deep-Inelastic Scattering and Related Subjects, DIS 2016. Hamburg, Germany 11-04-2016 – 15-04-2016

21. Ván P: Theories and heat pulse experiments of non-Fourier heat conduction. ***COMM APPL IND MATH*** 7:(2) 150-166 (2016)

22. Wolf G, Zétényi M: Dilepton and ϕ meson production in elementary and nuclear collisions at the NICA fixed-target experiment. ***EUR PHYS J A*** 52:(8) 258/1-3 (2016)

23. Albacete JL et al. incl. Barnaföldi GG, Lévai P (38 authors): Predictions for p + Pb Collisions at $\sqrt{s_{NN}}$= 5 TeV: Comparison with Data. ***INT J MOD PHYS E*** 25:(9) 1630005/1-6 (2016) 23rd European Physical Society Conference on High Energy Physics.

Conference proceedings

24. Djotyan GP, Bakos JS, Kedves MÁ, Ráczkevi B, Sörlei Zs, Lévai P, Czitrovszky A, Nagy A: Laser plasma generation and diagnostics at Wigner Centre for Physics. In: AWAKE

Workshop at Wigner, Budapest, Hungary, 08-04-2016 Paper lecture

25. Djotyan GP, Bakos JS, Kedves MÁ, Ráczkevi B, Sörlei Zs, Lévai P, Czitrovszky A, Nagy A, Kanetsyan EG, Kryuchkyan GYu: Plasma generation and diagnostics in the field of ultrashort laser pulses. In: 25th Annual International Laser Physics Workshop, Yerevan, Armenia, 11-07-2016 – 15-07-2016 Paper P.S2.3.

Book chapter

26. Montvay I, Biró T: Hungarian perspective. In: Rafelski J (Ed.): Melting Hadrons, Boiling Quarks - From Hagedorn Temperature to Ultra-Relativistic Heavy-Ion Collisions at CERN. Springer International Publishing, Berlin, 2016. pp. 37-40 (ISBN:978-3-319-17544-7)

Others

27. Bencze Gy: Akinek sokat köszönhet a hazai magfizika. ***TERMÉSZET VILÁGA*** 147:(8) 373 (2016)

28. Bencze Gy: Az elbűvölt fizikus nyomában (OLVASÓNAPLÓ). ***TERMÉSZET VILÁGA*** 147:(1) 46 (2016)

29. Bencze Gy: Marslakónak marslakó a lánya? ***TERMÉSZET VILÁGA*** 147:(9) 428 (2016)

30. Bencze Gy: Miért nem lett a taxisofőr Nobel-díjas? (OLVASÓNAPLÓ) ***TERMÉSZET VILÁGA*** 147:(4) 185 (2016)

31. Lévai P: Simonyi öröksége Csillebércen (Simonyi's heritage in Budapest, in Hungarian). ***TERMÉSZET VILÁGA*** 147 (Special edition 2): 74-77 (2016)

ALICE Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2016, here we list only a short selection of appearences in journals with the highest impact factor.

1. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (974 authors): Search for weakly decaying Λn and ΛΛ exotic bound states in central Pb-Pb collisions at $\sqrt{s_{NN}}$=2.76 TeV
PHYS LETT B **752:** 267-277 (2016)
2. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (985 authors): Elliptic flow of muons from heavy-flavour hadron decays at forward rapidity in Pb–Pb collisions at $\sqrt{s_{NN}}$= 2.76 TeV. ***PHYS LETT B*** **753:** 41-56 (2016)
3. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G,

Kiss G, Lévai P, Oláh L, Pochybova S (989 authors): Forward-central two-particle correlations in p–Pb collisions at $\sqrt{s_{NN}}$= 5.02 TeV. ***PHYS LETT B* 753:** 126-139 (2016)

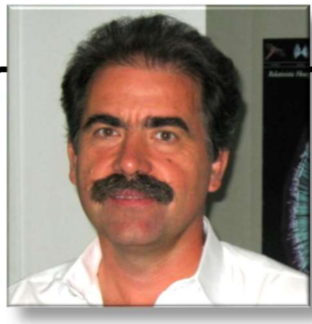
4. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (982 authors): Azimuthal anisotropy of charged jet production in $\sqrt{s_{NN}}$= 2.76 TeV Pb–Pb collisions. ***PHYS LETT B* 753:** 511-525 (2016)
5. Adam J et al. incl. Barnaföldi GG, Bencedi G, Berenyi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Olah L, Pochybova S (987 authors): Pseudorapidity and transverse-momentum distributions of charged particles in proton–proton collisions at $\sqrt{s}$= 13 TeV. ***PHYS LETT B* 753:** 319-329 (2016)
6. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (983 authors): Direct photon production in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***PHYS LETT B* 754:** 235-248 (2016)
7. Adam J et al. incl. Barnaföldi GG, Bencédi G, Bérenyi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (983 authors): Measurement of electrons from heavy-flavour hadron decays in p-Pb collisions at $\sqrt{s_{NN}}$=5.02TeV. ***PHYS LETT B* 754:** 81-93 (2016)
8. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (981 authors): HΛ3 and H[U+203E]Λ-3 production in Pb-Pb collisions at $\sqrt{s_{NN}}$=2.76 TeV. ***PHYS LETT B* 754:** 360-372 (2016)
9. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (982 authors): Centrality evolution of the charged-particle pseudorapidity density over a broad pseudorapidity range in Pb-Pb collisions at $\sqrt{s_{NN}}$= 2.76 TeV. ***PHYS LETT B* 754:** 373-385 (2016)
10. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (994 authors): Anisotropic flow of charged particles in Pb-Pb collisions at $\sqrt{s_{NN}}$= 5.02 TeV. ***PHYS REV LETT* 116:**(13) 132302/1-12 (2016)
11. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (996 authors): Multi-strange baryon production in pPb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS LETT B* 758:** 389-401 (2016)
12. □, Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (992 authors): Centrality dependence of the charged-particle multiplicity density at midrapidity in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT* 116:**(22) 222302/1-12 (2016)
13. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (982 authors): Measurement of an excess in the yield of J/psi at very low p(T) in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***PHYS REV LETT* 116:**(22) 222301/1-13 (2016)
14. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (993 authors): Multiplicity dependence of charged pion, kaon, and (anti)proton production at large transverse momentum in p–Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS LETT B* 760:** 720-735 (2016)
15. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (1002 authors): Pseudorapidity dependence of the

anisotropic flow of charged particles in Pb–Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***PHYS LETT B* 762:** 376-388 (2016)

16. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S, Vértesi R (1010 authors): Jet-like correlations with neutral pion triggers in pp and central Pb–Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***PHYS LETT B* 763:** 238-250 (2016)
17. Adam J et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (1000 authors): Correlated event-by-event fluctuations of flow harmonics in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***PHYS REV LETT* 117:**(18) 182301/1-14 (2016)

R-D. Femtoscopy

Tamás Csörgő, Gábor Kasza[1], Dávid Lucsányi[#], B. Lukács, Frigyes Nemes, András Ster, Róbert Vértesi



Exploring a new domain of QCD with elastic proton-proton scattering in the TOTEM experiment at LHC and theoretical studies in diffractive and low-x physics at LHC. — In the TOTEM experiment at CERN LHC, two special experimental results were achieved with our contributions. TOTEM determined the ρ parameter of elastic pp scattering with unprecendented precision, which allowed for the investigation of the impact parameter dependence (peripheriality) of elastic proton-proton scattering at LHC energies. This result was selected to the cove page of the European Physical Journal C in December 2016. In a conference contribution with primary Wigner authorship, we have also detailed, with significant Hungarian contribution from LHC beam optics calibration, the shape analysis of the differential pp cross-section in 8 TeV elastic pp collisions, which is found to be significantly different from a traditional exponential shape.

In 2016 we have successfully organized the 24th edition of the Low-x Meeting conference series in Gyöngyös, Hungary, one of the important meetings of diffraction and elastic scattering in close collaboration with Ch. Royon (chair, IAC) from Kansas University, Lawrence, US. We hosted a 5-day meeting that attracted 58 participants from 3 continents.

Search for the QCD Critical Point in the BNL RHIC experiment PHENIX and theoretical studies in fireball hydrodynamics. —In 2016, our PHENIX analysis on the Levy Analysis of Bose-Einstein correlations in 200 GeV Au+Au collisions received PHENIX preliminary status and a paper preparation group was formed. These PHENIX preliminary data indicate that the two-pion Bose-Einstein correlation is significantly different from a Gaussian shape in 200 GeV Au+Au collisions. The values of the intercept parameter λ are consistent with a significant in-medium mass modification of the η' mesons, and the value of the Levy exponent is significantly larger than 0.5, the expected maximum value of the exponent of the correlation function at the QCD critical point. We have published two theoretical results on the new exact solutions of fireball hydrodynamics with lattice QCD Equations of State, for rotating and exploding fireballs, for spheroidally and triaxially expanding ellipsoids, respectively. These solutions focus on relating the tilt ange of rotation to the search for the QCD critical point, providing important theoretical insight to the experimental data analysis in this mathematically very difficult area.

We have successfully organized the 2016 edition of our annual Zimányi Winter School on Heavy Ion Collisions. We hosted a 5-day meeting, with a common Zimányi-Ortvay Colloqium by R. Lacey (SUNY Stony Brook, USA).

[#] Ph.D student

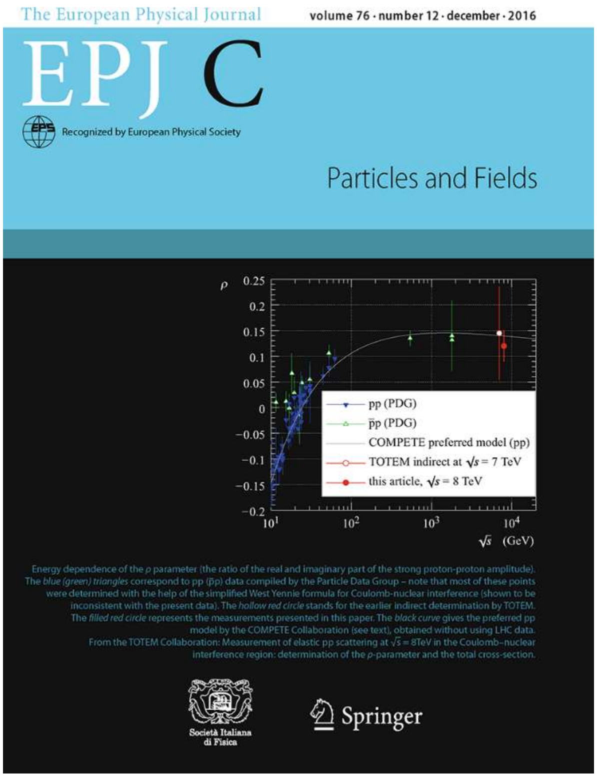


Figure 1. *In the TOTEM Collaboration, we have performed a precision measurement of the ratio of the real to the imaginary part of the forward scattering amplitude of elastic scattering, probing the nuclear-Coulomb interference region at very low four-momentum transfer. Our result excludes the simplified West-Yennie treatement of Coulomb –nuclear interference and allows for the experimental investigation of the impact parameter dependence of elastic proton-proton scattering. This TOTEM measurement was selected to the cover page of European Physical Journal C in December 2016, due to its unprecedented precision and novelty.*

Grants

KEK Visitor Fund, Tsukuba, Japan (T. Csörgő, 2016)

PHENIX Visitor Fund, Upton, BNL (J. Sziklai, T. Csörgő et al 2016)

Hungarian Academy of Sciences - Ukrainian Academy of Science bilateral grant NKM-082/2016

International cooperations:

PHENIX Collaboration (BNL, Upton, NY, USA):

Brookhaven National Laboratory, USA, Memorandum of Understanding between the PHENIX Experiment and KFKI representing the PHENIX-Hungary team (Hungarian Principal Investigator: T. Csörgő, participants from Wigner in 2016: T. Csörgő, G. Kasza, A. Ster, J. Sziklai)

TOTEM Collaboration (CERN LHC, Svájc)

CERN, Memorandum of Understanding for Collaboration in the Construction of the TOTEM detector and Memorandum of Understanding for the Maintenance and Operation of the TOTEM detector at LHC (Hungarian Principal Investigator T. Csörgő, participants from Wigner in 2016: F. Nemes, J. Sziklai, D. Lucsányi).

Bogoliubov Institute for Theoretical Physics (Kiev, Ukraine): bilateral grant NKM-082/2016

Lund University (Lund, Sweden) – Wigner RCP, Memorandum of Understanding on bilateral international collaboration (T. Csörgő, A. Ster, L. Lönnblad (Lund), G. Gustafson (Lund))

State University of New York at Stony Brook (Stony Brook, NY, USA) – Wigner RCP, Memorandum of Understanding on bilateral international collaboration (T. Csörgő, R. Lacey (SUNY SB))

Publications

Articles

1. Csörgő T, Nagy MI, Barna IF: Observables and initial conditions for rotating and expanding fireballs with spheroidal symmetry. ***PHYS REV C*** 93:(2) 024916/1-13 (2016)

2. Domjánné Nyizsalovszki R, Csörgő T, Novák T: AZ EINSTEIN TELESZKÓP PROJEKT és lehetséges hatásai a területfejlesztésre (The EINSTEIN TELESCOPE PROJECT and its possible effects on area development). ***ACTA CAROLUS ROBERTUS : KÁROLY RÓBERT FŐISKOLA GAZDASÁG- ÉS TÁRSADALOMTUDOMÁNYI KAR TUDOMÁNYOS KÖZLEMÉNYEI*** 6:(2) 120-144 (2016)

3. Karsai S, Pósfay P, Barnaföldi GG, Lukács B: Testing a possible way of geometrization of the strong interaction by a Kaluza-Klein star. ***INT J MOD PHYS A*** 31:(28-29) 1645031/1-9 (2016)

4. Lökös S, Csanád M, Tomášik B, Csörgő T: HBT radii from the multipole Buda-Lund model. ***ACTA PHYS POL B PROC SUPPL*** 9:(2) 269-274 (2016)
   Proc of the 11th Workshop on Particle Correlations and Femtoscopy (WPCF 2015). Warsaw, Poland: 03-10-2015 – 07-10-2015.

5. Lökös S, Csanád M, Csörgő T, Tomášik B: Higher order anisotropies in the Buda-Lund model -- disentangling flow and density field anisotropies. ***EUR PHYS J A*** 52:(10) 311. 20 (2016)

6. Nagy MI, Csörgő T: An analytic hydrodynamical model of rotating 3D expansion in heavy-ion collisions. ***INT J MOD PHYS A*** 31:(28-29) 1645017/1-10 (2016)

7. Nagy MI, Csörgő T: Simple solutions of fireball hydrodynamics for rotating and expanding triaxial ellipsoids and final state observables. ***PHYS REV C*** 94:(6) 064906/1-18 (2016)

8. Novák T, Csörgő T, Eggers HC, De Kock M: Model-independent analysis of nearly Lévy correlations. ***ACTA PHYS POL B PROC SUPPL*** 9:(2) pp. 289-292 (2016) Proc of the 11th Workshop on Particle Correlations and Femtoscopy (WPCF 2015). Warsaw, Poland: 03-10-2015 – 07-10-2015.

9. Vértesi R: Bottomonium production in heavy-ion collisions at STAR. ***NUCL PART PHYS P*** 276–278: 269-272 (2016)

10. Vértesi R: Production of quarkonia at RHIC. ***INT J MOD PHYS A*** 31:(28-29) 1645036. 8 (2016)

Others

11. Csörgő T, Kasza G: New exact solutions of hydrodynamics for rehadronizing fireballs with lattice QCD equation of state. Lecture presented at the Low-x 2016 conference, Gyöngyös, Hungary, June 6-11, 2016. https://arxiv.org/abs/1610.02197 pp. 1-16 (2016)

12. Csörgő T, Novák T: Quark Wars - a particle physics outreach game in the age of Star

Wars. Lecture presented at the Xth Workshop on Particle Correlations and Femtoscopy (WPCF-2014, Gyöngyös, Hungary), ***JCEGI*** 4:(4) 195-204 (2016)

See also: R-D ALICE 16

Phenix collaboration

1. Adare A et al. incl. Csörgő T, Nagy MI, Novak T, Sziklai J, Vértesi R (485 authors): Centrality-dependent modification of jet-production rates in deuteron-gold collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV LETT*** **116:** 122301/1-9 (2016)
2. Adare A et al. incl. Csörgő T, Nagy MI, Novák T, Ster A, Sziklai J, Vargyas M, Vértesi R (553 authors): Azimuthally anisotropic emission of low-momentum direct photons in Au + Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C*** 94: 064901/1-14 (2016)
3. Adare A et al. incl. Csörgő T, Nagy MI, Novák T, Ster A, Sziklai J, Vértesi R (447 authors): Dielectron production in Au + Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C*** **93:** 014904/1-34 (2016)
4. Adare A et al. incl. Csörgő T, Novák T, Ster A, Sziklai J, Vargyas M, Vértesi R (405 authors): Forward J/ψ production in U + U collisions at $\sqrt{s_{NN}}$ = 193 GeV. ***PHYS REV C*** **93:** 034903/1-12 (2016)
5. Adare A et al. incl. Csörgő T, Novak T, Ster A, Sziklai J, Vargyas M, Vértesi R (414 authors): Inclusive cross section and double-helicity asymmetry for π^0 production at midrapidity in p+p collisions at √s=510 GeV. ***PHYS REV D*** **93:** 011501/1-8 (2016)
6. Adare A et al. incl. Csörgő T, Nagy MI, Ster A, Sziklai J, Vértesi R (512 authors): Measurement of higher cumulants of net-charge multiplicity distributions in Au + Au collisions at $\sqrt{s_{NN}}$ = 7.7-200 GeV. ***PHYS REV C*** **93:**(1) 011901/1-8 (2016)
7. Adare A et al. incl. Csörgő T, Nagy MI, Novak T, Ster A, Sziklai J, Vargyas M, Vértesi R (452 authors): Measurement of parity-violating spin asymmetries in W± production at midrapidity in longitudinally polarized p+p collisions. ***PHYS REV D*** **93:** 051103/1-8 (2016)
8. Adare A et al. incl. Csörgő T, Sziklai J, Vértesi R (389 authors): Measurement of the higher-order anisotropic flow coefficients for identified hadrons in Au + Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C*** **93:**(5) 051902/1-8 (2016)
9. Adare A et al. incl. Csörgő T, Novák T, Ster A, Sziklai J, Vértesi R (405 authors): Measurements of directed, elliptic, and triangular flow in Cu+Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C*** **94:** 054910/1-18 (2016)
10. Adare A et al. incl. Csörgő T, Kőfaragó M, Novák T, Sziklai J, Vargyas M (335 authors): Measurements of double-helicity asymmetries in inclusive J/ψ production in longitudinally polarized p+p collisions at √s=510 GeV. ***PHYS REV D*** **94:**(11) 112008/1-10 (2016)
11. Adare A et al. incl. Csörgő T, Nagy MI, Novak T, Ster A, Sziklai J, Vértesi R, Zimányi J (631 authors): Scaling properties of fractional momentum loss of high-p_T hadrons in nucleus-nucleus collisions at $\sqrt{s_{NN}}$ from 62.4 GeV to 2.76 TeV. ***PHYS REV C*** **93:** 024911/1-20 (2016)
12. Adare A et al. incl. Csörgő T, Nagy MI, Novak T, Ster A, Sziklai J, Vértesi R (432 authors): Single electron yields from semileptonic charm and bottom hadron decays in Au+Au

collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 93:**(3) 034904/1-29 (2016)

13. Adare A et al. incl. Csörgő T, Nagy MI, Novák T, Ster A, Sziklai J, Vértesi R, Zimányi J (706 authors): Transverse energy production and charged-particle multiplicity at midrapidity in various systems from $\sqrt{s_{NN}}$ = 7.7 to 200 GeV706. ***PHYS REV C* 93:**(2) 024901/1-30 (2016)
14. Adare A et al. incl. Csörgő T, Nagy MI, Novák T, Ster A, Sziklai J, Vértesi R (512 authors): φ meson production in the forward/backward rapidity region in Cu + Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 93:**(2) 024904/1-13 (2016)

TOTEM Collaboration

Articles

1. Antchev G et al. incl. Csörgő T, Nemes F, Sziklai J (89 authors): Measurement of elastic pp scattering at √s=8 TeV in the Coulomb–nuclear interference region: determination of the ρ -parameter and the total cross-section. ***EUR PHYS J C* 76:**(12) 661/1-21 (2016)
2. Berretti M et al. incl. Csörgő T, Nemes F, Sziklai J (85 authors): The timing upgrade project of the TOTEM Roman Pots detectors. ***NUCL INSTRUM METH A* 824:**. 251-252 (2016)
3. Bossini E et al. incl. Csörgő T, Nemes F, Sziklai J (85 authors): Results on diamond timing detector for the TOTEM experiment. ***NUCL INSTRUM METH A* 824:** 87-88 (2016) Frontier Detectors for Frontier Physics: Proc. 13th Pisa Meeting on Advanced Detectors. La Biodola, Italy, 24-05-2015 – 30-05-2015
4. Cafagna FS et al. incl. Csörgő T, Nemes F, Sziklai J (85 authors): The TOTEM experiment at LHC for proton-proton cross section measurements. ***PoS (ICRC2015) 312*** 8 p (2016) The 34th International Cosmic Ray Conference ICRC2015. Hague, The Netherlands, 30-07-2015 – 06-08-2015
5. Csörgő T et al. incl. Nemes F, Sziklai J (85 authors): Evidence for Non-Exponential Differential Cross-Section of pp Elastic Scattering at Low |t| and √s = 8 TeV by TOTEM. ***EPJ WEB OF CONFERENCES* 120:** 02004/1-6 (2016) Proc. 45th International Symposium on Multiparticle Dynamics, ISMD 2015. Wildbad Kreuth, Germany, 04-10-2015 – 09-10-2015
6. Sen S et al. incl. Csörgő T, Nemes F, Sziklai J, Vesztergombi G (2396 authors): Results from combined CMS-TOTEM data. ***PoS (*DIS2016) 201**. 6 p (2016) Proc. 24th International Workshop on Deep-Inelastic Scattering and Related Subjects, DIS 2016. Hamburg, Germany, 11-04-2016 – 15-04-2016

Conference proceedings

7. Gallinaro M et al. incl. Csörgő T, Nemes F, Sziklai J (86 authors): Upgrades for the Precision Proton Spectrometer at the LHC: Precision Timing and Tracking Detectors. In: *Proc. 9th International Workshop on Diffraction in High Energy Physics (Diffraction 2016)* Santa Tecla, Italy, 2016.09.02-2016.09.08, pp. 1-4.
8. Nemes F et al. incl. Csörgő T, Sziklai J (85 authors): LHC optics and elastic scattering measured by the TOTEM experiment. In: *Proc. 17th Lomonosov Conference on Elementary Particle Physics*. Moscow, Russia, 20-08-2015 – 26-08-2015, pp. 1-4.

R-H. Hadron physics

Ferenc Siklér, László Boldizsár, Zoltán Fodor[A], Endre Futó[A], Sándor Hegyi, Gábor Jancsó[A], József Kecskeméti[A], Andrew John Lowe, Gabriella Pálla[E], Sona Pochybová[#], Zoltán Seres[A], Olivér Surányi, Róbert Vértesi, Anna Julia Zsigmond[#]

Our research group studies collisions of nucleons and nuclei, performs basic and advanced measurements, and tests theoretical ideas. We participate in several complementary experiments (mainly ALICE and CMS), both in data-taking and physics analysis.

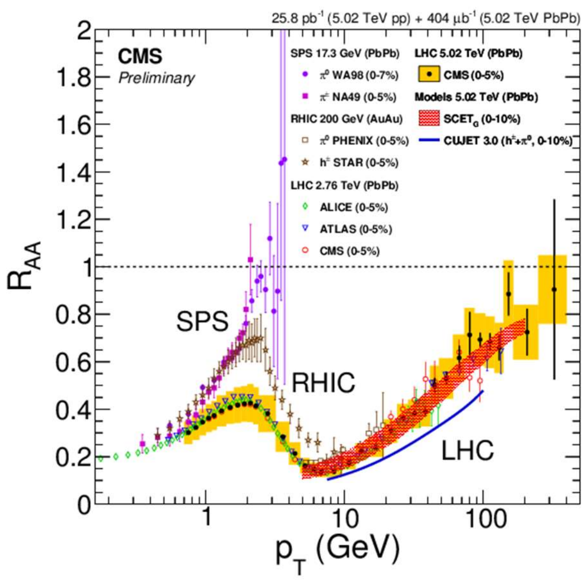
Spectra of identified hadrons. — We have measured the transverse momentum spectra of identified charged hadrons in proton-proton collisions at 13 TeV center-of-mass energy in CMS. Charged pions, kaons, and protons in the transverse-momentum range 0.1–1.7 GeV/*c* and for laboratory rapidities $|y| < 1$ were identified via their energy loss in the silicon tracker. The spectra and integrated yields are compared to lower center-of-mass energy pp results and to Monte Carlo simulations. The average transverse momentum increases with particle mass and the charged-particle multiplicity of the event. A comparison with lower energy data shows only a moderate dependence of the average transverse momentum on the center-of-mass energy. The Pythia8 CUETP8M1 event generator reproduces most features of the measured distributions, but EPOS LHC also gives a satisfactory description of several aspects. These results can be used to further constrain models of hadron production and the understanding of basic nonperturbative dynamics in hadron collisions.

Suppression of high momentum hadrons. — We have measured the spectra of charged particles produced within the pseudorapidity window $|\eta| < 1$ at a center-of-mass energy per nucleon pair of 5.02 TeV using Pb-Pb and proton-proton data from CMS. The spectra are given over the transverse momentum (p_T) ranges spanning 0.5–400 GeV/*c* in pp and 0.7–400 GeV/*c* in Pb-Pb collisions. The corresponding nuclear modification factor, R_{AA}, is measured in bins of collision centrality. The R_{AA} in the 5% most central collisions shows a maximal suppression by a factor of 7–8 in the p_T region of 6–9 GeV/*c*. This dip is followed by an increase, which continues up to the highest p_T measured, and approaches unity in the vicinity of 200 GeV/*c*. The modification factor is compared to theoretical predictions and earlier experimental results at lower collision energies. The newly measured pp spectrum is combined with the p-Pb spectrum previously published by the CMS Collaboration to construct the p-Pb nuclear modification factor, R_{pA}, up to 120 GeV/*c*. Above 20 GeV/*c*, R_{pA} exhibits weak momentum dependence and shows a moderate enhancement above unity.

Boson-jet correlations. — We have measured the production of Z-jet pairs for the first time in pp and central Pb-Pb collisions at a center-of-mass energy per nucleon pair of 5.02 TeV using the CMS detector. The Z-jet azimuthal angle correlations and transverse momentum imbalance are analyzed for events containing a Z boson with transverse momentum above 60 GeV/*c* and an associated jet above 30 GeV/*c*. A moderate shift in the jet p_T over Z boson

[A] Associate fellow
[E] Professor Emeritus
[#] Ph.D. student

p_T ratio is seen in central Pb-Pb collisions with respect to the ratio found using pp data, in agreement with expected jet quenching effects. The probability to find a back-to-back jet partner in Pb-Pb collisions is lower than in pp collisions, which suggests that in Pb-Pb collisions a larger fraction of partons associated with the Z boson lost energy and fell below the 30 GeV/*c* jet p_T threshold.



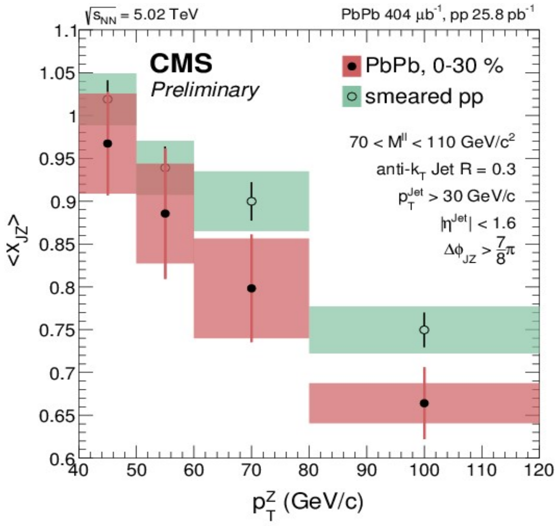


Figure 1. *Left: Measurements of the nuclear modification factors in central heavy-ion collisions at four different center-of-mass energies, for neutral pions (π^0) (SPS, RHIC), charged hadrons ($h^{\pm}$) (SPS, RHIC), and charged particles (LHC including CMS) compared to predictions of two models. The yellow band around the new 5.02 TeV CMS data shows the systematic uncertainties of the measurement. Right: The mean value of the jet p_T over Z boson p_T distribution (x_{JZ}) as a function of the Z boson transverse momentum.*

Identified hadron spectra with ALICE. — The Hungarian ALICE Group's main research direction is the measurements and analysis in connection with identified hadron production. We participated in the operation of the High Momentum Particle Identification Detector (HMPID) of the ALICE detector, the TPC upgrade and data analysis and the O2 DAQ upgrade projects.

Coordination of the ALICE upgrades. — We coordinate the Hungarian contribution to CERN's largest heavy-ion experiment ALICE. This activity is two-folded: In addition to data analysis, our group plays key role in the construction of the world largest, 90 m3-volume, GEM-based TPC in collaboration with group R-I and several international partners.

Our group has leading activity in the ALICE Offline & Online (O2) Upgrade Project, together with the Wigner DAQ Laboratory and Wigner GPU Laboratory.

Grants

OTKA K 109703: Consortional main: Hungary in the CMS experiment of the Large Hadron Collider (F. Siklér, 2013-2016)

Swiss National Science Foundation, SCOPES 152601: Preparation for and exploitation of the CMS data taking at the next LHC run (G. Dissertori ETHZ, 2014-2017)

International cooperation

ALICE, CMS, FOPI, NA61 (CERN) and STAR (RHIC)

Publications

Others

1. Siklér F: Gyorsítók és részecskék (Accelerators and particles, in Hungarian). ***TERMÉSZET VILÁGA*** 147:(Special edition 2) 82-85 (2016)

2. Siklér F: Egy életút (A course of life, in Hungarian). ***FIZIKAI SZEMLE*** 66:(9) 287-289 (2016)

3. Boldizsár L: Generációm mentora (The mentor of my generation, in Hungarian). ***FIZIKAI SZEMLE*** 66:(9) 292-293 (2016)

See also: R-I.8

CMS Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2015, here we list only a short selection of appearences in journals with the highest impact factor.

1. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ, Bartók M (2285 authors): Measurement of long-range near-side two-particle angular correlations in pp collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **116:**(17) 172302/1-19 (2016)
2. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ, Bartók M (2297 authors): Measurement of the top quark pair production cross section in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **116:**(5) 052002/1-18 (2016)
3. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ, Bartók M (2271 authors): Search for narrow resonances decaying to dijets in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **116:**(7) 071801/1-17 (2016)
4. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2268 authors): Search for narrow resonances in dijet final states at $\sqrt{s}$ = 8 with the novel CMS technique of data scouting. ***PHYS REV LETT*** **117:**(3) 031802/1-27 (2016)
5. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2264 authors): Search for resonant production of high-mass photon pairs in proton-proton collisions at $\sqrt{s}$ = 8 and 13 TeV. ***PHYS REV LETT*** **117:**(5) 051802/1-19 (2016)
6. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ, Bartók M (2311 authors): Study of B meson production in p+Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV using exclusive hadronic decays. ***PHYS REV LETT*** **116:**(3) 032301/1-18 (2016)

7. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2311 authors): A search for pair production of new light bosons decaying into muons. ***PHYS LETT B* 752:** 146-168 (2016)
8. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2310 authors): Angular analysis of the decay $B^0 \rightarrow K^{*0}\mu^+\mu^-$ from pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 753:** 424-448 (2016)
9. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2276 authors): Combined search for anomalous pseudoscalar HVV couplings in VH($H \rightarrow b\bar{b}$) production and $H \rightarrow VV$ decay. ***PHYS LETT B* 759:** 672-696 (2016)
10. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2316 authors): Inclusive and differential measurements of the charge asymmetry in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 757:** 154-179 (2016)
11. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2308 authors): Measurement of spin correlations in production using the matrix element method in the muon+jets final state in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 758:** 321-346 (2016)
12. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2311 authors): Measurement of the CP-violating weak phase φ_s and the decay width difference $\Delta\Gamma_s$ using the decay channel in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 757:**97-120 (2016)
13. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2316 authors): Measurement of the inelastic cross section in proton–lead collisions at $\sqrt{s_{NN}}$=5.02 TeV. ***PHYS LETT B* 759:** 641-662 (2016)
14. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2144 authors): Measurement of the $B(B_s^0 \rightarrow J/\psi f_0(980))/B(B_s^0 \rightarrow J/\psi\varphi(1020))$ in pp collisions at $\sqrt{s}$ = 7 TeV. ***PHYS LETT B* 756:** 84-102 (2016)
15. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2258 authors): Measurement of the W boson helicity fractions in the decays of top quark pairs to lepton + jets final states produced in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 762:** 512-534 (2016)
16. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2269 authors): Measurement of the ZZ production cross section and $Z \rightarrow \ell^+\ell^-\ell'^+\ell'^-$ branching fraction in pp collisions at $\sqrt{s}$ = 13 TeV. ***PHYS LETT B* 763:** 280-303 (2016)
17. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2273 authors): Measurement of the $Z\gamma \rightarrow \nu\bar{\nu}\gamma$ production cross section in pp collisions at $\sqrt{s}$ = 8 TeV and limits on anomalous ZZγ and Zγγ trilinear gauge boson couplings. ***PHYS LETT B* 760:** 448-468 (2016)
18. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F,

Veszprémi V, Vesztergombi G, Zsigmond AJ (2292 authors): Measurements of $t\bar{t}$ charge asymmetry using dilepton final states in pp collisions $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 760:** 365-386 (2016)

19. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2312 authors): Search for a Higgs boson decaying into $\gamma^*\gamma \rightarrow \ell\ell\gamma$ with low dilepton mass in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 753:** 341-362 (2016)
20. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2310 authors): Search for a low-mass pseudoscalar Higgs boson produced in association with a pair in pp collisions at $\sqrt{s}$ = 8 TeV. ***PHYS LETT B* 758:** 296-320 (2016)
21. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2314 authors): Search for exotic decays of a Higgs boson into undetectable particles and one or more photons. ***PHYS LETT B* 753:** 363-388 (2016)
22. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2287 authors): Search for lepton flavour violating decays of the Higgs boson to eτ and eμ in proton–proton collisions at √s=8 TeV. ***PHYS LETT B* 763:** 472-500 (2016)
23. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2311 authors): Search for neutral MSSM Higgs bosons decaying to μ+μ- in pp collisions at √s=7 and 8 TeV. ***PHYS LETT B*752:** 221-246 (2016)
24. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2290 authors): Search for neutral resonances decaying into a Z boson and a pair of b jets or τ leptons. ***PHYS LETT B* 759:** 369-394 (2016)
25. Khachatryan V et al. incl. Bencze G, Hajdu C, Házi A, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2140 authors): Search for new phenomena in monophoton final states in proton-proton collisions at √s=TeV. ***PHYS LETT B* 755:** 102-124 (2016)

NA49 Collaboration

1. Anticic T et al. incl. Fodor Z, László A, Pálla G, Siklér F, Veres GI, Vesztergombi Gy (65 authors): Production of deuterium, tritium, and He 3 in central Pb + Pb collisions at 20A, 30A, 40A, 80A, and 158A GeV at the CERN Super Proton Synchrotron. ***PHYS REV C* 94:**(4) 044906/1-20 (2016)

NA61 Collaboration

1. Abgrall N et al. incl. Fodor Z, László A, Márton K, Vesztergombi G (151 authors): Measurements of pi(+/-), K-+/-, K-S(0), Lambda and proton production in proton-carbon interactions at 31 GeV/c with the NA61/SHINE spectrometer at the CERN SPS. ***EUR PHYS J C* 76:**(2) 84/1-49 (2016)
2. Abgrall N et al. incl. Fodor Z, László A, Márton K, Vesztergombi G (158 authors):

Measurements of π± differential yields from the surface of the T2K replica target for incoming 31 GeV/c protons with the NA61/SHINE spectrometer at the CERN SPS: NA61/SHINE Collaboration. ***EUR PHYS J C* 76:**(11) 617/1-27 (2016)

3. Aduszkiewicz A et al. incl. Fodor Z, László A, Márton K, Vesztergombi G (140 authors): Production of ΛΛ-hyperons in inelastic p+p interactions at 158 GeV/c. ***EUR PHYS J C* 76:**(4) 198/1-18 (2016)
4. Aduszkiewicz A et al. incl. Fodor Z, László A, Márton K, Vesztergombi G (132 authors): Multiplicity and transverse momentum fluctuations in inelastic proton–proton interactions at the CERN Super Proton Synchrotron. ***EUR PHYS J C* 76:**(11) 635/1-17 (2016)

FOPI Collaboration

1. Gasik P et al. incl. Fodor Z, Kecskeméti J, Seres Z (66 authors): Strange meson production in Al plus Al collisions at 1.9 AGeV. ***EUR PHYSL J A* 52:**(6) 177/1-13 (2016)
2. Piasecki K et al. incl. Fodor Z, Kecskeméti J, Seres Z (73 authors): Centrality dependence of subthreshold ϕ meson production in Ni + Ni collisions at 1.9A GeV. ***PHYS REV C* 94:**(1) 014901/1-8 (2016)

R-J. Standard model and new physics

Viktor Veszprémi, Dániel Barna[A], Lajos Diósi, Csaba Hajdu, Dezső Horváth[E], Ádám Hunyadi, József Tóth, Tamás Vámi[#], István Wágner[A]

Physics analyses and theoretical work. — We have continued the study of supersymmetric processes leading to strongly boosted top quark decays. We performed the inclusive simulation of such processes, worked out a method for background estimation, and demonstrated its sensitivity in simulation.

The group also participated in the ASACUSA experiment at the Antimatter Factory of CERN which resulted in a break-through in the test of the CPT invariance, the theorem stating the equivalence of matter and antimatter. By installing a new kind of cooling system the difference between the masses of protons and anti-protons was shown to be less than 10^{-9}. Using laser spectroscopy, 13 transitions were measured with the precision of a few times 10^{-9} on about 10^{9} anti-protonic helium atoms cooled down below 1.7 K in cryogenic low-pressure helium gas. This result was reported at several conferences including the Vienna Symmetry Festival, published in Science, and mentioned in a special press announcement at CERN.

We provide also a member for the Publication Committee of the CMS Experiment at CERN and play important role in publishing CMS results of low-x QCD studies.

Work on instrumentation. — During the 2016 data-taking, we have monitored the radiation damage induced performance changes in the CMS pixel detector. We have updated the calibration data-bases used in the offline data-reconstruction in order to improve the hit resolution. We participated in the alignment of the CMS tracker, and improved the alignment technique by identifying misalignment components as residues of the calibrations in pixel local hit reconstruction. We studied the collision pile-up dependent efficiency of the pixel detector in 2016, which is a major determining factor for the CMS luminosity measurement used in all physics analyses. By identifying nuclear interactions inside the pixel detector, we participated in the position measurement of the beam-pipe and various mechanical components of the detector in order to survey the status of the envelope in which the Phase I Pixel Upgrade detector is going to be installed in the beginning of 2017. The group has manufactured the control and read-out electronics for the Phase I Pixel Upgrade detector according to the design we completed in 2015. We played a major role in the commissioning of the data acquisition system to be used for the new detector, in the construction of the Geant modeling of the new detector within the CMS software framework, and the preparation of the local reconstruction with the new geometry.

[A] Associate fellow
[E] Professor Emeritus
[#] Ph.D. student

Stable operation of the T2_HU_Budapest grid site continued in 2016. Our site is used extensively by the entire collaboration including our group for reconstructing collision data in physics analyses. The disk capacity committed to CMS has increased to 700 TB, and our computation power commitments to 933 CPU cores.

Within the framework of the SuShi (Superconducting Shield) Septum for the FCC project, the first two superconducting shield prototypes were designed, and the first one - made of MgB2 - was constructed by an Italian company. Our detailed computer simulation studies showed that it is possible to find a wire configuration around the shield to produce a homogeneous magnetic field in a wide range of field strengths. The CERN Accelerator School (CAS) was organized in Budapest between 2-14 October.

Outreach. — The Hungarian Teachers programme at CERN (15-21 August 2016) was organized by Wigner RCP, on the initiative of our group, with the participation of 20 Hungarian physics teachers. It was followed by a general meeting on November 12 for the participants of all previous trainings taking place between 2006 and 2016 at Sapientia College of Theology, Budapest. We also participated in the organization of the annual Hands-on Particle Physics Master-classes on two occasions with 22 high-school students attending each session. In addition to conference talks and university teaching, many popular lectures were given by our group.

Grants

OTKA K 109703: Consortional main: Hungary in the CMS experiment of the Large Hadron Collider (V. Veszprémi, Cs. Hajdu, D. Horváth, T. Vámi)

OTKA K103917 (D. Barna, L. Diósi, D. Horváth)

International cooperation

CMS Collaboration (199 institutes), ATLAS Collaboration (182 institutes),

University of Tokyo, Japan;

RIKEN, Wako, Japan;

Max-Planck-Institut für Quantenoptik, Germany;

Università di Brescia & Istituto Nazionale di Fisica Nucleare, Italy

Publications

Articles

1. Diósi L: Nonlinear Schrödinger equation in foundations: Summary of 4 catches. ***J PHYS CONF SER*** 701:(1) 012019/1-5 (2016)

2. Diósi L: Structural features of sequential weak measurements. ***PHYS REV A*** 94:(1) 010103/1-4 (2016)

3. Hori M, Aghai-Khozani H, Soter A, Barna D, Dax A, Hayano R, Kobayashi T, Murakami Y, Todoroki K, Yamada H, Horvath D, Venturelli L: Buffer-gas cooling of antiprotonic helium to 1.5 to 1.7 K, and antiproton-to-electron mass ratio. ***SCIENCE*** 354:(6312) 610-

614 (2016)

4. Horváth D: Ultra-fast neutrinos: What can we learn from a false discovery? ***INT J MOD PHYS A*** 31:(28-29) 1645037/1-11 (2016)

5. Levy A, Diosi L, Kosloff R: Quantum flywheel. ***PHYS REV A*** 93:(5) 052119/1-9 (2016)

6. Tilloy A, Diosi L: Sourcing semiclassical gravity from spontaneously localized quantum matter. ***PHYS REV D*** 93:(2) 024026/1-12 (2016)

7. Todoroki K, Barna D, Hayano RS, Aghai-Khozani H, Soter A, Corradini M, Leali M, Lodi-Rizzini E, Mascagna V, Venturelli L, Prest V, Vallazza L, De Salvador D, Hori M: Instrumentation for measurement of in-flight annihilations of 130 keV antiprotons on thin target foils. ***NUCL INSTRUM METH A*** 835 110-118 (2016)

Others

8. Horváth D: A CERN nagy hadronütköztetôje, 2016 (The Large Hadron Collider of CERN, in Hungarian) ***FIZIKAI SZEMLE*** 66:(11) 364-372 (2016)

9. Barna D: Magyar részvétel a jövő részecskegyorsítójának fejlesztésében (Hungarian participation in the development of future's particle accelerator, in Hungarian). ***TERMÉSZET VILÁGA*** 147:(Special edition 2) 86-89 (2016)

10. Horváth Dezső: Neutrínóoszcilláció és neutrínótömeg. Fizikai Nobel-díj, 2015 (Neutrino oscillation and neutrino mass. Physical Nobel Prize, 2015, in Hungarian). ***MAGYAR KÉMIKUSOK LAPJA*** 71:(2) 38-40 (2016)

See also: R-I.8, R-H NA49 Collaboration, R-H NA61 collaboration (Vesztergombi G)

ATLAS collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2016, here we list only a short selection of appearances in journals with the highest impact factor.

1. Aaboud M et al. incl. Pásztor G, Tóth J (2851 authors): Search for charged Higgs bosons produced in association with a top quark and decaying via $H\pm \rightarrow \tau\nu$ using pp collision data recorded at $\sqrt{s}$ = 13 TeV by the ATLAS detector. ***PHYS LETT B*** **759:** 555-574 (2016)
2. Aaboud M et al. incl., Pásztor G, Tóth J (2854 authors): Search for resonances in the mass distribution of jet pairs with one or two jets identified as b-jets in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***PHYS LETT B*** **759:** 229-246 (2016)
3. Aaboud M et al. incl. Pásztor G, Tóth J (2863 authors): Search for TeV-scale gravity signatures in high-mass final states with leptons and jets with the ATLAS detector at $\sqrt{s}$=13 TeV. ***PHYS LETT B*** **760:** 520-537 (2016)
4. Aaboud M et al. incl. Pásztor G, Tóth J (2857 authors): Search for heavy long-lived charged R-hadrons with the ATLAS detector in 3.2 fb(-1) of proton-proton collision data at $\sqrt{s}$=13 TeV. ***PHYS LETT B*** **760:** 647-665 (2016)

5. Aaboud M et al. incl. Pásztor G, Tóth J (2859 authors): Search for Higgs and Z boson decays to phi gamma with the ATLAS detector. ***PHYS REV LETT*** **117:**(11) 111802/1-19 (2016)
6. Aaboud M et al incl. Pásztor G, Tóth J (2864 authors): Measurement of the W±Z boson pair-production cross section in pp collisions at √{ s} = 13 TeV with the ATLAS detector. ***PHYS LETT B*** **762:** 1-22 (2016)
7. Aaboud M et al. incl. Pásztor G, Tóth J (2862 authors): Search for high-mass new phenomena in the dilepton final state using proton-proton collisions at √{ s} = 13TeV with the ATLAS detector. ***PHYS LETT B*** **761:** 372-392 (2016)
8. Aaboud M et al. incl. Pásztor G, Tóth J (2857 authors): Measurement of the top quark mass in the t t bar →dilepton channel from √{ s} = 8 TeV ATLAS data. ***PHYS LETT B*** **761:** 350-371 (2016)
9. Aaboud M et al. incl. Pásztor G, Tóth J (2861 authors): Measurement of the total cross section from elastic scattering in pp collisions at √{ s} = 8 TeV with the ATLAS detector. ***PHYS LETT B*** **761:** 158-178 (2016)
10. Aaboud M et al. incl. Pásztor G, Tóth J (2855 authors): Measurement of the t t bar production cross-section using eμ events with b-tagged jets in pp collisions at √{ s} = 13TeV with the ATLAS detector. ***PHYS LETT B*** **761:** 136-157 (2016)
11. Aaboud M et al. incl. Pásztor G, Tóth J (2852 authors): Search for scalar leptoquarks in pp collisions at \sqrt{s} = 13 TeV with the ATLAS experiment. ***NEW J PHYS*** **18:** 093016/1-26 (2016)
12. Aaboud M et al. incl. Pásztor G, Tóth J (2855 authors): Measurement of W+W− production in association with one jet in proton–proton collisions at with the ATLAS detector. ***PHYS LETT B*** **763:** 114-133 (2016)
13. Aaboud M et al. incl. Pásztor G, Tóth J (2858 authors): Search for dark matter produced in association with a hadronically decaying vector boson in pp collisions at with the ATLAS detector. ***PHYS LETT B*** **763:** 251-268 (2016)
14. Aaboud M et al. incl. Pásztor G, Tóth J (2864 authors): Search for new resonances in events with one lepton and missing transverse momentum in pp collisions at √s=13 TeV with the ATLAS detector. ***PHYS LETT B*** **762:** 334-352 (2016)
15. Aaboud M et al. incl. Pásztor G, Tóth J (2858 authors): Measurement of the inelastic proton-proton cross section at √s=13 TeV with the ATLAS detector at the LHC. ***PHYS REV LETT*** **117:**(18) 182002/1-19 (2016)
16. Aad G et al. incl. Pásztor G, Tóth J (2865 authors): Constraints on non-Standard Model Higgs boson interactions in an effective Lagrangian using differential cross sections measured in the H → γγ decay channel at with the ATLAS detector. ***PHYS LETT B*** **753:** 69-85 (2016)
17. Aad G et al. incl. Pásztor G, Tóth J (2864 auhors): Measurements of four-lepton production in pp collisions at with the ATLAS detector. ***PHYS LETT B*** **753:** 552-572 (2016)
18. Aad G et al. incl. Pásztor G, Tóth J (2868 authors): Dijet production in √s=7 TeV pp collisions with large rapidity gaps at the ATLAS experiment. ***PHYS LETT B*** **754:** 214-234 (2016)
19. Aad G et al. incl. Pásztor G, Tóth J (2871 authors): Combination of searches for WW,

WZ, and ZZ resonances in pp collisions at with the ATLAS detector. ***PHYS LETT B* 755:** 285-305 (2016)

20. Aad G et al. incl. Pásztor G, Tóth J (2836 authors): Search for new phenomena in dijet mass and angular distributions from pp collisions at $\sqrt{s}=13$ TeV with the ATLAS detector. ***PHYS LETT B* 754:** 302-322 (2016)
21. Aad G et al. incl. Pásztor G, Tóth J (2853 authors): Measurement of the charge asymmetry in highly boosted top-quark pair production in $\sqrt{s}=8$ TeV pp collision data collected by the ATLAS experiment. ***PHYS LETT B* 756:** 52-71 (2016)
22. Aad G et al. incl. Pásztor G, Tóth J (2865 authors): Measurement of the dependence of transverse energy production at large pseudorapidity on the hard-scattering kinematics of proton-proton collisions at $\sqrt{s}=2.76$ TeV with ATLAS. ***PHYS LETT B* 756:** 10-28 (2016)
23. Aad G et al. incl. Pásztor G, Tóth J (2872 authors): Evidence for single top-quark production in the s-channel in proton-proton collisions at $\sqrt{s}=8$ TeV with the ATLAS detector using the Matrix Element Method. ***PHYS LETT B* 756:** 228-246 (2016)
24. Aad G et al. incl. Pásztor G, Tóth J (2850 authors): Measurement of the ZZ production cross section in pp collisions at $\sqrt{s}=13$ TeV with the ATLAS detector. ***PHYS REV LETT* 116:**(10) 101801/1-19 (2016)
25. Aad G et al. incl. Pásztor G, Tóth J (2856 authors): Search for new phenomena in final states with large jet multiplicities and missing transverse momentum with ATLAS using $\sqrt{s}=13$ TeV proton-proton collisions. ***PHYS LETT B* 757:** 334-355 (2016)
26. Aad G et al. incl. Pásztor G, Tóth J (2870 authors): Charged-particle distributions in $\sqrt{s}=13$ TeV pp interactions measured with the ATLAS detector at the LHC. ***PHYS LETT B* 758:** 67-88 (2016)
27. Aad G et al. incl. Pásztor G, Tóth J (2845 authors): Search for single production of a vector-like quark via a heavy gluon in the 4b final state with the ATLAS detector in pp collisions at $\sqrt{s}=8$ TeV. ***PHYS LETT B* 758:** 249-268 (2016)
28. Aad G et al. incl. Pásztor G, Tóth J (2870 authors): Observation of long-range elliptic azimuthal anisotropies in $\sqrt{s}=13$ and 2.76 TeV pp collisions with the ATLAS detector. ***PHYS REV LETT* 116:**(17) 172301/1-20 (2016)
29. Aad G et al. incl. Pásztor G, Tóth J (2850 auhors): Measurement of W± and Z-boson production cross sections in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector. ***PHYS LETT B* 759:** 601-621 (2016)
30. Aad G et al. incl. Pásztor G, Tóth J (2827 authors): A search for an excited muon decaying to a muon and two jets in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector. ***NEW J PHYS* 18:**(7) 073021/1-21 (2016)
31. Aad G et al. incl. Pásztor G, Tóth J (2849 authors): Transverse momentum, rapidity, and centrality dependence of inclusive charged-particle production in p + Pb collisions measured by the ATLAS experiment.. ***PHYS LETT B* 763:** 313-336 (2016)

R-L. Functional nanostructures

Dániel Géza Merkel, Gábor Bazsó[#], László Bottyán[A], István Dézsi[E], Márton Major, Dénes Lajos Nagy[E], Szilárd Sajti

The structure and magnetism of Fe/FeO/Fe/FeV characterized by magnetometry and polarized neutron reflectometry. — The ferromagnet/metal Fe/V system displays remarkable magnetic properties over a wide range of temperatures, particularly with regards to induced magnetization near the interface. Here, we use argon ion-bombardment during Fe layer deposition as a way to tailor the structural and magnetic properties of bilayer and multilayer systems containing Fe/FeV components. We present structural and magnetic results on Fe/FeV bilayer and Fe/Fe-oxide/Fe/FeV multilayer systems. Magnetization measurements were taken over a range of temperatures and show the expected ferromagnetic behaviour for the Fe/FeV bilayer. The Fe/Fe-oxide/Fe/FeV multilayer demonstrates an enhanced coercivity and exchange bias at low temperatures, both due to the presence of the antiferromagnetic Fe-oxide layer. Polarized neutron reflectometry (PNR) results (scattering length density (SLD) depth profile and neutron spin asymmetry) were used to identify mixed interfacial layers resulting from ion-bombardment. These demonstrated a lower magnetic moment than bulk Fe layers and may undergo a reversal process that differs from non-mixed layers within the sample. (Fig. 1)

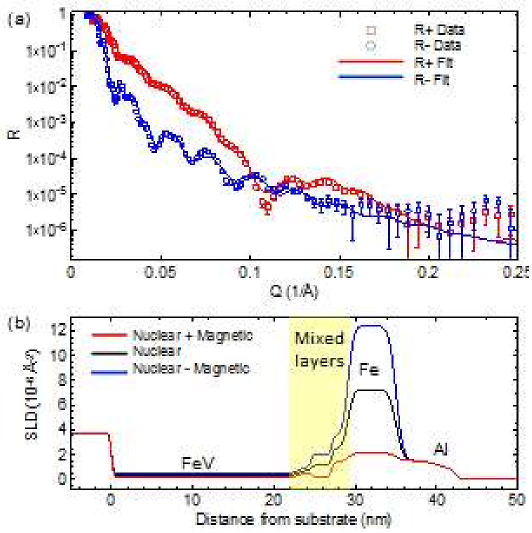


Figure 1. *PNR results for the Fe/FeV bilayer sample. (a) PNR data and fits for saturation (~8000 A/m) field at 5 K. (b) Profile of the SLD across the sample. The difference between the red and blue curves is proportional to the magnetic moment. The yellow region denotes mixed layers between FeV and Fe due to ion-bombardment.*

Roughness replication in neutron supermirrors and multilayers. — In collaboration with the S-L group, the interface roughness and its evolution within the layer sequence of various multilayers was investigated by means of off-specular neutron reflectometry. Neutron supermirrors (SMs), the major components of neutron optical devices, are depth-graded d-spacing multilayers of several hundreds to several thousands of bilayers. Experimental

[#] Ph.D student
[A] Associate fellow
[E] Professor Emeritus

evidence was found for long range roughness replication in the investigated DC-sputtered Ni(Mo)-Ti aperiodic SM structures by observation of resonant diffuse scatter peaks and plateaus. The first order incident beam RDS is missing in the neutron off-specular scatter of normal but is present in reverse layer sequence supermirrors. The different character of the diffuse neutron scattering from normal and reverse sequence SMs is explained using theoretical considerations and confirmed by numerical calculation by the Distorted Wave Born Approximation. A good agreement of experiment and simulation was found for a common interface roughness, depth-independent in-plane and out-of-plane correlation lengths and Hurst parameter of □=7Å, ξ_{II} =450 Å and $□_{out}$=4000 Å and *h*=0.5. The total off-specular intensity of the supermirrors was found non-monotonous with respect to the specular reflectivity at the corresponding angle of incidence. Further studies of roughness correlation in Ni-Ti multilayers are in progress. (Fig. 2)

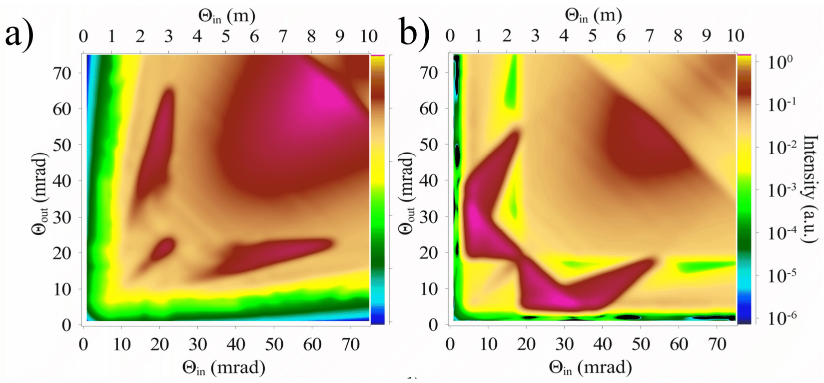


***Figure 2**. Simulated Θ_{in} – Θ_{out} intensities for normal sequence m=3 a) and reverse sequence m=2.5 b) neutron supermirrors using the distorted-wave Born approximation.*

International cooperation

Department of Physics, California State University, San Bernardino, CA 92407, USA

Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia

Department of Materials Science and Engineering, National Chung Hsing University, Taichung 402, Taiwan

Institute for Superconducting and Electronic Materials, University of Wollongong, Wollongong NSW 2252, Australia

Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, China

Long term visitors

Hartmut Spiering, Johannes Gutenberg-Universität Mainz, Institute of Inorganic and Analytical Chemistry, Germany, two weeks, 2016, (host: DL Nagy)

Publications

Articles

1. Gong J, Paul N, Nagy B, Dolgos M, Bottyán L, Müller-Buschbaum P, Böni P, Zheng J-G, Paul A: Morphology of Fe nanolayers with Pt overlayers on low-temperature annealing. ***J APPL CRYSTALLOGR*** 49:(5) 1682-1692 (2016)

2. Layek S, Greenberg E, Xu WM, Rozenberg GK, Pasternak MP, Itie JP, Merkel DG:

Pressure-induced spin crossover in disordered alpha-LiFeO2. ***PHYS REV B*** 94:(12) 125129/1-7 (2016)

3. Li XN, Yuan LH, Wang JH, Jiang LH, Rykov AI, Nagy DL, Bogdan Cs, Ahmed MA, Zhu KY, Sun GQ, Yang WS: A "copolymer-co-morphology" conception for shape-controlled synthesis of Prussian blue analogues and as-derived spinel oxides. ***NANOSCALE*** 8:(4) 2333-2342 (2016)

4. Nagy B, Khaydukov Y, Efremov D, Vasenko AS, Mustafa L, Kim JH, Keller T, Zhernenkov K, Devishvili A, Steitz R, Keimer B, Bottyan L: On the explanation of the paramagnetic Meissner effect in superconductor/ferromagnet heterostructures. ***EUROPHYS LETT*** 116:(1) 17005/1-6 (2016)

5. Patterson EA, Major M, Donner W, Durst K, Webber KG, Rodel J: Temperature-dependent deformation and dislocation density in SrTiO3 (001) Single Crystals. ***J AM CERAM SOC*** 99:(10) 3411-3420 (2016)

6. Pforr F, Major M, Donner W, Stuhr U, Roessli B: Influence of tetragonal platelets on the dielectric permittivity of 0.964Na1/2Bi1/2TiO3-0.036BaTiO3. ***PHYS REV B*** 94:(1) 014105/1-10 (2016)

7. Pradip R, Piekarz P, Bosak A, Merkel DG, Waller O, Seiler A, Chumakov AI, Rüffer R, Oleś AM, Parlinski K, Krisch M, Baumbach T, Stankov S: Lattice dynamics of EuO: Evidence for giant spin-phonon coupling. ***PHYS REV LETT*** 116:(18) 185501/1-5 (2016)

8. Seiler A, Piekarz P, Ibrahimkutty S, Merkel DG, Waller O, Pradip R, Chumakov AI, Rüffer R, Baumbach T, Parlinski K, Fiederle M, Stankov S: Anomalous lattice dynamics of EuSi2 nanoislands: Role of interfaces unveiled. ***PHYS REV LETT*** 117:(27) 276101/1-6 (2016)

9. Spiering H, Ksenofontov V, Leupold O, Kusz J, Deák L, Németh Z, Bogdán C, Bottyán L, Nagy DL: Line shape of 57Co sources exhibiting self absorption. ***HYPERFINE INTERACT*** 237: 58/1-9 (2016)

11. Yazdi MB, Major M, Wildes A, Wilhelm F, Rogalev A, Donner W, Alff L: Possible evidence for a spin-state crossover in the Verwey state in Fe3 O4 thin films. ***PHYS REV B*** 93:(1) 014439/1-5 (2016)

See also: S-E.1

R-M. Ion beam physics

Edit Szilágyi, István Bányász, Pál Kostka[A], Endre Kótai[A], Imre Kovács, Attila Németh, Zoltán Szőkefalvi-Nagy[E]

Microlens fabrication. — In collaboration with Nuclear Physics Institute (Řež, Czech Republic) and Atomki (Debrecen, Hungary) microlenses were designed and fabricated in thin films of polydimethylsiloxane (PDMS) polymer (thickness = 30 µm). Focused beams of 10.5 MeV N^{4+} ions obtained from a 2.2-MeV High Voltage Tandetron were used to produce the microlenses. Rings of 15, 25 and 75 µm inner diameter were irradiated with the focused ion beam with very low fluences, between 7.8×10^{11} and 4.68×10^{13} ions/cm^2. Due to the elasticity of the PDMS, compaction of the irradiated ring resulted in non-uniform swelling of the enclosed disk thus producing a quasi-spherical object, i.e. a microlens. As shown by atomic force microscopy (AFM) images, lenses irradiated by low and moderate fluence were found to be spherical, while the highest fluences resulted in flat top profiles. Focal lengths as a function of fluence ranged 1400–100 µm for the 25µm lenses and 450–75 µm for the 15 µm lenses as calculated based on the curvatures obtained from AFM. Intensity distributions at the focal planes of the lenses were recorded using a microscope equipped with a 50 x Long Working Distance objective at a wavelength of 632.8 nm. Focal spot of a 25 µm diameter microlens (fluence = 5×10^{12} ions/cm^2) is presented in Fig. 1. Light intensity distribution in the focal spot is close to diffraction limited, i.e., almost as good as the theoretical limit for the microlens.

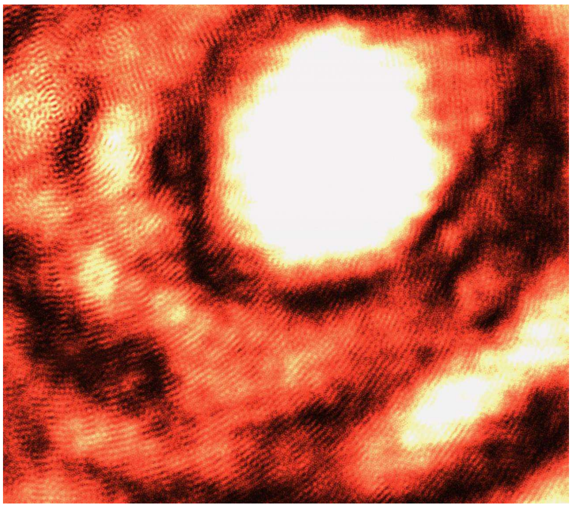


Figure 1. *Microphotograph of the focal spot of a 25 µm microlens.*

Advanced cultural heritage research. — The composition of silicate glass practically has not changed from antiquity, its ingredients are mainly silicon dioxide or quartz, fluxes - soda (sodium carbonate) or potash (potassium carbonate) and stabilizers – calcium carbonate. Ancient glass-makers developed an extensive empirical knowledge on colouring, decolouring and opacifying glass products. Small amounts of minerals were added during manufacturing to obtain the colour and modify the optical properties of the glass, such as opacity etc. The traces of opacifiers, pigments, colouring and de-colouring agents in the glass artefacts can be used to identify the recipe applied and may help to find the glass-maker workshop. As a contribution to IPERION CH (*Integrated Platform for the European Research Infrastructure ON Cultural Heritage)* HORIZON 2020 project external milli-beam PIXE was applied to determine the

[A] Associate fellow

[E] Professor Emeritus

composition of bulk, to analyse the colorants and opacifier in painted bracelets from various 10th-12th Centuries AD Byzantine archaeological sites situated along Danube and late medieval (17th-18th Centuries AD) glass artefacts discovered during architectural restoration of two churches in Bucharest. As a reference painted modern Murano glass pieces and glass samples from different archaeological sites in Central Europe were also analysed. The study demonstrated an impressive continuity in glass recipes from 10th to 18th Century and confirmed the use of small quantities of cobalt oxide for blue colour, indicated manganese combined with iron for dark glass, copper for green, lead for yellow and, only in modern Murano glass, selenium together with zinc to obtain a reddish colour.

Figure 2. Painted Murano glass sample positioned on the PIXE spectrometer.

Grants

OTKA K 101225: Development and optical monitoring of nanostructures for sensing (P. Petrik, 2015-2018)

EC H2020 Grant No. 654028: Integrated Platform for the European Research Infrastructure on Culture Heritage (IPERION CH, 2015-2019)

MTA Infrastructure Development: modernization of the vacuum system of the heavy ion implanter (E. Szilágyi 2016)

International cooperation

Nuclear Physics Institute (Řež, Czech Republic, I. Bányász)

Instituto di Fisica Applicata "Nello Carrara" (Sesto Fiorentino, Italy, I. Bányász)

Publications

Articles

1. Battistig G, Zolnai Z, Németh A, Panjan P, Menyhárd M: Nanoscale SiC production by ballistic ion beam mixing of C/Si multilayer structures. ***J PHYS D APPL PHYS*** 49:(18) 185303/1-8 (2016)

2. Battistig G, Gurbán S, Sáfrán G, Sulyok A, Németh A, Panjan P, Zolnai Z, Menyhárd M: Wafer-scale SiC rich nano-coating layer by Ar+ and Xe+ ion mixing. ***SURF COAT TECH*** 302: 320-326 (2016)

3. Palamara E, Zacharias N, Xanthopoulou M, Kasztovszky Zs, Kovács I, Palles D, Kamitsos EI: Technology issues of Byzantine glazed pottery from Corinth, Greece. ***MICROCHEMICAL JOURNAL*** 129: 137-150 (2016)

Conference proceedings

4. Bányász I, Pelli S, Nunzi-Conti G, Righini GC, Berneschi S, Szilágyi E, Németh A, Fried M, Lohner T, Petrik P, Zolnai Z, Khanh NQ, Rajta I, Nagy GUL, Havranek V, Vosecek V, Lavrentiev V, Veres M, Himics L: Design and fabrication of integrated optical elements in glasses and crystals by various ion beam techniques. In: *Proc. 12th International Topical Meeting on Nuclear Applications of Accelerators (AccApp '15)*. Washington, USA, 10-11-2015 -13-11-2015 Ed.: .Cole P, Kensington:American Nuclear Society, 2016. pp. 389-415.

5. Bányász I, Berneschi S, Fried M, Havranek V, Khanh NQ, Nagy GUL, Németh A, Nunzi-Conti G, Pelli S, Rajta I, Righini C, Szilágyi E, Veres M, Zolnai Z: The use of ion beam techniques for the fabrication of integrated optical elements. In: *Proc. 18th International Conference on Transparent Optical Networks (ICTON)*. Trento, Italy, 10-07-2016 – 14-07-2016, Eds.: Ferrari M, Dorosz D, Marciniak M, pp. 1-4.

Book chapter

6. Balabanski DL, Blümich B, Gelli N, Iancu V, Iovea M, Kriznar A, Massi M, Mazzinghi A, Ortega-Feliu I, Respaldiza MA, Ruberto C, Scrivano S, Suliman G, Szőkefalvi-Nagy Z, Ur CA, Zia W: Complementary Methods: γ-beam Techniques, X-Ray Fluorescence (XRF) and Nuclear Magnetic Resonance (NMR)Nuclear physics for cultural heritage. In: *Nuclear Physics for Cultural Heritage* Eds.: Mackova A, MacGregor D, Azaiez F, Nyberg J, Piasetzky E, Mulhouse: European Physical Society (EPS), 2016. pp. 37-53. (ISBN:978-2-7598-2091-7)

Others

9. Keszthelyi L: Simonyi Károlyra emlékezem (I remember Charles Simonyi, in Hungarian). ***TERMÉSZET VILÁGA*** 147:(KSz) pp. 54-56 (2016)

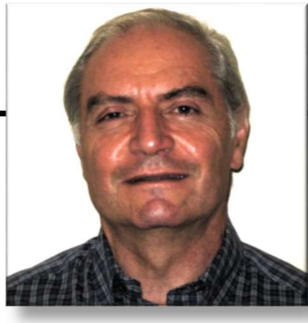
10. Kostka P: A hazai fizikatörténet jeles emléke (Exemplary memory of the history of domestic physics, in Hungarian). ***TERMÉSZET VILÁGA*** 147:(KSz) 57-59 (2016)

11. Szőkefalvi-Nagy Z: "Simonyi"-gyorsítóval a kulturális örökség tudományban (With a

“Simonyi”-accelerator in the science of cultural heritage, in Hungarian). ***TERMÉSZET VILÁGA*** 147:(KSz). 90-92. (2016)

See also: S-M.12, S-M.21

R-N. Cold plasma and atomic physics in strong field



Gagik P. Dzsotjan, József Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós Kedves, Béla Ráczkevi, Zsuzsanna Sörlei[A]

Generation and real-time diagnostics of homogeneous laser plasma – Our research in this direction was intensively continued in 2016 aiming at development of novel schemes of real-time diagnostics of Rb plasma created in the field of strong laser pulses in the femtosecond duration range. Our research is closely connected and correlated with the AWAKE (advanced wake acceleration) experiment at CERN. This novel plasma-based accelerator currently under construction in CERN will utilize the proton bunch available at Large Hadron Collider (LHC) to accelerate electrons (positrons) to TeV energies in one acceleration stage. An extended volume of extremely homogeneous plasma is an indispensable part of the acceleration scheme. This plasma will be used for splitting the LHC proton bunch into micro-bunches using self-modulation instability in the plasma to provide coherent wake-field acceleration of electrons by the proton bunch. Our experimental setup (see Fig. 1) may be considered as a tabletop analogy of the laser plasma source of the AWAKE experiment.

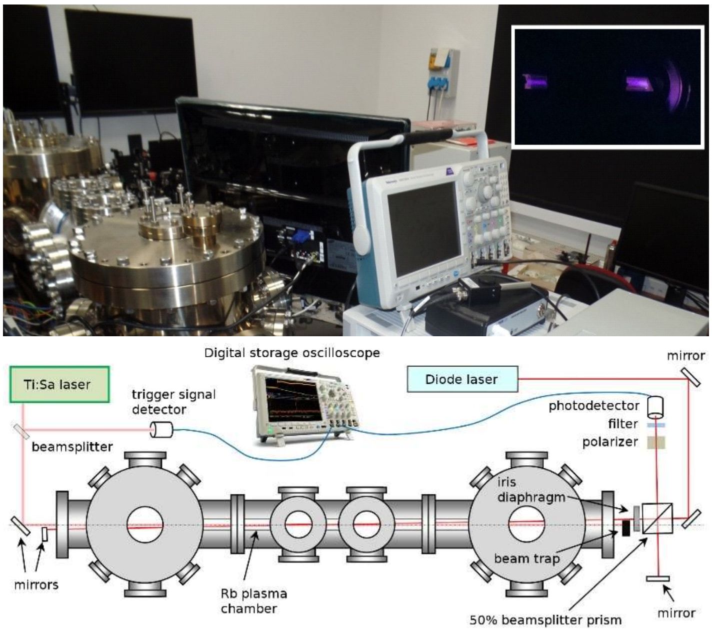


Figure 1. *The experimental setup with the scheme of the real-time interferometric diagnostic system. The inset: the generated plasma (side view).*

The plasma is created by ultra-short (30-40 fs) laser pulses (with pulse energy about 25 mJ) from Ti:Sa laser system Hydra of Coherent Co.

A new diagnostic scheme of the created Rb plasma based on the interferometry has been development in our group in the longitudinal direction (forming a small angle with direction of propagation of the ionizing laser pulses) allowing for measurements of the density and recombination time of the plasma. This method along with the laser absorption spectroscopy method in the transverse direction has allowed us to reveal the physics of generation of the Rb plasma, its space- and time- behavior and to measure the plasma parameters including its density, recombination time and transverse expansion velocity.

[A] Associate fellow

An example of the interferometry signal is shown in Fig. 2 with the cosine fitting function applied.

Results of our studies allow us to understand the physical mechanisms of generation of *extended* laser plasma in Rubidium vapors as well as to understand and describe the induced plasma instabilities. These results (in collaboration with the AWAKE team) will be used to create optimal conditions for generation of highly homogeneous plasma for application in the AWAKE project at CERN

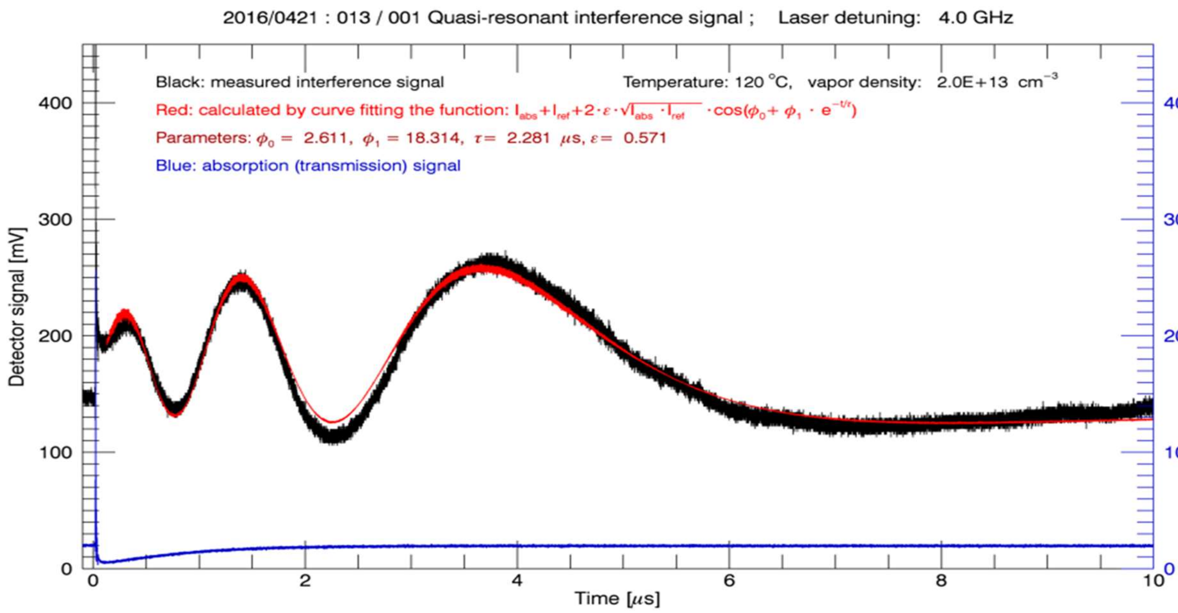


Figure 2. *An example of an interferometry signal measured by the fast detector with a cosine fitting curve.*

Coherent control of atomic states mediated by metallic nanostructures–The coherent manipulation of quantum systems is an important challenge in modern science and engineering, with significant applications in quantum optics and information processing, nuclear magnetic resonance, nonlinear optics, laser controlled chemistry and many others. Controlling quantum emitters (atoms, molecules, quantum dots, etc.), light, and its interactions is a key issue for implementing all-optical devices and information processing at the quantum level. This generally necessitates a strong coupling of emitters to photonic modes. We show that strong coupling in quantum plasmonics can be used to mediate efficiently the interaction between emitters via a decoherence-free channel, immune to the strong plasmon dissipation. We have demonstrated an efficient and robust population transfer between ground states of spatially separated atoms in the scheme of stimulated Raman adiabatic passage (STIRAP) mediated by a spherical metallic nanoparticle, see Fig. 3. These results pave the way for an efficient use of the quantum plasmonic platform without its inherent losses.

We have shown, in particular, that the considered scheme displays strong coupling and can be used to transfer quantum information efficiently between quantum emitters (atoms, molecules, quantum dots, etc) by STIRAP processes. It is important to note that the inherent robustness of such adiabatic passage techniques guarantees high transfer efficiencies.

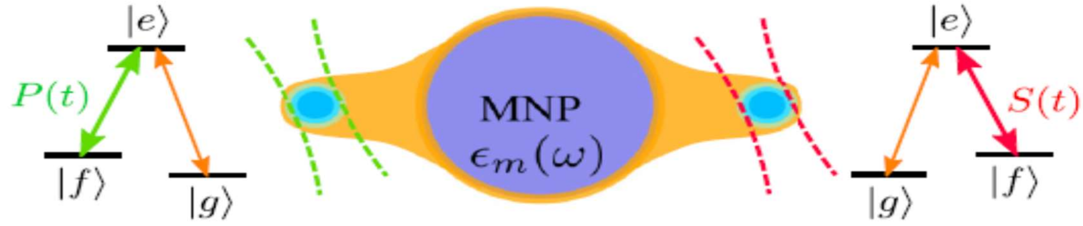


Figure 3. *Two three-level atoms in the vicinity of a metal nanoparticle of permittivity $\varepsilon m(\omega)$.*

In 2016, the design and development of composite pulse sequences for the high fidelity inversion of inhomogeneously broadened, optically dense atomic ensembles was continued. Such pulse sequences are very useful in the field of quantum information processing and quantum communication, because they enable the construction of single photon memories based on the photon echo phenomenon. The effect of the pulse sequence is parametrized by a set of relative phases between the elementary pulses that the composite pulse is built up of and the effect of the entire sequence can be optimized using these phases. Properties like ensemble bandwidth that the composite pulse inverts, optical depth up to which it is effective, peak intensity and minimum time required for the inversion process are the most important properties that can be considered in the optimization process.

A project started in 2016 is the modeling of the propagation of an ionizing laser pulse in rubidium vapor. This project is associated with the AWAKE program in CERN which aims to construct a novel type of particle accelerator based on plasma wake-field acceleration. The work started with the development of a relatively simple atomic model that can be used to calculate the strong nonlinear optical response of the atomic medium. Such a model is essential if the complex propagation of the ionizing pulse through a spatially extended vapor is to be computed.

Grants and international cooperation

The Excellence Program Grant of the Hungarian Academy of Sciences, II and III phases (G.P. Dzsotjan, 2015-2016, 2016-2017)

AWAKE Collaboration Agreement, Max Planck Institute for Physics, München, Germany (2015), (contact person: G.P. Dzsotjan)

Agreement of Academic Cooperation between Wigner Research Center and the Yerevan State University (2015-), (contact person: G.P. Dzsotjan)

Collaboration with the Technical University of Kaiserslautern, Kaiserslautern, Germany

Collaboration with the University of Bourgogne, Dijon, France

Collaboration with the Jagiellonian University of Krakow, Poland

Publications

Articles

1. Demeter G: Composite pulses for high-fidelity population inversion in optically dense, inhomogeneously broadened atomic ensembles. ***PHYS REV A*** 93:(2) 023830/1-8 (2016)

2. Dzsotjan D, Rousseaux B, Jauslin HR, Des Francs GC, Couteau C, Guérin S: Mode-selective quantization and multimodal effective models for spherically layered systems. ***PHYS REV A*** 94:(2) 023818/1-15 (2016)

3. Rousseaux B, Dzsotjan D, des Francs GC, Jauslin HR, Couteau C, Guerin S: Adiabatic passage mediated by plasmons: A route towards a decoherence-free quantum plasmonic platform. ***PHYS REV B*** 93:(4) 045422/1-7 (2016)

4. Varga-Umbrich K, Bakos JS, Djotyan GP, Ignácz PN, Ráczkevi B, Sörlei Z, Szigeti J, Kedves MÁ: Stabilization and time resolved measurement of the frequency evolution of a modulated diode laser for chirped pulse generation. ***LASER PHYSICS*** 26:(5) 055006/1-7 (2016)

5. Varguet H, Rousseaux B, Dzsotjan D, Jauslin HR, Guérin S, Colas Des Francs G: Dressed states of a quantum emitter strongly coupled to a metal nanoparticle. ***OPT LETT*** 41:(19) 4480-4483 (2016)

Book chapter

6. Ráczkevi B: Nagy elmozdulások mérése holografikus interferometriával (Measuring big shifts by holographic interferometry, in Hungarian). GlobeEdit, 2016. 92 p.(ISBN:978-3-330-71327-7)

R-O. ITER and fusion diagnostic development

Gábor Veres, wih 11 engineers and 4 technicians

Subtitle. — In support of a successful ITER and other fusion oriented projects worldwide.

In the ITER Bolometer project, which aims at the development of the whole ITER bolometry camera system, the main results of the group were: establishment of a suitable qualification method for the cameras trough compilation and processing of various loads and assembly requirements, development of candidate designs for vacuum vessel cameras fulfilling the foreseen requirements, and development of an optimisation method for the architecture of the 3DPCB of divertor cameras.

In the Tokamak Services for Diagnostics project the group has designed (in cooperation with its IO colleagues) several prototypes of the ITER in-vessel looms and had is also manufacture in the local, Wigner workshop. The elements are now ready for testing.

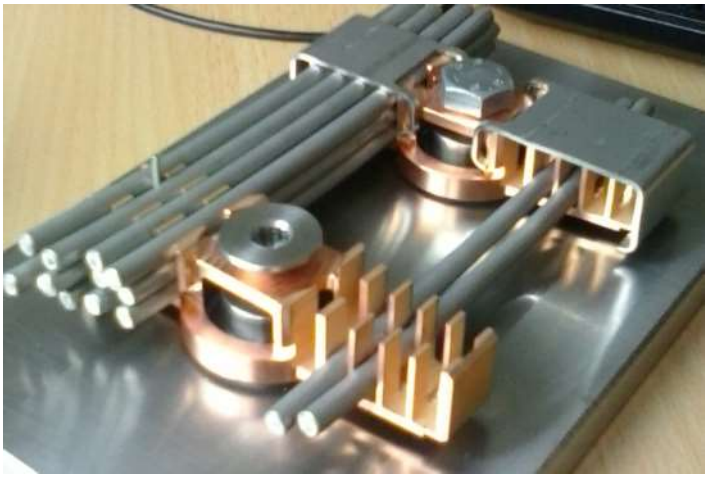


Figure 1. Prototypes of ITER cable looms ready to be tested.

Another activity that occupied us during the year was the preparation and definition of a series of tests that will be carried out in 2017 on several manufacturers' mineral insulated cables (MIC, a reference cable for the ITER in-vessel environment). The tests include electric, outgassing, bending and a so called TIEMF test, where the electric noise generated in the cable (of nano-Volt order) and driven by thermal gradients will be quantified.

In the EUROfusion Consortium we largely contributed to two work packages: to the WP on the Breeding Blanket (targeting the development of a Tricium breeder unit) and the WP on the Early Neutron Source (targeting the development of a high flux 14 MeV neutron source for fusion material testing).

Grants

F4E-FPA-328 Tokamak Services for Diagnostics (G. Veres, 2012-18)

F4E-FPA-384 Diagnostic Development: ITER Bolometers (G. Veres, 2014-18)

IO/15/TR/11457/JTR Engineering Design Expertise for Diagnostic Electrical Services (G. Veres, 2016-17)

International cooperation

Max Planck Institute of Plasma Physics (Garching, Germany), Development of ITER bolometers (G. Veres)

The European Joint Undertaking for ITER and the Development of Fusion Energy (Barcelona, Spain), Tokamak Services (G. Veres)

ITER International Organization (St. Paul-lez-Durance, France), In-vessel Electrical Services (G. Veres)

Publications

Articles

1. Anda G, Bencze A, Berta M, Dunai D, Hacek P, Krbec J, Réfy D, Krizsanóczi T, Bató S, Ilkei T, Kiss IG, Veres G, Zoletnik S: Lithium beam diagnostic system on the COMPASS tokamak. ***FUSION ENG DES*** 108: 1-6 (2016)

2. Ilkei T, Bodnár G, Baross T, Kiss B, Piros A, Porempovics G, Recski J, Rovni I: Trícium szaporításhoz kapcsolódó fejlesztések (Developments connected to tritium propagation, in Hungarian). ***NUKLEON*** 9: 197/1-5 (2016)

3. Náfrádi G, Kovácsik Á, Németh J, Pór G, Zoletnik S: Preliminary neutron shielding calculations of the electronics in the EAST BES systems focusing on neutron induced displacement damage. ***FUSION ENG DES*** 112: 225-231 (2016)

4. Nagy D, Baross T, Bendefy A, Darányi F, Kiss IG, Pataki Á, Szalai J, Veres G: ITER diagnosztikák elektromos infrastruktúrájának fejlesztése (Development of electronic infrastructure of ITER diagnostics, in Hungarian). ***NUKLEON*** 9: 198/1-4 (2016)

5. Son SH, Hong S−H, Kim Junghee, Kim Jun Young, Kim HS, Ding F, Luo G−N, Németh J, Zoletnik S, Fenyvesi A, Pitts R: Multi-purpose mid-plane manipulator for plasma surface interaction research in KSTAR. ***FUSION ENG DES*** 109–111, Part A: 286-289 (2016)

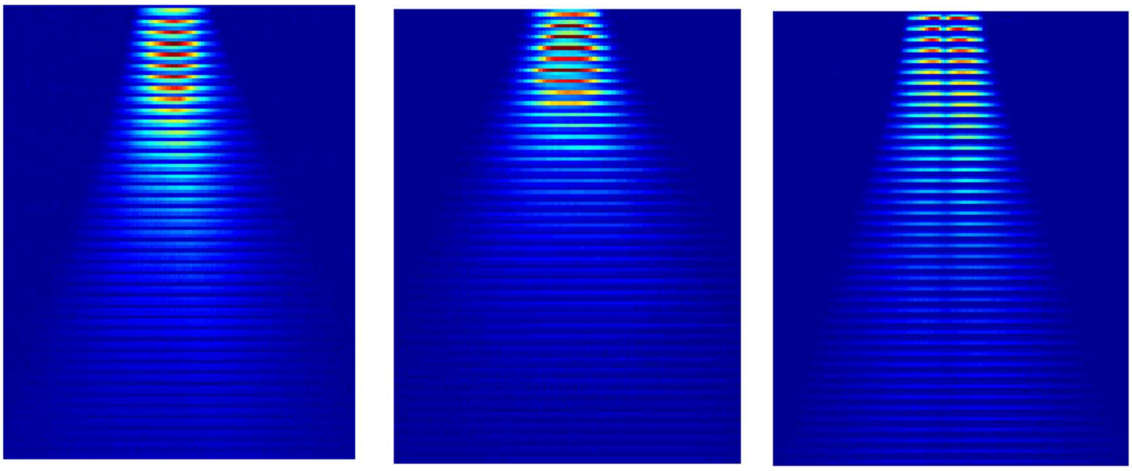
6. Veres G: Az ITER projekt (The ITER project, in Hungarian). ***NUKLEON*** 9:Paper 196/1-3 (2016)

See also: R-H NA49 Collaboration, R-Q Jet Collaboration

R-P. Laser plasma

István B. Földes, Márk Aladi#, Imre Ferenc Barna, Róbert Bolla#, Zsolt Kovács#, Mihály Pocsai#

Cluster characterization from different nozzles for high harmonic generation. — Rayleigh-scattering diagnostic was used to measure the features and sizes of the clusters from different nozzles. Simple Parker valves, Parker valves with home-made nozzles and supersonic De Laval nozzles of different sizes have been compared. Fig. 1 shows the scattered light at different distances downward from the orifice of 3 different nozzles. The intensity and thus the cluster sizes are similar but there is a significant difference in the spatial propagation. These results allow more precise high harmonic and Coulomb explosion experiments because the propagation effects can be well separated from the single cluster behavior.



a) b) c)

Figure 1. *Rayleigh scattered intensity from a Parker valve of 1 mm (a), from a Parker valve with extra 0.7 mm nozzle (b) and from a De Laval nozzle of 1 mm diameter (c) in case of 2 bar Xe backing pressure.*

Fast ions from Coulomb explosion of clusters irradiated by KrF laser. — When clusters are irradiated by short-pulse radiation, after the first ionization the clusters explode due to the large space charge which is called Coulomb explosion. Ions up to several keV have been observed in case of 10^{15} W/cm^2 KrF laser intensity. Experiments to investigate the ion spectra for different laser intensities and laser polarization is in progress.

Relativistic harmonics and carrier-envelope phase dependence with a 2-cycle laser. — Collaborative experiments with the Max Planck Institute of Quantum Optics was continued using the less than 5fs pulses of the LWS20 laser system there. High-harmonics were

Ph.D. student

generated up to 100 eV photon energy, the observed spectrum by using ~10^{20} W/cm^2 focused intensity. The observed $I_n \sim n^{8/3}$ dependence of the harmonic spectrum on the order of harmonics is in good agreement with the theory of the relativistic oscillating mirror (ROM) model.

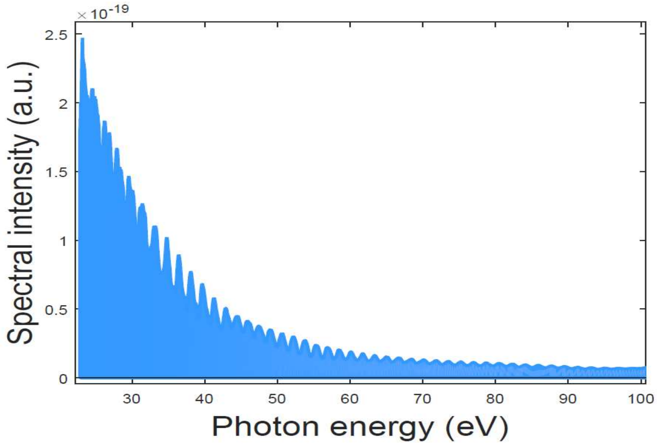


Figure 2. *High harmonics spectrum with a <5 fs laser, I≈10^{20} W/cm^2.*

Carrier-envelope phase (CEP) is essential for 2-cycle laser pulses, therefore it was monitored for each shot. It was found that the harmonics can be shifted shot by shot which corresponds to the theoretical expectations due to the varying CEP phase. Data acquisition to have a shot-to-shot correspondence between spectra and CEP is in progress.

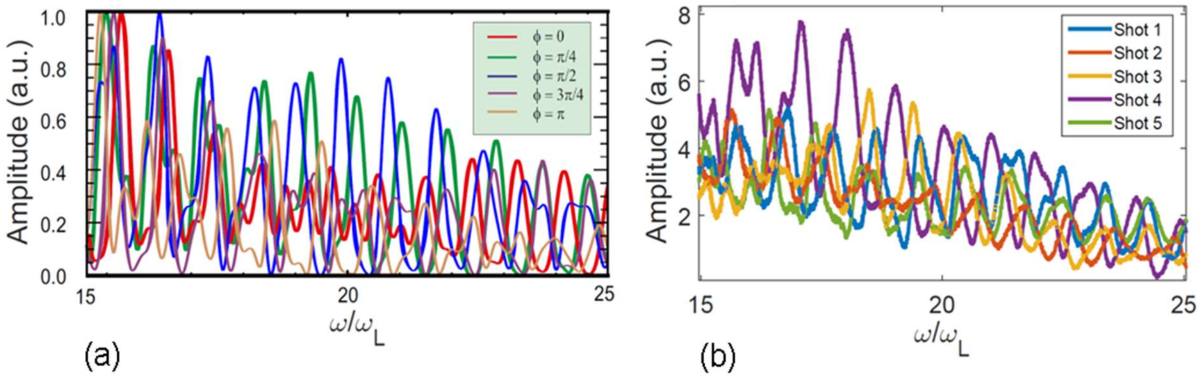


Figure 3. *PIC simulation results on harmonics spectra for various CEP (a) and experimental spectra with shot-to-shot varying CEP phase(b).*

Homogeneous rubidium plasma generation for novel particle accelerators. — The theoretical possibility of generating homogenous rubidium plasma for the AWAKE experiment in CERN for electron acceleration is investigated. Instead of particle-in-cell (PIC) simulations classical Maxwell equations are used including *ab-initio* quantum mechanical information. The ionization process of Rb atoms by the infrared laser radiation has been investigated. First the bound and continuous atomic structure of the Rb atom was evaluated with *ab-initio* quantum mechanical means, applying a linear combination of atomic orbitals of Slater wave functions and regular Coulomb wave packets for the discretized electron continuum. More than 30 low lying bound sates of Rb can be calculated together with additional ionization states for l=0,5 angular momenta.

The ionization process is under investigation in the field of a 800 μm wavelength 120 fs long laser pulse with peak intensity of 10^{14} W/cm^2. Beyond ionization probabilities, ionization cross sections, above threshold ionization peaks, angular differential electron distribution, and high harmonic generation spectra will be calculated and compared to similar experimental data and other theoretical models. These ionization probabilities will give the input data for the next propagation studies where the interaction of laser impulse and Rb plasma will be investigated.

Grants

EUROFUSION, Enabling Research ToIFE project

International cooperation

Max Planck Institute of Quantum Optics (MPQ, Garching, Germany).

AWAKE Experiment CERN.

Publications

Articles

1. Aladi M, Bolla R, Rácz P, Földes IB: Noble gas clusters and nanoplasmas in high harmonic generation. ***NUCL INSTRUM METH B*** 369: pp. 68-71. (2016) Proc. of International Workshop on Photon and fast Ion induced Processes in Atoms, Molecules and Nanostructures (PIPAMON) Debrecen, Hungary, .24-03-2015 – 26-03-2015.

2. Barna IF, Varró S: Proton scattering on carbon nuclei in bichromatic laser field at moderate energies. ***NUCL INSTRUM METH B*** 366: pp. 77-82. (2016) Proc. of International Workshop on Photon and fast Ion induced Processes in Atoms, Molecules and Nanostructures (PIPAMON) Debrecen, Hungary, .24-03-2015 – 26-03-2015.

3. Barna IF, Kersner R: Heat conduction: hyperbolic self-similar shock-waves in solid medium. ***J LIE THEORY*** 10:(S2) 010/1-4 (2016)

4. Barna IF, Bognár G, Hriczó K: Self-similar analytic solution of the two-dimensional Navier-Stokes equation with a non-Newtonian type of viscosity. ***MATH MODEL ANAL*** 21:(1) 83-94 (2016)

5. Gilicze B, Barna A, Kovács Z, Szatmári S, Földes IB: Plasma mirrors for short pulse KrF lasers. ***REV SCI INSTRUM***87:(8) 083101 (2016)

6. Pocsai MA, Varró S, Barna IF: Electron acceleration by a bichromatic chirped laser pulse in underdense plasmas. ***NUCL INSTRUM METH B*** 369: 50-54 (2016) Proc. of International Workshop on Photon and fast Ion induced Processes in Atoms, Molecules and Nanostructures (PIPAMON) Debrecen, Hungary, .24-03-2015 – 26-03-2015.

7. Szatmari S, Dajka R, Barna A, Gilicze B, Foldes IB: Improvement of the temporal and spatial contrast of high-brightness laser beams. ***LASER PHYS LETT*** 13:(7) 075301/1-5 (2016)

See also: R-D.1

R-Q. Beam emission spectroscopy

Dániel Dunai, Gábor Anda, Attila Bencze, Sándor Hegedűs, Tibor Krizsanóczi, Máté Lampert[#], Gábor Petravich[A], Dániel Réfy[#], Balázs Tál, Sándor Zoletnik

The Beam Emission Spectroscopy (BES) experimental technique has been used in fusion plasma experiments for decades. Nearly all major fusion experiments are equipped with BES diagnostics, and a variety of applications have been developed. The basic idea is that an atomic beam can penetrate the magnetic field of fusion devices and the beam fluorescence is measured. The light emission originates from excitation by plasma particle collisions; hence the light intensity gives information primarily on local plasma density.

Our group designs, manufactures, installs and operates BES diagnostics in several major fusion devices around the globe. Heating beam BES diagnostics were installed at MAST, KSTAR and EAST tokamaks, while alkali beams are operated in collaborations at JET, KSTAR, EAST, Compass and ASDEX Upgrade tokamaks. Wendelstein 7-X stellarator is also being equipped with an alkali beam BES diagnostic. This diversity gives a unique opportunity for multi machine comparison of several important physics phenomena.

An alkali beam diagnostic is being designed and manufactured for the Wendelstein 7-x stellarator in the framework of the Eurofusion WPS1 project in collaboration between Wigner RCP Budapest and IPP Greifswald. The ion gun was manufactured and tested in 2016 and planned to be installed in 2017. The primary objective of the diagnostic is to measure density profiles, island structures, turbulence and turbulence flow properties in the SOL as well as the edge region of Wendelstein 7-X. The main target is to measure upstream densities at high spatial (1cm) and temporal (1µs) resolutions.

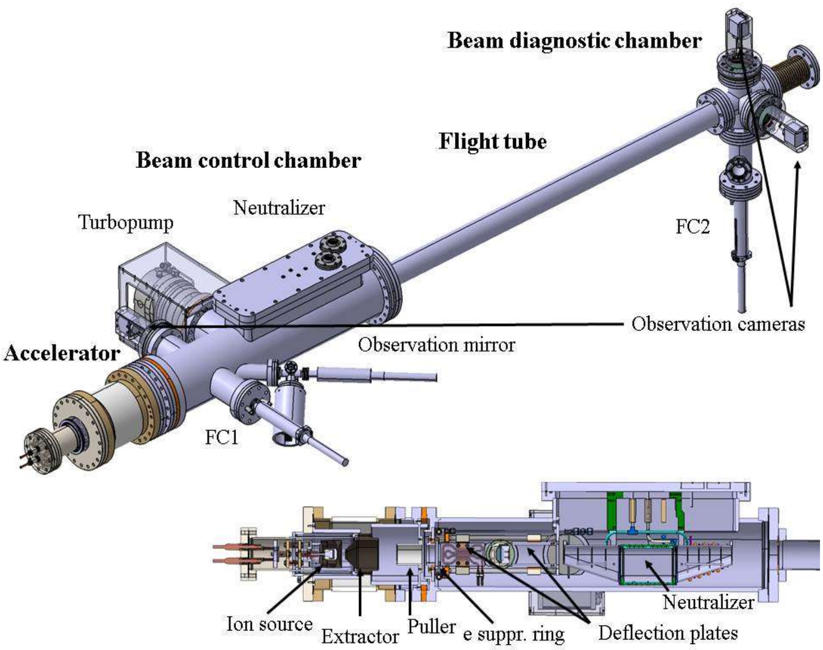


Figure 1. *The engineering drawings of the ion gun built for Wendelstein 7X stellarator.*

[#] Ph.D. student
[A] Associate fellow

Grants

Eurofusion Grants

International cooperation

CCFE UK, IPP Prague CZ, Max Planck Institute, IPP Garching D, Max Planck Institute IPP Greifswald D, ASIPP China, NFRI Korea

Publications

Articles

1. Anda G, Bencze A, Berta M, Dunai D, Hacek P, Krbec J, Réfy D, Krizsanóczi T, Bató S, Ilkei T, Kiss IG, Veres G, Zoletnik S: Lithium beam diagnostic system on the COMPASS tokamak. ***FUSION ENG DES*** 108: 1-6 (2016)

2. Kim J, Nam YU, Lampert M, Ghim Y-C: Reliability of the two-point measurement of the spatial correlation length from Gaussian-shaped fluctuating signals in fusion-grade plasmas. ***NUCL FUSION*** 56:(10) 106016/1-15 (2016)

3. Náfrádi G, Kovácsik Á, Németh J, Pór G, Zoletnik S: Preliminary neutron shielding calculations of the electronics in the EAST BES systems focusing on neutron induced displacement damage. ***FUSION ENG DES*** 112: 225-231 (2016)

4. Son SH, Hong S−H, Kim Junghee, Kim Jun Young, Kim HS, Ding F, Luo G−N, Németh J, Zoletnik S, Fenyvesi A, Pitts R: Multi-purpose mid-plane manipulator for plasma surface interaction research in KSTAR. ***FUSION ENG DES*** 109–111, Part A: 286-289 (2016)

5. Zoletnik S: Az európai fúziós útiterv (The European Fusion Roadmap, in Hungarian) ***NUKLEON*** 9: 195/1-8 (2016)

JET Collaboration

According to the list published in the Appendix of F. Romanelli and JET Contributors, ***NUCL FUSION*** 55: 104001, 2015, there are 1106 JET participants. Contributors from the Wigner RCP are Bodnár G, Cseh G, Dunai D, Kocsis G, Petravich G, Réfy D, Szabolics T, Tál B, Zoletnik S.

1. Hillesheim JC et al. incl. JET Contributors: Stationary zonal flows during the formation of the edge transport barrier in the JET tokamak. ***PHYS REV LETT*** 116:(6) 065002/1-6 (2016)
2. Batistoni P et al. incl. JET Contributors: Technological exploitation of Deuterium-Tritium operations at JET in support of ITER design, operation and safety. ***FUSION ENG DES*** **109:** 278-285 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
3. Boyer H et al. incl. JET Contributors: JET Tokamak, preparation of a safety case for tritium operations. ***FUSION ENG DES*** **109:** 1308-1312 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea

4. Giegerich T et al. incl. JET Contributors: Advanced design of the Mechanical Tritium Pumping System for JET DTE2. ***FUSION ENG DES*** **109:** 359-364 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
5. Horton L et al. incl. JET Contributors: JET experiments with tritium and deuterium-tritium mixtures. ***FUSION ENG DES*** **109:** 925-936 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
6. Lengar I et al. incl. JET Contributors: Radiation damage and nuclear heating studies in selected functional materials during the JET DT campaign. ***FUSION ENG DES*** **109:** 1011-1015 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
7. Pillon M et al. incl. JET Contributors: Characterization of a diamond detector to be used as neutron yield monitor during the in-vessel calibration of JET neutron detectors in preparation of the DT experiment. ***FUSION ENG DES*** **106:** 93-98 (2016)
8. Ratta GA et al. incl. JET Contributors: Global optimization driven by genetic algorithms for disruption predictors based on APODIS architecture. ***FUSION ENG DES*** **112:** 1014-1018 (2016) Proc. 10th IAEA Technical Meeting on Control, Data Acquisition, and Remote Participation for Fusion Research, 20–24 April 2015, Ahmedabad, India
9. Reynolds S et al. incl. JET Contributors: JET experience on managing radioactive waste and implications for ITER. ***FUSION ENG DES*** **109:** 979-985 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
10. Snoj L et al. incl. JET Contributors: Neutronic analysis of JET external neutron monitor response. ***FUSION ENG DES*** **109:** 99-103 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
11. Villari R et al. incl. JET Contributors: Neutronics experiments and analyses in preparation of DT operations at JET. ***FUSION ENG DES*** **109:** 895-905 (2016) Proc. 12th International Symposium on Fusion Nuclear Technology 14 - 18 September 2015, Jeju Island, South Korea
12. Murari A et al. incl. JET Contributors: Upgrades of Diagnostic Techniques and Technologies for JET Next D-T Campaigns
    IEEE T NUCL SCI **63:**(3) pp. 1674-1681. (2016)
    ANIMMA Conference. Lisbon, Portugália: 2015
13. Budny RV, JET Contributors: Alpha heating and isotopic mass effects in JET plasmas with sawteeth. ***NUCL FUSION*** **56:**(3) 036013/1-15 (2016)
14. Budny RV, Cordey JG, TFTR Team, JET Contributors: Core fusion power gain and alpha heating in JET, TFTR, and ITER. ***NUCL FUSION*** **56:**(5) 056002/1-18 (2016)
15. Buratti P et al. incl. JET Contributors: Diagnostic application of magnetic islands rotation in JET. ***NUCL FUSION*** **56:**(7) 076004/1-11 (2016)
16. Clairet F, Sirinelli A, Meneses L, JET Contributors: Plasma turbulence measured with fast frequency swept reflectometry in JET H-mode plasmas. ***NUCL FUSION*** **56:**(12) 126019/1-9 (2016)
17. Den Harder N et al. incl. JET Contributors: ELM-resolved divertor erosion in the JET

ITER-Like Wall. ***NUCL FUSION*** **56:**(2) 026014/1-9 (2016)

18. Gao Y et al. incl. JET Contributors: Characteristics of pre-ELM structures during ELM control experiment on JET with n=2 magnetic perturbations. ***NUCL FUSION*** **56:**(9) 092011/1-8 (2016) Proc. Joint Meeting of the 597th Wilhelm and Else Heraeus Seminar / 7th International Workshop on Stochasticity in Fusion Plasmas. Greifswald, Germany, 10-12 September 2015
19. Hender TC et al. incl. JET Contributors: The role of MHD in causing impurity peaking in JET hybrid plasmas. ***NUCL FUSION*** **56:**(6) 066002/1-15 (2016)
20. Jaervinen AE et al. incl. JET Contributors: Comparison of H-mode plasmas in JET-ILW and JET-C with and without nitrogen seeding. ***NUCL FUSION*** **56:**(4) 046012/1-19 (2016)
21. Lennholm M et al. incl. JET Contributors: Real-time control of ELM and sawtooth frequencies: similarities and differences. ***NUCL FUSION*** **56:**(1) 016008/1-21 (2016)

22 Lerche E et al. incl. JET Contributors: Optimization of ICRH for core impurity control in JET-ILW. ***NUCL FUSION*** **56:**(3) 036022/1-19 (2016)

23. de la Luna E et al. incl. JET Contributors: Understanding the physics of ELM pacing via vertical kicks in JET in view of ITER. ***NUCL FUSION*** **56:**(2) 026001/1-22 (2016)
24. Murari A et al. incl. JET Contributors: Application of transfer entropy to causality detection and synchronization experiments in tokamaks. ***NUCL FUSION*** **56:**(2) 026006/1-11 (2016)
25. Murari A et al. incl. JET Contributors: How to assess the efficiency of synchronization experiments in tokamaks. ***NUCL FUSION*** **56:**(7) 076008/1-12 (2016)
26. Paz-Soldan C et al. incl. JET Contributors: The non-thermal origin of the tokamak low-density stability limit. ***NUCL FUSION*** **56:**(5) 056010/1-12 (2016)
27. Roccella R et al. incl. JET Contributors: Asymmetric toroidal eddy currents (ATEC) to explain sideways forces at JET. ***NUCL FUSION*** **56:**(10) 106010/1-11 (2016)
28. Salewski M et al. incl. JET Contributors: Fast-ion energy resolution by one-step reaction gamma-ray spectrometry. ***NUCL FUSION*** **56:**(4) 046009/1-11 (2016)
29. Silva C et al. incl. JET Contributors: Experimental investigation of geodesic acoustic modes on JET using Doppler backscattering. ***NUCL FUSION*** **56:**(10) 106026/1-10 (2016)
30. Stan-Sion C et al. incl. JET Contributors: Tritium retention measurements by accelerator mass spectrometry and full combustion of W-coated and uncoated CFC tiles from the JET divertor. ***NUCL FUSION*** **56:**(4) 046015/1-8 (2016)

See also R-P ASDEX Upgrade Collaboration

R-S. Space physics

Zoltán Németh, Zsófia Bebesi, Melinda Dósa[#], Géza Erdős, Lajos Földy, Antal Juhász, Károly Kecskeméty, Péter Király[A], Andrea Opitz, Károly Szegő[A], Mariella Tátrallyay[A], Anikó Timár[#]

Solar System Bodies and Magnetospheres

Cometary physics. — The Rosetta spacecraft continued the exploration of the environment of comet 67P/Churyumov-Gerasimenko. Our research group contributed to several important results concerning the induced magnetosphere of the comet. We investigated the interaction of the solar wind and the cometary plasma, and found several relationships between the angular distributions of the interacting plasma populations. We also studied the response of the cometary environment to the arrival of abrupt solar wind disturbances. Our researchers participated in the discovery of the diamagnetic cavity of this comet (a region around the nucleus, from which the strong cometary activity "blows away" the magnetic field – a phenomenon observed only once at comet 1P/Halley earlier). We worked out a method, which can be used to find diamagnetic cavity crossing events on a magnetically dirty spacecraft, where residual fields render the usual methods very difficult. We used this method to detect more than a hundred cavity crossing events, and to build an event database. We analyzed the properties of these events, revealed and explained the plasma signatures accompanying the crossing of the cavity boundary, described the probable shape of the cavity and showed that an old model – refined and with proper input parameters – provides a good fit for the average extent of the cavity (Fig. 1). We also contributed to the discovery of a new type of plasma boundary; the analysis of the distribution of suprathermal electrons; and to the study of magnetic pile-up and mirror-mode waves around the comet.

The magnetosphere and moons of Saturn. — Based on the observations of the Cassini spacecraft we studied the magnetodisc of Saturn (a complex magnetized plasma phenomenon, which influences almost every property of the magnetosphere of Saturn). In addition to our contribution to a book, which reviews the properties of the magnetodiscs and aurorae of giant planets, we have also found that the complex time dependence of the magnetic and plasma measurements in the vicinity of the magnetodisc can be simultaneously explained by a simple model, which takes into account the planetary period oscillations (PPO) of the magnetodisc and the position of the spacecraft relative to the central sheet of the magnetodisc.

Using Cassini observations, we have followed the orbital evolution of E-ring dust particles, through their entire lifetime, starting at moon Enceladus, and ending in: a) a collision with the A-ring or any of the satellites; or b) losing all their mass due to sputtering; or c) leave the magnetosphere of Saturn. Using an updated version of our model (which included a noon-

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[A] Associate fellow

midnight electric field in the magnetosphere and a refined plasma model) we calculated the deposition rates and maps of E-ring particles to surfaces of the moons of Saturn.

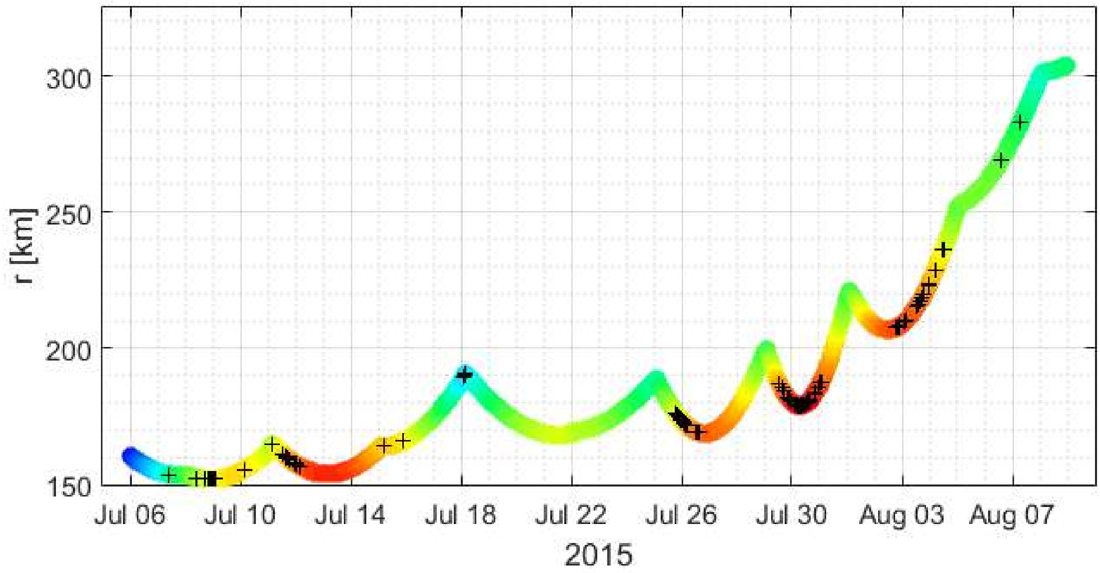

*Figure 3 The distance between Rosetta and the nucleus. Black **+** signs mark the sites where Rosetta encountered the cavity; the color of the line represents the distance from the nucleus in r_{cs} units, where r_{cs} is the time dependent theoretical boundary distance.*

Space Weather

Space weather propagation. — Our analysis of the interplanetary magnetic field, measured by satellites during the declining phase of the solar cycle 23, have shown that significant modulation of the magnetic flux were present in association with the solar rotation. The recurrent magnetic flux increases, lasting for several years, may have impact on the terrestrial environment and can contribute to space weather events.

Space weather effects on Solar System bodies. — We participated in the statistical analysis of global polarity reversals of the Venusian induced magnetosphere in response to the polarity change in the interplanetary magnetic field; and also in a multi-instrument study of the topside ionosphere of Mars under different solar wind conditions.

Suprathermal ions. — By studying the energy spectra of various ions at suprathermal energies during quiet solar conditions in fast solar wind streams from near-equatorial coronal holes we found that the bulk wind ions serve as a seed population subsequently accelerated to high energies.

Grants

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ESA PECS Cluster Science Data System (M. Tátrallyay, 2015-2017)

János Bolyai Research Scholarship (Z. Németh, 2016-2019)

International cooperation

International team of the Cassini Plasma Spectrometer (CAPS) (K. Szegő, Z. Németh)

International team of the Cassini Magnetometer (MAG), (G. Erdős)

International team of the Rosetta Plasma Consortium (RPC) (K. Szegő, Z. Németh)

International team of the Cluster mission (M. Tátrallyay)

Europlanet2020-RI, integrating the European planetary science community (K. Szegő, A. Opitz)

University of Colorado, Boulder, USA (A. Juhász)

Lomonosov Moscow State University, Russia (K. Kecskeméty)

Publications

Articles

1. Behar E, Nilsson H, Wieser G Stenberg, Németh Z, Broiles T W, Richter I: Mass loading at 67P/Churyumov-Gerasimenko: A case study. ***GEOPHYS RES LETT*** 43:(4) 1411-1418 (2016)

2. Broiles TW, Burch JL, Chae K, Clark G, Cravens TE, Eriksson A, Fuselier SA, Frahm RA, Gasc S, Goldstein R, Henri P, Koenders C, Livadiotis G, Mandt KE, Mokashi P, Németh Z, Odelstad E, Rubin M, Samara M: Statistical analysis of suprathermal electron drivers at 67P/Churyumov–Gerasimenko. ***MON NOT R ASTRON SOC*** 462:(Suppl_1) S312-S322 (2016)

3. Daibog E, Kecskeméty K, Lazutin L, Logachev Y: Jovian electrons as an instrument of investigation of the interplanetary medium structure. ***J PHYS CONF SER*** 675 032024/1-4 (2016) International Conference on Particle Physics and Astrophysics (ICPPA). Moscow, Russia, 05-10-2015 – 10-10-2015

4. Dálya Zs, Opitz A: Improvement of background solar wind predictions. ***GEOPHYS RES ABSTR*** 18 145471-1 (2016) EGU General Assembly Conference Abstracts. Vienna, Austria: 18-04-2016 – 22-04-2016

5. Vech D, Stenberg G, Nilsson H, Edberg N, Opitz A, Szegő K, Zhang T, Futaana Y: On the global polarity reversal of the induced magnetosphere of Venus: a statistical study. ***GEOPHYS RES ABSTR*** 18: 116/1-1 (2016) EGU General Assembly Conference Abstracts. Vienna, Austria: 18-04-2016 – 22-04-2016

6. Edberg N J T, Eriksson A I, Odelstad E, Vigren E, Andrews D J, Johansson F, Burch J L, Carr C M, Cupido E, Glassmeier K-H, Goldstein R, Halekas J S, Henri P, Koenders C, Mandt K, Mokashi P, Németh Z, Nilsson H, Ramstad R, Richter I, Wieser G Stenberg: Solar wind interaction with comet 67P: Impacts of corotating interaction regions. ***J GEOPHYS RES-SPACE*** 121:(2) 949-965 (2016)

7. Goetz C, Koenders C, Richter I, Altwegg K, Burch J, Carr C, Cupido E, Eriksson A, Güttler

C, Henri P, Mokashi P, Németh Z, Nilsson H, Rubin M, Sierks H, Tsurutani B, Vallat C, Volwerk M, Glassmeier K-H: First detection of a diamagnetic cavity at comet 67P/Churyumov-Gerasimenko. ***ASTRON ASTROPHYS*** 588 A24/1-6 (2016)

8. Mandt KE, Eriksson A, Edberg NJT, Koenders C, Broiles T, Fuselier SA, Henri P, Németh Z, Alho M, Biver N, Beth A, Burch J, Carr C, Chae K, Coates AJ, Cupido E, Galand M, Glassmeier K-H, Goetz C, Goldstein R, Hansen K C, Haiducek J, Kallio E, Lebreton J-P, Luspay-Kuti A, Mokashi P, Nilsson H, Opitz A, Richter I, Samara M, Szegő K, Tzou C-Y, Volwerk M, Wedlund CS, Wieser GS: RPC observation of the development and evolution of plasma interaction boundaries at 67P/Churyumov-Gerasimenko. ***MON NOT R ASTRON SOC*** 462:(Suppl1) S9-S22 (2016)

9. Németh Z, Burch J, Goetz C, Goldstein R, Henri P, Koenders C, Madanian H, Mandt K, Mokashi P, Richter I, Timar A, Szegő K: Charged particle signatures of the diamagnetic cavity of comet 67P/Churyumov–Gerasimenko. ***MON NOT R ASTRON SOC*** 462:(Suppl_1) S415-S421 (2016)

10. Németh Z, Szegő K, Földy L, Cowley SWH, Provan G, Thomsen M: Periodic motion of the magnetodisk as a cause of quasi-periodic variations in the Kronian magnetosphere. ***PLANET SPACE SCI*** 130:(1) 54-59 (2016)

11. Vech D, Stenberg G, Nilsson H, Edberg NJT, Opitz A, Szegő K, Zhang T, Futaana Y Statistical features of the global polarity reversal of the Venusian induced magnetosphere in response to the polarity change in interplanetary magnetic field ***J GEOPHYS RES-SPACE*** 121:(5) 3951-3962 (2016)

12. Volwerk M, Richter I, Tsurutani B, Götz C, Altwegg K, Broiles T, Burch J, Carr C, Cupido E, Delva M, Dósa M, Edberg N J T, Eriksson A, Henri P, Koenders C, Lebreton J-P, Mandt K E, Nilsson H, Opitz A, Rubin M, Schwingenschuh K, Stenberg Wieser G, Szegö K, Vallat C, Vallieres X, Glassmeier K-H: Mass-loading, pile-up, and mirror-mode waves at comet 67P/Churyumov-Gerasimenko. ***ANN GEOPHYS*** 34:(1) 1-15 (2016)

13. Withers Paul, Matta M, Lester M, Andrews D, Edberg N J T, Nilsson H, Opgenoorth H, Curry S, Lillis R, Dubinin E, Fränz M, Han X, Kofman W, Lei L, Morgan D, Pätzold M, Peter K, Opitz A, Wild J A, Witasse O: The morphology of the topside ionosphere of Mars under different solar wind conditions: Results of a multi-instrument observing campaign by Mars Express in 2010. ***PLANET SPACE SCI*** 120 24-34 (2016)

14. Zel'dovich MA, Logachev YI, Surova GM, Kecskeméty K, Veselovskii IS: Suprathermal ions in solar-wind outflows from coronal holes at 1 AU. ***ASTRON REP+*** 60:(7) 687-693 (2016)

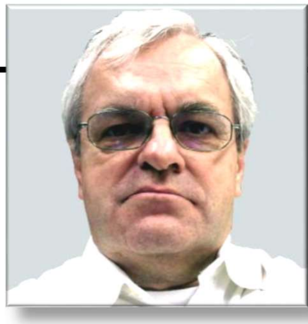
Book

15. Szegő K, Achilleos N, Arridge Ch, Badman S, Delamere P, Grodent D, Kivelson MG, Louarn Ph (eds.): The Magnetodiscs and Aurorae of Giant Planets. Springer Verlag, New York 2016. (Space Sciences Series of ISSI) 50. (ISBN:978-1-4939-3394-5)

Other

16. Szegő K: A Naprendszer kutatása az RMKI/RMI-ben (Research of the Solar System in the RMKI/RMI). ***TERMÉSZET VILÁGA*** 147:(Special edition 2) 93-96 (2016)

R-T. Space technology



János Zoltán Nagy#, András Balázs, Attila Baksa, László Hevesi, István Horváth, Zoltán Pálos, Bálint Sódor, Sándor Szabó, Lajos Szalai, Sándor Szalai[E], Gábor Tróznai, Pál Gábor Vizi#

Our team supports our space exploration with technical background, development of onboard electronics, flight software and special ground equipment to test and calibration of flying instruments. Our intensive job starts with instrument and software development years prior to mission launch. During flight we take part in data evaluation, mission steering job and upload fly software with patches in case of eventual unexpected circumstances.

Interplanetary missions

Rosetta. — The greatest historic mission in which we have ever participated is the Rosetta mission of ESA ended as planned on 30th September, 2016. The mission ended with controlled impact onto the comet it had been investigating for more than two years. Rosetta's final maneuver set it on a collision course with the comet from an altitude of about 19 km. Two months before descending, Orbiters camera, Osiris took pictures of the Lander Philae the onboard computer of which was developed by us (Fig. 1). The processing of scientific and housekeeping data of the landing unit is still in progress.

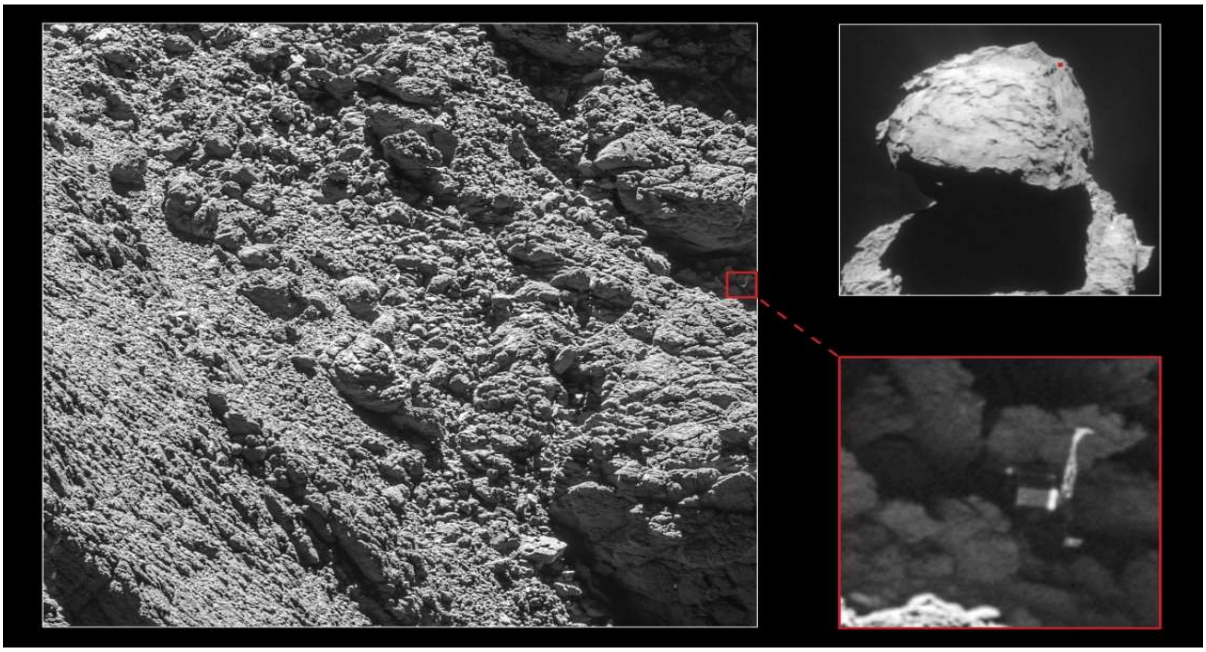


Figure 1. *On 5th September, 2016 Rosetta's high-resolution camera found the Philae lander wedged into a dark crack on Comet 67P/Churyumov–Gerasimenko.*

Ph.D. student

E Professor Emeritus

The results of Rosetta make probable that comets are ancient leftovers of early Solar System formation rather than fragments of collisions between larger bodies later on. During 12 years, until the end of the mission the power switch module developed and designed as a spatial structure by our team worked and supplied several sensors on orbiter unit continuously (Fig. 2).

Figure 2. *Power switch module developed by our team which switched the power for five sensors of Rosetta Plasma Consortium instrument.*

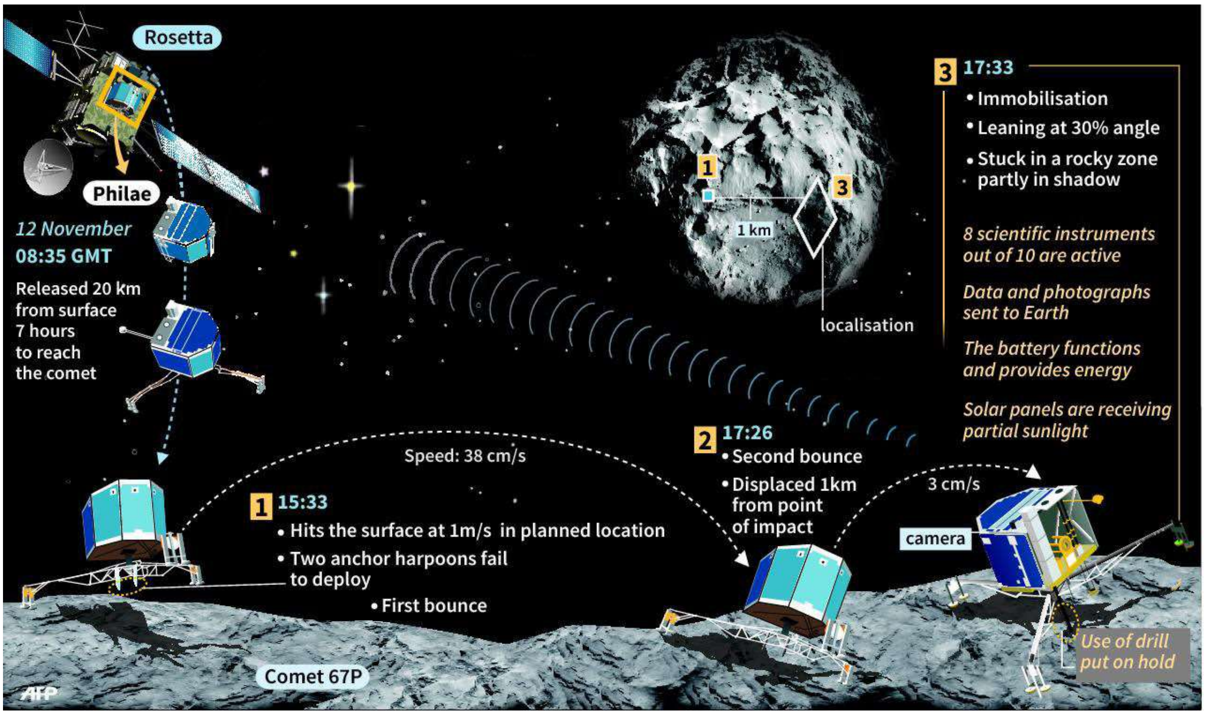


Figure 3. *Landing of the Philae lander on 12th November, 2014. Examining housekeeping and solar sensor illumination data, we reconstructed the movement, direction and trajectories of lander path.*

BepiColombo PICAM. — We developed the DC/DC power supply unit for PICAM experiment of BepiColombo mission. The QM (qualification model), FM (flight model) and SFM (spare flight model, Fig. 4) of DC/DC converter are delivered and went through all tests and wait for launch of BepiColombo (Fig. 4).

Particle Environment Package (PEP) for Juice. — The JUpiter ICy moons Explorer spacecraft will emergence of habitable words around gas giant. Currently we are developing DC/DC converter for the project JUICE goal of which is to explore icy moons of Jupiter (Figs. 5 and 6). The planned launch is 2022.

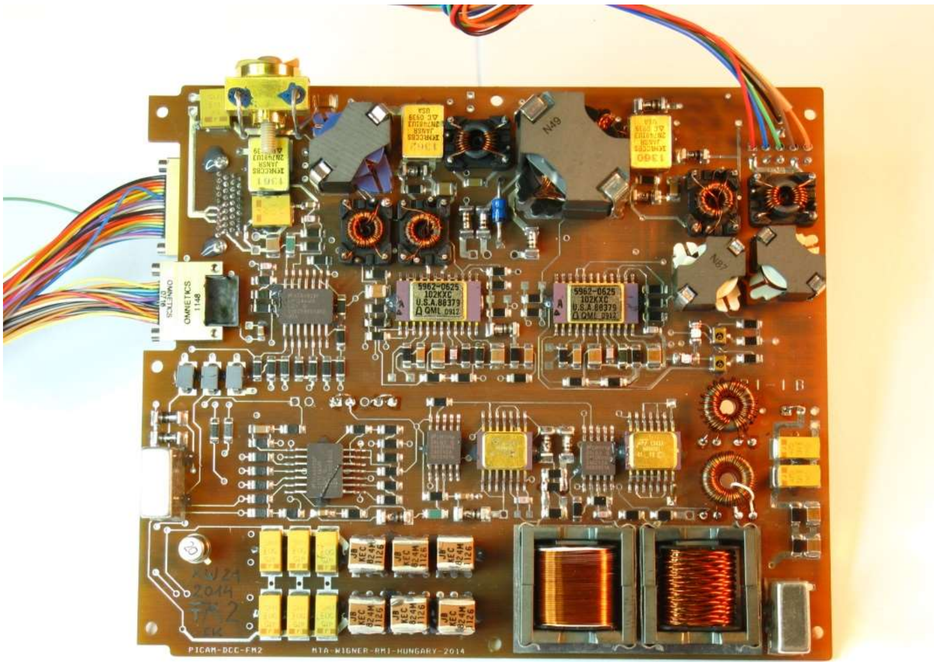
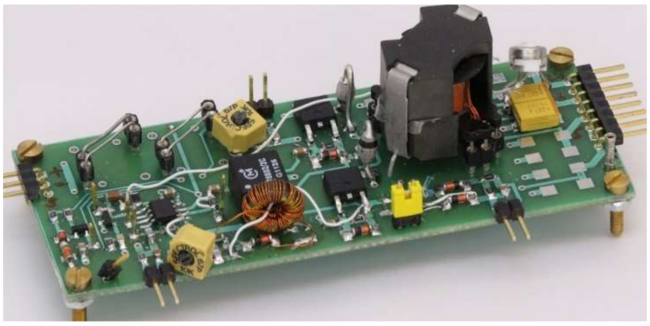


Figure 4. *Delivered SFM model of PICAM DC/DC converter*



⇧***Figure 5.*** *Prototype model of one PS unit for PEP Juice.*

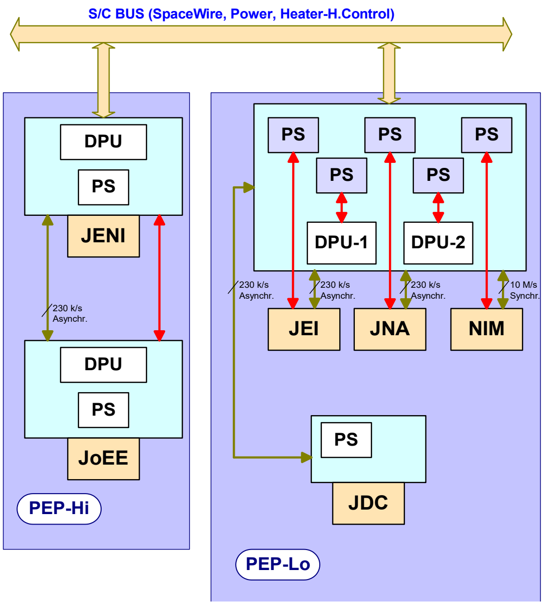
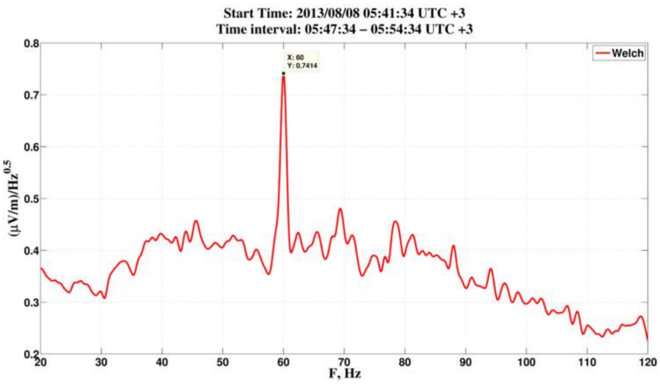


Figure 6. *The yellow units are the sensors and the units marked with PS in PEP-Lo are the power supply units developed by our team.* ⇨

Missions around the Earth

Obstanovka. — The Obstanovka experiment works in the Russian segment of the International Space Station. Its scientific job is to explore near-Earth space and space weather phenomena in high atmosphere. It was put in work in April 2013. We developed three onboard computers for this experiment. Surprisingly, Obstanovka discovered that the 50- or 60-Hz signal from power lines on Earth can appear in the spectra of electric and magnetic signals above Earth (Figs. 7 and 8).



⇧***Figure 7****. 60 Hz signal from power lines on Earth in spectra of electric signals.*

Figure 8. *During overflight the blue color indicates area where the 60 Hz and the red line where 50 Hz was indicated in electric spectra.*⇨

New application area. — We have developed a special interface card for the Leon-microprocessor, developed for European space projects to meet future requirements of performance, software compatibility and low system costs (Fig. 9).

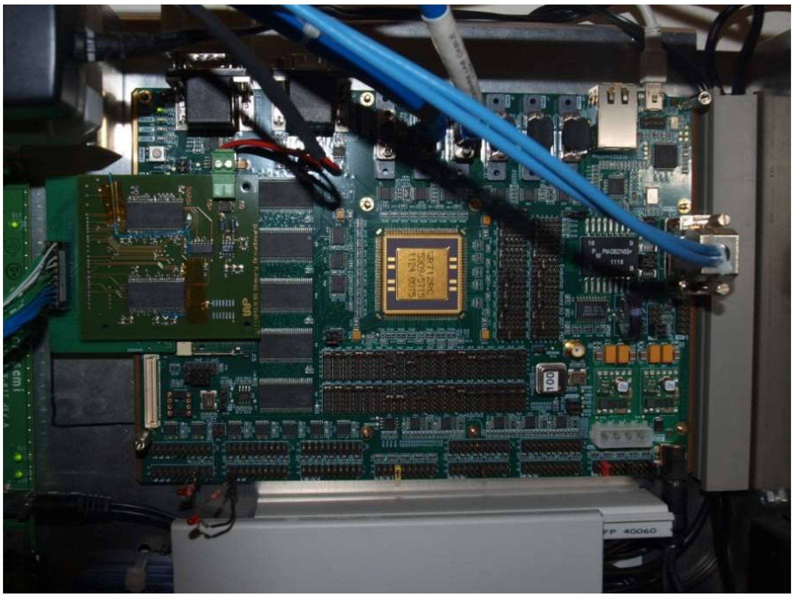


Figure 9. *The Leon3 development board in the picture.*

Zero Magnetic Field Laboratory (ZBL). — ZBL realization begins in mid-2017 and it will be finalized in two years. Our team participated in the preparation of the space technology related aspects of this important infrastructure.

Grants

ESA PECS- 4000109793 (we are subcontractor in this contract) Juice; PECS-4200098091 BepiColombo; PECS 4200098078 CDNS; PECS 4200098080 RPC

International cooperation

IRF (Swedish Institute of Space Physics, Kiruna), Imperial College, London, IKI Moszkva, DLR Köln, ESOC Darmstadt, MPS Lindau), CNES Touluse, IRAP Touluse, IWF Gratz, FMI Helsinki

Publications

Articles

1. Baksa A, Balazs A, Palos Z, Spanyi P, Szalai S, Varhalmi L: Software on a comet: The philae lander's central onboard computer. ***IEEE SOFTWARE*** 33:(2) 81-84 (2016)

2. Balázs A, Baksa A, Bitterlich H, Hernyes I, Küchemann O, Pálos Z, Rustenbach J, Schmidt W, Spányi P, Sulyán J, Szalai S, Várhalmi L: Command and data management system (CDMS) of the Philae lander. ***ACTA ASTRONAUT*** 125: 105-117 (2016)

3. Nagy J, Balajthy K, Szalai S, Sodor B, Horvath I, Lipusz C: Obstanovka: Exploring nearby space. ***IEEE SOFTWARE*** 33:(4) 101-105 (2016)

4. Szalai S, Nagy J, Horváth I, Sódor B, Tróznai G, Balajthy K, Sulyán J: An overview of low-cost EGSE architectures improvement. ***ACTA POLYTECH HUNG*** 13:(3) 139-158 (2016)

5. Szalai S: A Rosetta–Philae sikere magyarok részvételével (Success of Rosetta-Philae with the participation of Hungarians, in Hungarian). ***FIZIKAI SZEMLE*** 66:(10) 322-327 (2016)

Conference proceedings

6. Sipos A, Vizi GP: Ten years of the simulated Mars rover model competition. In: *Proc. H-SPACE 2016: 2nd International Conference on Research, Technology and Education of Space* Budapest, Hungary, 25-02-2016 – 26-02-2016, Eds.: Bacsárdi L, Kovács K, Magyar Asztronautikai Társaság, 2016, pp. 61-62. (ISBN:9789637367106)

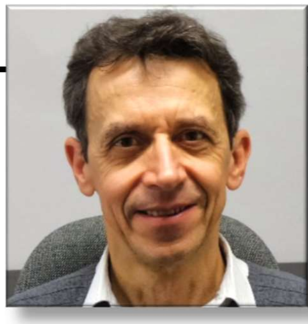
7. Vizi GP: Application of the fleet of micro sized space-motherships (MSSM) deploying nano, pico space devices and robots (NPSDR) in space. In: *Proc. H-SPACE 2016: 2nd International Conference on Research, Technology and Education of Space* Budapest, Hungary, 25-02-2016 – 26-02-2016, Eds.: Bacsárdi L, Kovács K, Magyar Asztronautikai Társaság, 2016, pp. 43-44 (ISBN:9789637367106)

8. Horvath A, Berczi Sz, Vizi PG: Nano and pico landing space probe swarm to search the possibility of life at the southern pole of Mars with an environmental friendly structure. In: *Proc. 47th Lunar and Planetary Science Conference*, The Woodlands, USA, 21-03-2016 – 26-03-2016. Houston (TX): Lunar and Planetary Institute, Paper 2570. 2 p. (LPI Contribution Series, 1903.)

9. Sipos A, Vizi PG: 10 years of the simulated Mars rover model competition. In: *Proc. 47th Lunar and Planetary Science Conference*, The Woodlands, USA, 21-03-2016 – 26-03-2016. Houston (TX): Lunar and Planetary Institute, Paper 2098. 2 p. (LPI Contribution Series, 1903.)

10. Vizi PG, Berczi Sz, Csizmadia S, Hegedüs T: Extended meteor hunting with smartphones as surveillance cameras. In: *Proc. 47th Lunar and Planetary Science Conference*, The Woodlands, USA, 21-03-2016 – 26-03-2016. Houston (TX): Lunar and Planetary Institute, Paper 1797. 2 p. (LPI Contribution Series, 1903.)

Laboratory of rehabilitation-technology



József Laczkó, András Arató, Norbert Márkus, Szabolcs Malik, Mariann Mravcsik[#], Lilla Botzheim[#]

For studying the natural and artificial control of human movements, we conducted kinematic and muscle-activity (electromyograms) measurements on human arm movements of able-bodied participants. The effect of external resistances and body positions on variances of repetitively executed movements was examined. The motor variances were examined at the level of hand position, at angular changes in the joints, and at muscle activities, the latter ones were represented and studied in high dimensional, "natural biological" spaces. This allows us to describe movement-stability, to better understand motor control and to define and refine rehabilitation methods. Based on our results in the control of lower limb movements, in 2016 we substituted missing neural control, by multichannel functional electrical muscle stimulation, and made it possible for 10 spinal cord injured (SCI), lower-limb paralyzed individuals to perform cycling movements against various loads on a stationary bike. We recorded and tracked the power and energy output of the SCI participants. The power output produced during FES cycling by spinal cord injured individuals depends on many factors, such as cycling cadence, crank resistance and the current amplitude, pulse with and frequency of the stimulating current. We found that power output is significantly higher when more muscles (4 per limbs instead of 2) are stimulated. The advantage is that in this case the current amplitude per muscles is lower while the achieved power output is higher. Power output can be increased by increasing cycling velocity or by cycling against higher crank resistance. It was observed in the National Institute for Medical Rehabilitation in Budapest that the paralyzed people who volunteered to participate in our FES assisted rehabilitation program with 4 (per legs) stimulated muscles, preferred to cycle against higher crank resistance but for shorter total cycling time, thus achieving greater power output but maintaining the level of energy output.

Another field of rehabilitation research for helping people with sensory disabilities and for facilitating communication abilities of blind and deaf-blind people. We compared the efficiency of braille input devices and methods. We provided the use of our TalkPad speech prosthesis software for 40-50 new users. We educated 4 amateur radio operator for using morse code with a speed of at least 20wpm to extend previous studies at the station HA5RST. We advanced the MOST (Mobile Slate Talker) devices for the blind and deaf-blind due to the challenges given by continuously changing operating system.

Grants:

Austrian – Hungarian Scientific and Educational Cooperation Action Fund, Project number: 94ou7, Development of rehabilitation protocols for spinal cord injured people (J. Laczko, 2016-2017)

[#] Ph.D. student

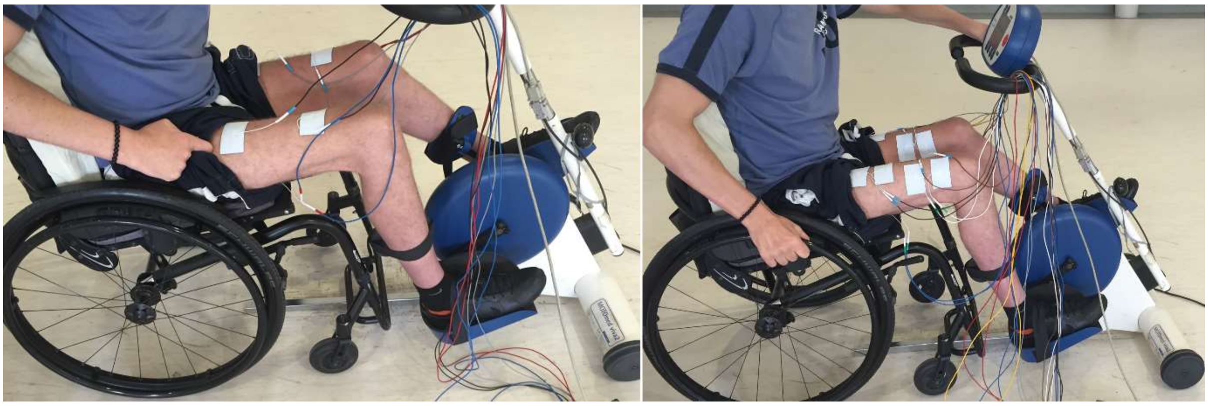


Figure 1. Spinal cord injured (lower limb paralysed) person performs cycling movements generated by functional electrical stimulation of 2 muscles per legs (left) and by 4 muscles per legs (right). The achieved power output depends on the number of muscles and on the applied stimulation pattern. This rehabilitation method is advantageous for physical and physiological (cardiovascular and respiratory) well-being.

International cooperation

Medical University Vienna, Center for Medical Physics and Biomedical Technics (W. Mayr).

Rehabilitation Institute of Chicago (R. Scheidt and F. Mussa-Ivaldi)

Studying movement coordination deficits after stroke and spinal cord injury.

Publications

Article

1. Laczko J, Mravcsik M, Katona P: Control of cycling limb movements: aspects for rehabilitation. ***ADV EXP MED BIOL*** 957: 273-289 (2016) Progress in Motor Control: Theories and Translations. (ISBN 978-3-319-47313-0)

Conference proceedings

2. Katona Péter, Mravcsik M, Laczkó J: Fejlesztések a gerincsérültek terápiájában alkalmazott Funkcionális Elektromos Stimulációs (FES) kerékpározó edzés módszerében (Developments in the Functional Electric Stimulation (FES) bycicling training method applied in the therapy of spinal cord injuries, in Hungarian). In: *Proc. Sokszínű sporttudomány*, Szombathely, Hungary, 04-12-2015 – 05-12-2015. Magyar Sporttudományi Füzetek (Magyar Sporttudományi Szemle különszáma) 14., Eds.: Szmodis M and Szőts G, Magyar Sporttudományi Társaság, Budapest, 2016, pp. 65-79. (ISBN:978-615-5187-10-0)

3. Mravcsik M, Klauber A, Laczkó J: FES driven lower limb cycling by four and eight channel stimulations – a comparison in a case study. In: *Proc. 12th Vienna International Workshop on Functional Electrical Stimulation*, Vienna, Austria, 08-09-2016 – 09-09-2016. Eds.: Bijak M, Mayr W, Pichler M, International FES Society, Milano, 2016 pp. 89-93. (ISBN:978-3-900928-12-4)

Book

4. Laczko J, Latash ML (Eds.): Progress in Motor Control: Theories and Translations.: Springer International Publishing, Cham 2016. 388 p. (ISBN:978-3-319-47313-0)

INSTITUTE FOR
SOLID STATE PHYSICS AND OPTICS

S-E. Non-equilibrium alloys

Judit Balogh, László Bujdosó, Dénes Kaptás, Tamás Kemény[A], László Ferenc Kiss, Imre Vincze[E]

Magnetic properties of nanoscale multilayers. — The superparamagnetic nature of ultrathin Fe layers between Ag layers has been investigated for a long time, but the dependence of the superparamagnetic properties on the number of the alternating Fe and Ag layers in a multilayer stack has not yet been studied. Superparamagnetism of a nominally few monolayer thick magnetic layer appears due to the island growth mode of the layer and multilayers of such discontinuous layers are called granular multilayers. The effects of dipole interactions on the superparamagnetic behavior have long been intensively studied, but only a few granular multilayer systems were studied from this point of view experimentally.

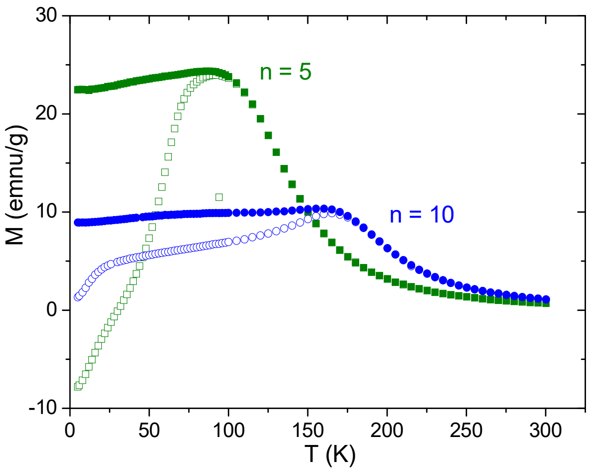
We have studied the blocking temperature, T_B, – the temperature above which the relaxation frequency of the magnetic moment exceeds the frequency characteristic to the measurement – in Fe/Ag granular multilayers with different number (n=1, 2, 5, 10, 20) of Fe/Ag bilayers. T_B was determined from magnetization measurements in a superconducting quantum interference device (SQUID) and it is defined as the cusp temperature of the magnetization measured after cooling the sample from 300K to 5K in zero field. The average size of the Fe granules were estimated from Mössbauer spectroscopy measurements. The role of the dipolar interactions and a perpendicular magnetic anisotropy component in the observed unusually large variation of T_B was investigated by Monte-Carlo (MC) simulations in collaboration with the Democritos Research Center, Athens.

Two representative FC/ZFC magnetization curves are shown for the n=1 and 10 samples in Fig. 1. The T_B values measured in different applied fields are shown for all the samples in Fig. 2. As can be seen from the figures there is a large, almost an order of magnitude increase of T_B as the number of bilayers is increased from 1 to 10. Upon further increasing the number of bilayers (n=20), no change of the blocking temperature is observed.

In case of a non-interacting particle assembly, the increase of T_B can result from the increase of the average grain size and/or the anisotropy energy. Significant changes of these factors for our samples could be ruled out by the Mössbauer spectroscopy measurements. The Monte Carlo simulations indicated that the dipolar interactions between the neighboring layers and the out-of-plane anisotropy should play a decisive role in the observed large variation of the blocking temperature.

[A] Associate fellow

[E] Professor Emeritus



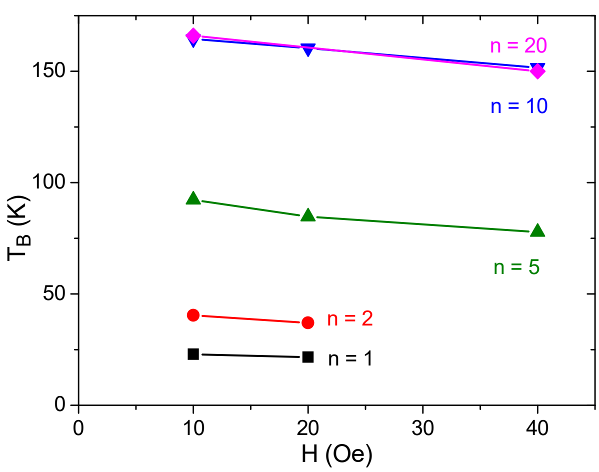


***Figure 1.** Magnetization of granular multi-layers with the indicated number of Fe/Ag bilayers measured after cooling in 10 Oe field (full symbols) and in zero field (empty symbols).*

***Figure 2.** Dependence of the temperature of the maxima of the measured ZFC curves (T_B) on the measuring field for different number of Fe/Ag bilayers.*

Grants

OTKA K101456 Mössbauer and Magnetic Study of Intermetallic Compounds (I. Vincze, 2012-2017)

OTKA K112811 Magnetic Multilayers Modified by Amorphous Alloys (J. Balogh, 2015-2019)

International cooperation

Department of Condensed Matter Physics at the University of Seville (Seville, Spain) (L.F. Kiss)

National Center for Scientific Research "Demokritos" (Athens, Greece) (J. Balogh)

Department of Physics, Shiga University of Medical Science (Shiga, Japan) (J. Balogh)

Publications

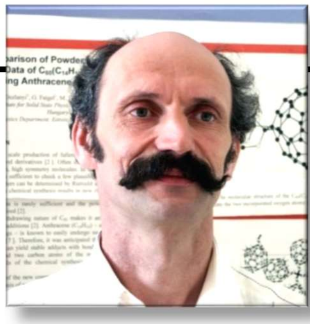
Articles

1. Balogh J, Kaptás D, Kiss LF, Dézsi I, Nakanishi A, Devlin E, Vasilakaki M, Margaris G, Trohidou KN: Increase of the blocking temperature of Fe-Ag granular multilayers with increasing number of the layers. ***J MAGN MAGN MATER*** 401: 386-390 (2016)

2. Kiss LF, Kemény T, Bednarčík J, Gamcová J, Liermann H-P: Influence of the critical Fe atomic volume on the magnetism of Fe-rich metallic glasses evidenced by pressure-dependent measurements. ***PHYS REV B*** 93:(21) 214424/1-14 (2016)

3. Náfrádi B, Antal A, Fehér T, Kiss LF, Mézière C, Batail P, Forró L, Jánossy A: Frustration-induced one-dimensionality in the isosceles triangular antiferromagnetic lattice of δ -(EDT-TTF- CONMe$_2$)$_2$AsF$_6$. ***PHYS REV B*** 94:(17) 174413/1-6 (2016)

S-F. Laboratory for advanced structural studies



Gyula Faigel, Gábor Bortel, Dániel Datz#, László Gránásy, Judit Horváth#, Zoltán Jurek, Katalin Kamarás, Gyöngyi Klupp, Bálint Korbuly#, Éva Kováts, Gergely Németh#, Katalin Németh, Gábor Oszlányi, Áron Pekker, Sándor Pekker, Frigyes Podmaniczky#, Tamás Pusztai, László Rátkai#, Bence Szabados#, Zsolt Szekrényes#, Hajnalka-Mária Tóháti#, Gyula Tóth, György Tegze, Miklós Tegze

The Laboratory of Advanced Structural Studies (LASS) carries out research in three areas: carbon based materials, the theory of phase transformations and X-ray related methods. In the last year, we have reached significant results in all of these fields.

Carbon-based systems. — Lately, various carbon-based materials have become the center of intensive research. Earlier, we concentrated on fullerenes and related compounds whereas metal organic framework (MOF) materials, carbon nanotubes and nanotube-based hybrid systems are our center of interest currently.

Metal-organic frameworks. Metal-organic frameworks are porous coordination polymers with large inner cavities. The rigid, metal-containing clusters at the nodes (inorganic Secondary Building Units, inorganic SBUs) are joined by organic linkers. In our recent work, we have successfully prepared six new MOF structures with zinc-containing secondary building units and cubane-1,4-dicarboxylic acid linkers. This year, we have continued the study of this new family of materials. We scaled up the preparation in order to get homogeneous, high quality samples in large quantities. We have elaborated the safe storage of water-sensitive samples, and the activation of MOF structures. We started to examine the absorption properties of our new materials. We have characterized the structure of high-symmetry MOF-5 and analogue materials with various solvents in their voids by single-crystal X-ray diffraction. Recently, we have also prepared a new four-nuclear MOF with spiro[3.3]heptane-2,6-dicarboxylic acid linkers with similar structure to our highest symmetry frameworks.

Infrared spectroscopy on carbon-based systems: Our research concentrated on fullerenes, nanotubes, nanotube-based hybrids and two-dimensional systems. We introduced new methods: synchrotron-based infrared spectroscopy, near-field infrared microscopy and photoinduced spectroscopy. Materials studied were carbon and boron nitride nanotubes, both pristine and filled with small molecules, graphene and solar cell materials based on methylamine-PbI_3 perovskite (Fig. 1) and carbon nanotubes. We also studied the luminescence properties of another prospective solar-cell material, silicon carbide.

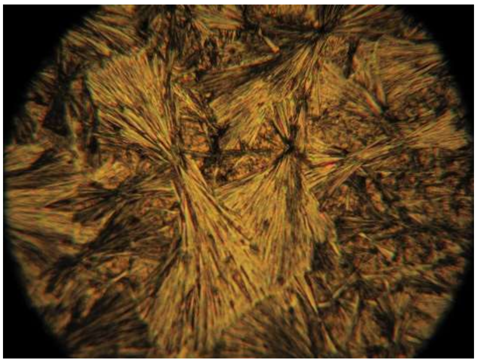


Figure 1. *Methylamine-lead iodide (MA-PbI_3) deposited on carbon nanotube film.*

Ph.D student

Theory of phase transformations. – We have investigated various aspects of crystalline freezing within atomistic and coarse-grained continuum models:

(1) We used two differently formulated orientation-field-based phase-field models (termed as KWC model and HMP model) to study polycrystalline solidification. First, we studied the grain coarsening process including the determination of the limiting grain-size distribution and compared the results to those from experiments on thin films to the models of Hillert and Mullins, and to predictions by multiphase-field theories. In contrast to the other models mentioned, the results of the orientation-field-based phase-field models were in agreement with the experiments. Then, as we did earlier with the KWC model, we extended the orientation field to the liquid state in the HMP model, and applied it to describe multi-dendritic solidification, polycrystalline growth, including the formation of "dizzy" dendrites disordered via the interaction with foreign particles (Fig. 2).

Figure 2. *Interaction of a growing dendrite with foreign particles represented by 'orientation pinning centers' in the HMP model. From left to right: composition, phase-field, and orientation maps.*

(2) We studied heteroepitaxy, two-step nucleation, and nucleation at the growth front within the framework of a simple dynamical density functional theory, the Phase-Field Crystal (PFC) model. We investigated the misfit dependence of the critical thickness in the Stranski-Krastanov growth mode in isothermal studies. The simulation results for stress release via the misfit dislocations fit better to the People-Bean model than to the one by Matthews and Blakeslee. Next, we investigated structural aspects of two-step crystal nucleation at high undercoolings, where an amorphous precursor forms in the first stage. Finally, we modelled the formation of new grains at the solid–liquid interface at high supersaturations/supercoolings, a phenomenon termed Growth Front Nucleation (Fig. 3).

X-ray related methods. — We have carried out X-ray diffraction experiments by inside X-ray sources. The atoms which we used as point sources were exited by a very intense focused synchrotron-generated X-ray beam. The diffraction pattern, which consists of lines (called Kossel lines) were detected by a 2D position-sensitive detector. Using the results of the dynamical diffraction of X-rays, we analyzed the line profiles of the Kossel lines and determined experimentally the phase of the structure factors of all the measured diffraction lines (Fig. 4). This opens the way to single-pulse structure determination by X-ray free-electron lasers.

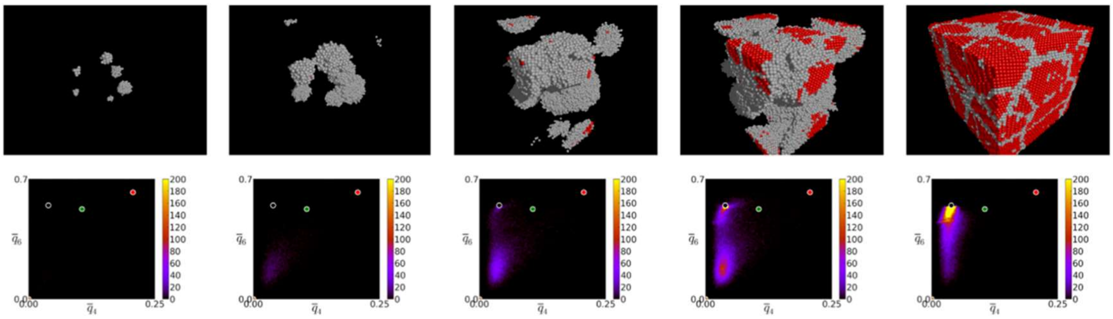


Figure 3. *Two-step nucleation in the PFC model. Time increases from left to right. Upper row: grey and red spheres corresponds to atoms with bcc-like and amorphous neighbourhood, respectively, while atoms in the liquid are transparent. Lower row: the corresponding* $\bar{q}_4$ *vs.* $\bar{q}_6$ *bond-order parameter maps. Solidification appears to start with the nucleation of amorphous domains.*

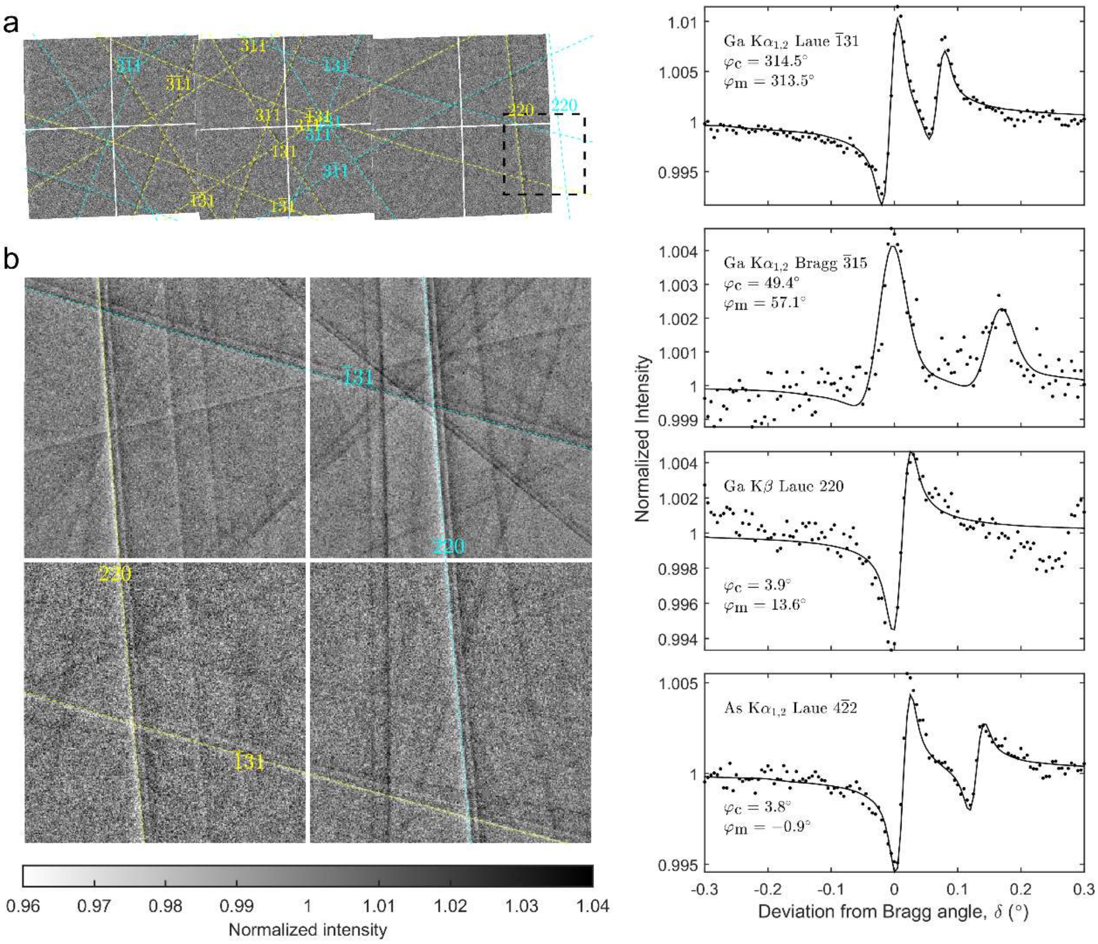


Figure 4. *Measured Kossel pattern (left panel) of GaAs. On the upper part three consecutive detector positions are shown, while in the lower part a selected region given on the upper part by the dashed rectangle. Profiles of selected Kossel lines (right panel). The fitted curves are depicted by continuous lines and the measured and theoretically calculated phases are also given in the figure.*

Grants

ESA PECS Contract No. 40000110759/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2015–2016).

ESA PECS Contract No. 40000110756/11/NL/KML: MAGNEPHAS III – Modelling of growth and transformation kinetics (L. Gránásy, 2015–2016).

EU FP7 NMP-2011-LARGE-5/280421: EXOMET – Physical processing of molten light alloys under the influence of external fields (L. Gránásy, 2012–2016).

OTKA NK- 105691, Science in nanolaboratories (K. Kamarás 2013-2017)

OTKA ANN-107580, Nanoscale investigation of molecular scaffolding (K. Kamarás 2013-2016)

OTKA K-115504. Structure determination of biological particles with X-ray free electron laser (Tegze Miklós 2015- 2019).

OTKA K-115959, Pattern formation in far-from equilibrium systems (László Gránásy, 2016–2019)

International cooperations

CNR-IMEM Institute, Parma, Prof. Cesare Frigeri

Faculty of Physics, University of Vienna, Prof. Jannik C. Meyer

Department of Chemistry, Durham University, Prof. Kosmas Prassides

Institut de Physique de la Matière Complexe, EPFL, Lausanne, Prof. László Forró

Physics of Condensed Matter Laboratory, École Polytechnique, Palaiseau, France: Mathis Plapp and Hervé Henry

Access e.V., Technical University of Aachen, Achen, Germany: Markus Apel

ELI Beamline, Prague: Andreasson Jakob, Angelov Borislav; common measurements at ESRF

Publications

Articles

1. Bortel G, Faigel G, Tegze M, Chumakov A: Measurement of synchrotron-radiation-excited Kossel patterns. ***J SYNCHROTRON RADIAT*** 23: 214-218 (2016)

2. Faigel G, Bortel G, Tegze M: Experimental phase determination of the structure factor from Kossel line profile. ***SCI REP-UK*** 6: 22904/1-8 (2016)

3. Ho PJ, Knight C, Tegze M, Faigel G, Bostedt C, Young L: Atomistic three-dimensional coherent x-ray imaging of nonbiological systems. ***PHYS REV A*** 94:(6) 063823/1-14 (2016)

4. Müller C, Németh K, Vesztergom S, Pajkossy T, Jacob T: The interface between HOPG and 1-butyl-3-methyl-imidazolium hexafluorophosphate. ***PHYS CHEM CHEM PHYS*** 18:(2) 916-925 (2016)

5. Németh G, Datz D, Tóháti HM, Pekker Á, Kamarás K: Scattering near-field optical microscopy on metallic and semiconducting carbon nanotube bundles in the infrared. ***PHYS STATUS SOLIDI B*** 253:(12) 2413-2416 (2016)

6. Oszlányi G, Sütő A: Volumic omit maps in ab initio dual-space phasing. ***ACTA CRYSTALLOGR A*** 72:(4) 480-488 (2016)

7. Parajdi-Losonczi PL, Bényei AC, Kováts É, Timári I, Muchova TR, Novohradsky V, Kasparkova J, Buglyó P: $[(\eta^6\text{-p-cymene})Ru(H_2O)_3]^{2+}$ binding capability of aminohydroxamates - A solution and solid state study. ***J INORG BIOCHEM*** 160: 236-245 (2016)

8. Pekker Á, Németh G, Botos Á, Tóháti HM, Borondics F, Osváth Z, Biró LP, Walker K, Khlobystov AN, Kamarás K: Cloaking by π-electrons in the infrared. ***PHYS STATUS SOLIDI B*** 253:(12) 2457-2460 (2016)

9. Podmaniczky F, Tóth GI, Pusztai T, Gránásy L: Investigating nucleation using the phase-field method. ***J INDIAN I SCI*** 96:(3) 161-178 (2016)

10. Quintavalle D, Márkus BG, Jánossy A, Simon F, Klupp G, Gyori MA, Kamarás K, Magnani G, Pontiroli D, Riccò M: Electronic and ionic conductivities in superionic Li_4C_{60}. ***PHYS REV B*** 93:(20) 205103/1-8 (2016)

11. Saftics A, Kurunczi S, Szekrényes Zs, Kamarás K, Khánh NQ, Sulyok A, Bősze Sz, Horvath R: Fabrication and characterization of ultrathin dextran layers: time dependent nanostructure in aqueous environments revealed by OWLS. ***COLLOID SURFACE B*** 146: 861-870 (2016)

12. Spina M, Náfrádi B, Tóháti HM, Kamarás K, Bonvin E, Gaal R, Forró L, Horváth E: Ultrasensitive 1D field-effect phototransistors: $CH_3NH_3PbI_3$ nanowire sensitized individual carbon nanotubes. ***NANOSCALE*** 8:(9) 4888-4893 (2016)

13. Tegze M, Bortel G: Coherent diffraction imaging: Consistency of the assembled three-dimensional distribution. ***ACTA CRYSTALLOGR A*** 72:(4) 459-464 (2016)

14. Toth GI: Phase-field modeling of isothermal quasi-incompressible multicomponent liquids. ***PHYS REV E*** 94:(3) 033114/1-9 (2016)

15. Tóth GI, Zarifi M, Kvamme B: Phase-field theory of multicomponent incompressible Cahn-Hilliard liquids. ***PHYS REV E*** 93:(1) 013126/1-13 (2016)

Book chapter

16. Apel M, Spatschek R, Roters F, Larsson H, Gandin C-A, Guillemot G, Podmaniczky F, Gránásy L, Schmitz GJ, Chen Q: Microstructure Modeling. In: Schmitz GJ, Prahl U (eds.): Handbook of Software Solutions for ICME. Weinheim: Wiley-VCH Verlag GmbH & Co. KGaA (ISBN:978-3-527-33902-0) pp. 269-323 (2016)

See also: S-D.1

S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Dorina Ágner, Dávid Iván[#], Kálmán Tompa[E], Francis I.B. Williams[A]

Intrinsically disordered p53 transactivation domain and its helically pre-structured segment. — The strengths of the water-protein interactions for intrinsically disordered proteins (IDPs) vary in a narrow range, and are nearer to the bulk-phase water-water interactions than to that for globular proteins (GPs, e.g. bovine serum albumin, BSA). The "surface" of IDPs is more open to the water, and the amount of the bound water molecules involved is much greater than for GPs. Wide-line ^{1}H NMR intensity and differential scanning calorimetry (DSC) measurements were carried out on the intrinsically disordered 73-residue full transactivation domain (TAD) of the p53 tumor suppressor protein and two peptides: one a wild type p53 TAD peptide with a helix pre-structuring property, and a mutant peptide with a disabled helix-forming propensity. The number of the interacting protein-water connections were quantified. The wild-type p53 TAD has a highly disordered structure as compared to BSA, a reference GP. We found the degree of disorder (being less structured) to increase as BSA < wild type full p53 TAD < wild type p53 TAD helix peptide < mutant p53 TAD peptide. The DSC measurements show the interactions of the proteins with the other solutes, especially with sodium and chloride ions. The full p53 TAD and the peptides bind a considerably greater amount of NaCl than the globular BSA. Both methods, wide-line ^{1}H-

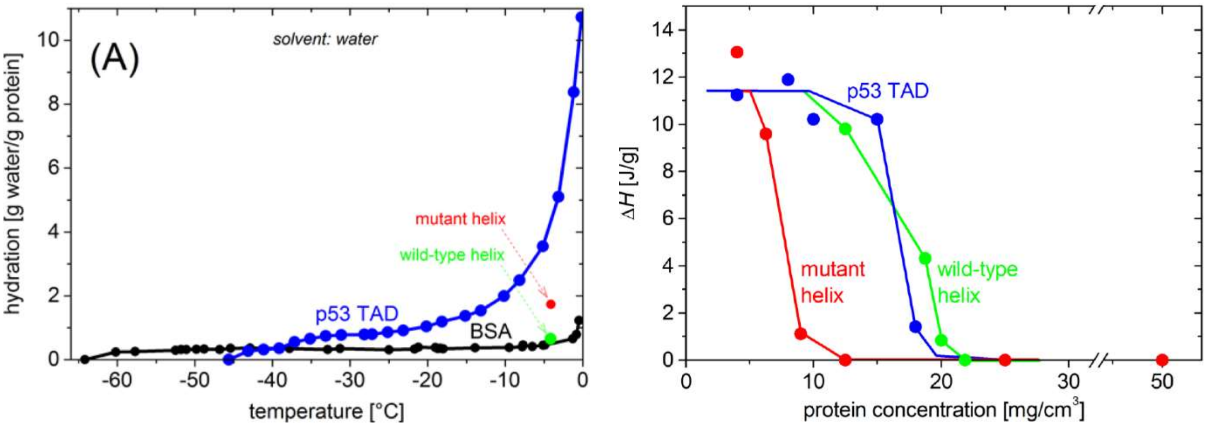


Figure 1. *Left panel: Hydration measured by the ^{1}H-NMR signal intensities of the mobile water for 50 mg/ml p53 TAD (blue) and 50 mg/ml BSA (black) dissolved in water. T = −4 °C data for the helices are shown for comparison (green and red). Right panel: Enthalpy changes associated with the eutectic melting of the H_2O-NaCl system measured as a function of protein concentration for full p53 TAD (blue), wild type p53 TAD helix peptide (green) and mutant peptide (red) dissolved in the buffer solution of 150 mM NaCl, 50 mM Tris, 1 mM EDTA, pH = 7.5. The lines are guides to the eye.*

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NMR and DSC, are not only capable of distinguishing IDPs against GPs, but are also able to differentiate two structural states of IDPs in terms of their interactions with water molecules or other chemical entities, such as salt ions (Fig. 1).

International cooperation

Joint Project supported by the Korean Research Council of Fundamental Science & Technology (KRFC) and Hungarian Academy of Sciences (Hungarian project leader: P. Tompa, Institute of Enzymology, Research Centre for Natural Sciences; participating scientists of Wigner RCP: K. Tompa, M. Bokor, 2014-2016)

Publications

Articles

1. Pisoni A, Katrych S, Arakcheeva A, Verebélyi T, Bokor M, Huang P, Gaál R, Matus P, Karpinski J, Forró L: Single crystals of superconducting SmFeAsO H_x: Structure and properties. ***PHYS REV B*** 94:(2) 024525/1-9 (2016)

2. Tompa P, Han KH, Bokor M, Kamasa P, Tantos A, Fritz B, Kim DH, Lee C, Verebélyi T, Tompa K: Wide-line NMR and DSC studies on intrinsically disordered p53 transactivation domain and its helically pre-structured segment. ***BMB REPORTS*** 49:(9) 497-501 (2016)

S-H. Partially ordered systems

Tamás Börzsönyi, Ágnes Buka[E], Nándor Éber, Katalin Fodor-Csorba[A], Katalin Gillemot, Antal Jákli, István Jánossy[A], Péter Salamon, Ellák Somfai, Balázs Szabó[#], Tibor Tóth-Katona

Granular materials. — Grain alignment has been investigated in hopper flows using X-ray CT measurements.

The packing fraction, grain alignment, orientational order parameter, and flow field in a 3D hopper has been investigated (Fig. 1a) based on X-ray CT measurements. We analyzed subsequent clogged states for 6 materials (Fig. 1b-g) including elongated particles (pegs), lentils, and nearly spherical grains (peas). We have shown that for elongated particles the grains get ordered in the flowing parts of the silo. Similarly to the case of simple shear flows, the average orientation of the rods is not parallel to the streamlines but encloses a small angle with it. The order parameter increases as the grains travel downwards the silo and the local shear deformation grows (Fig. 1h). In most parts of the hopper, the orientational distribution of the grains did not reach the stationary orientational distribution observed for simple shear.

Modeling of soft materials. — The limit of validity of linear elasticity has been tested in athermal soft-sphere packings.

The shear response of soft solids can be described with linear elasticity, provided the applied deformation is slow and weak. However, both of these approximations break down when the material loses rigidity, such as in foams and emulsions near their jamming point. When deformations are applied too quickly, the material becomes stiffer. On the other hand, when deformations are too large, the material softens and eventually flows. Using computer simulations of athermal soft-sphere packings we identified characteristic strain and time scales that quantify the limit of validity of linear elasticity, and related these scales to changes in the microscopic contact network. Our findings indicate that the mechanical response of jammed solids are generically nonlinear and rate-dependent on experimentally accessible strain and time scales. (Fig. 1i).

Electric-field-induced patterns in nematic liquid crystals. – The effect of superimposed dc and ac applied voltages has been studied on two types of spatially periodic instabilities in nematic liquid crystals, flexoelectric domains (FD) and electroconvection (EC).

Determining the onset characteristics (threshold voltage and critical wave vector), we found that, unexpectedly, the superposition of driving with different time symmetries inhibits the pattern-forming mechanisms for FD and EC as well. As a consequence, the onset shifts to much higher voltages than the individual dc or ac thresholds. A dc-bias-induced reduction of

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the crossover frequency from the conductive to the dielectric EC regimes and a peculiar transition between two types of flexodomains with different wavelengths were detected. Independent impedance measurements have proved that the applied dc voltage component substantially affects both the electrical conductivity and its anisotropy. Taking into account the experimentally detected variations of these parameters in the linear stability analysis of the underlying nematohydrodynamic equations, a qualitative agreement with the experimental findings on the onset behavior of spatially periodic instabilities was obtained.

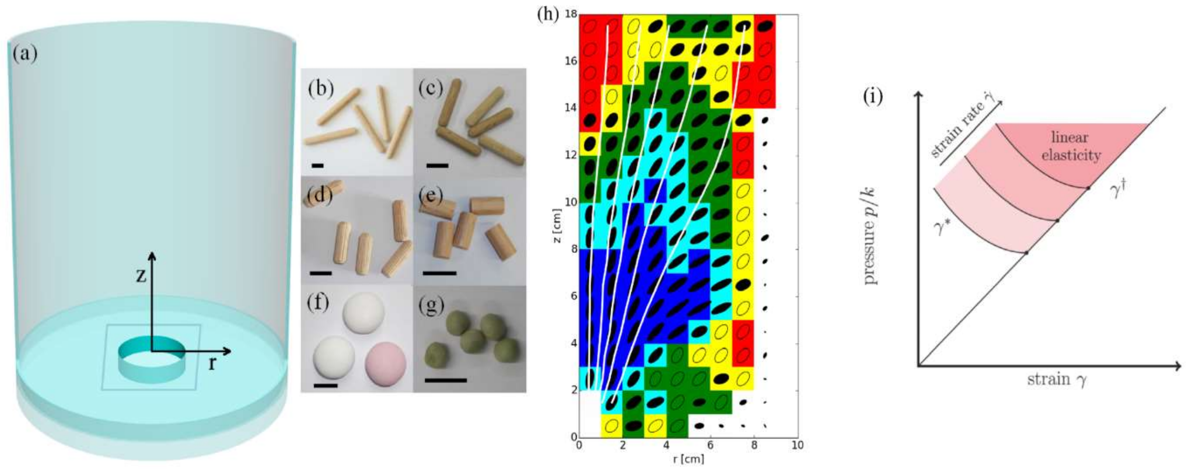

Figure 1. *(a-h) The packing and orientation of anisometric grains has been determined by X-ray CT. (i) The limits of validity of linear elasticity in athermal soft-sphere packings.*

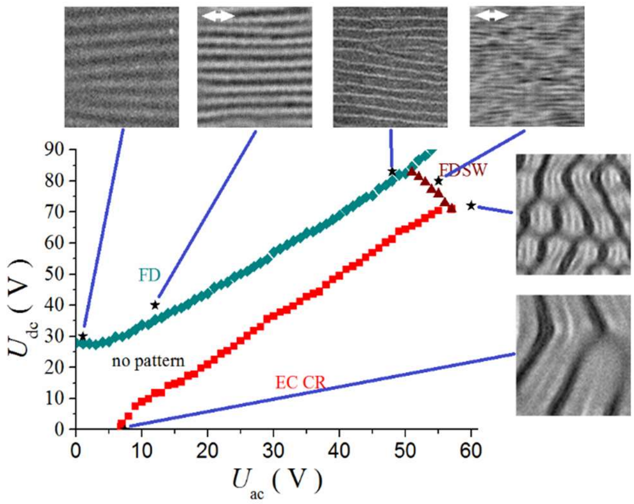

Figure 2. *Stability limit curves in the ac–dc voltage plane for the instabilities in the nematic liquid crystal 1OO8 at 5 Hz with typical pattern snapshots of 64 μm × 64 μm. FD and FDSW are flexodomains, EC CR denotes conductive regime of electroconvection.*

Carbon nanotube/epoxy composites. – The effect of temperature and filler concentration on the electrical parameters of a composite (carbon nanotubes dispersed in an epoxy matrix has been investigated).

We found that the electric and dielectric behavior of these composites follows Jonscher's universal dielectric response. The frequency dependence could be interpreted by a fractal model. The fractal dimension evaluated from the impedance data are close to that obtained by neutron scattering. The critical exponents describing the concentration dependence of the conductivity and the dielectric constant obtained in the vicinity of the percolation threshold are in good agreement with the theoretical values. The temperature coefficient of the resistivity is typically negative, except for composites with nanotube concentration exceeding the percolation threshold, where at temperatures below the glass transition a positive temperature coefficient was detected.

Synthesis of mesogenic compounds. — A series of five-ring pyridine-based bent-core compounds has been synthesized, bearing different substituents at the peripheral phenyl rings (CH_3O, Cl and NO_2). Their mesomorphic behaviour has been investigated by polarizing optical microscopy, differential scanning calorimetry and X-ray scattering, and then compared with the unsubstituted parent compound. The introduction of the methoxy groups at the peripheral phenyl rings of the bent core results in a non-mesomorphic compound, whereas the chloro- and nitro-substituted compounds form enantiotropic B1-like phases. Significant changes of the textures and transition temperatures of the mesophase have been observed under UV light indicating the possibility to design self-organized molecules suitable for UV indicators (see Figure 3.).

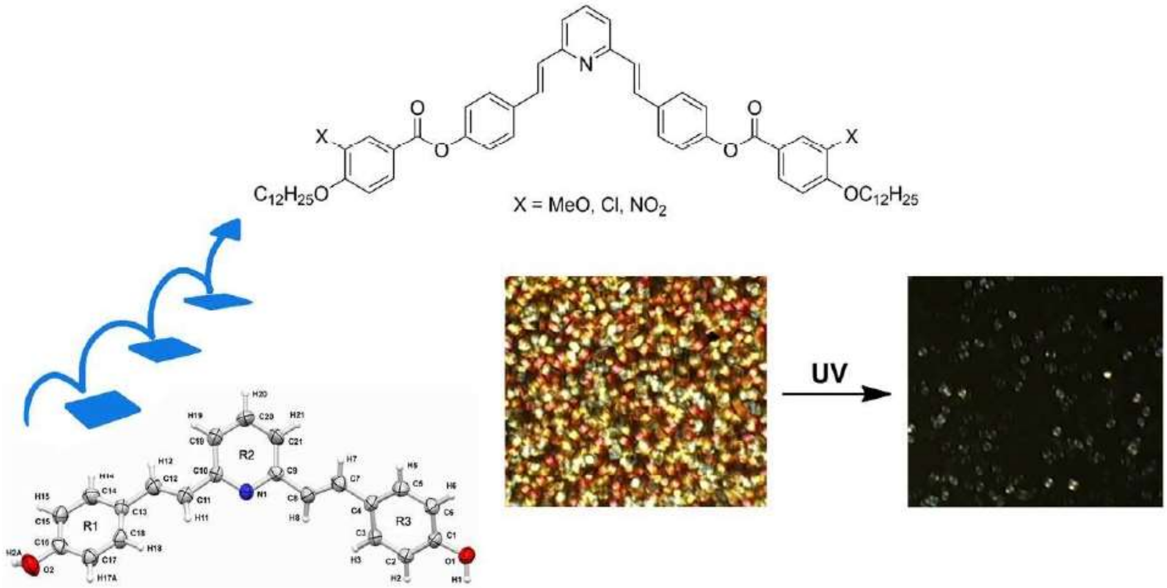

Figure 3. *Molecular structure of the synthesized pyridine-based bent-core compounds and demonstration of their sensitivity to UV light.*

Liquid crystal composite materials. — Magnetic properties of a ferronematic, i.e., a nematic liquid crystal doped with magnetic nanoparticles in low volume concentration have been studied, with the focus on the ac magnetic susceptibility. A weak dc bias magnetic field (a few Oe) applied to the ferronematic in its isotropic phase increases the ac magnetic susceptibility considerably. Passage of the isotropic-to-nematic phase transition resets this enhancement irreversibly (unless the dc bias field is applied again in the isotropic phase). A phenomenological explanation has been proposed which associates the discovered effect with the aggregation of nanoparticles in the course of the isotropic-to-nematic phase transition and their disaggregation under the influence of a dc (bias) magnetic field.

Grants

OTKA NN 107737: Anisometric granular materials (T. Börzsönyi, 2013-2016)

EU M-ERA.NET FP7 (OTKA NN 110672): Magnetically active anisotropic composite systems, (T. Tóth-Katona, 2013-2016)

OTKA K 116036: Flow and rheology of non-spherical particles (E. Somfai, 2016-2020)

International cooperation

COST Action IC1208: Integrating devices and materials: a challenge for new instrumentation in ICT (Management Committee Member: N. Éber, 2013-2017)

COST Action ES1404: A European network for a harmonised monitoring of snow for the benefit of climate change scenarios, hydrology and numerical weather prediction (Management Committee Member: K. Gillemot, 2014-2018)

Otto Von Guericke Universität Magdeburg (Magdeburg, Germany): Flow properties of suspensions and granular materials (T. Börzsönyi, 2015-2016)

Ecole Supérieure de Physique et de Chimie Industrielles de Paris (France): Rheology of elongated grains and suspensions of fibers (T. Börzsönyi, 2016-2017)

Cadi Ayyad University (Marrakech, Morocco): Composite materials from natural resources (N. Éber, 2014-2016)

Institute of Experimental Physics, SAS (Košice, Slovakia): Magnetic properties of anisotropic composite nanosystems (N. Éber, 2015-2016)

RIKEN (Wako, Japan): Creation, active control, and possible application of topological defects in advanced soft matter systems (Á. Buka, 2016-2018)

Jožef Stefan Institute (Ljubljana, Slovenia): Microfluidic systems based on anisotropic soft matter (P. Salamon, 2016-2018)

Publications

Articles

1. Antanasijević J, Antanasijević D, Pocajt V, Trišović N, Fodor-Csorba K: A QSPR study on the liquid crystallinity of five-ring bent-core molecules using decision trees, MARS and artificial neural networks. ***RSC ADVANCES*** 6:(22) 18452-18464 (2016)

2. Antanasijević J, Pocajt V, Antanasijević D, Trišović N, Fodor-Csorba K: Prediction of clearing temperatures of bent-core liquid crystals using decision trees and multivariate adaptive regression splines. ***LIQUID CRYSTALS*** 43:(8) 1028-1037 (2016)

3. Boschan J, Vågberg D, Somfai E, Tighe BP: Beyond linear elasticity: Jammed solids at finite shear strain and rate. ***SOFT MATTER*** 12:(24) 5450-5460 (2016)

4. Börzsönyi T, Somfai E, Szabó B, Wegner S, Mier P, Rose G, Stannarius R: Packing, alignment and flow of shape-anisotropic grains in a 3D silo experiment. ***NEW J PHYS*** 18:(9) 093017/1-9 (2016)

5. Cvetinov M, Stojanovic M, Obadovic D, Ristic I, Vajda A, Fodor-Csorba K, Eber N: Phase behavior and molecular self-assembly of some calamitic/bent-core nematic mixtures. ***MOL CRYST LIQ CRYST*** 630:(1) 28-36 (2016)

6. Éber N, Salamon P, Buka Á: Electrically induced patterns in nematics and how to avoid

them. ***LIQ CRYST REV*** 4:(2) 101-134 (2016)

7. Éber N, Salamon P, Fekete BA, Karapinar R, Krekhov A, Buka Á: Suppression of spatially periodic patterns by dc voltage. ***PHYS REV E*** 93:(4) 042701/1-14 (2016)

8. Finger T, Von Rüling F, Lévay S, Szabó B, Börzsönyi T, Stannarius R: Segregation of granular mixtures in a spherical tumbler. ***PHYS REV E*** 93:(3) 032903/1-9 (2016)

9. Fischer D, Börzsönyi T, Nasato DS, Pöschel T, Stannarius R: Heaping and secondary flows in sheared granular materials. ***NEW J PHYS*** 18:(11) 113006/1-19 (2016)

10. Novotná V, Hamplová V, Sasnouski G, Salamon P: Lactic acid derivatives with terphenyl molecular core. ***LIQUID CRYSTALS*** 43:(9) 1251-1258 (2016)

11. Popov P, Honaker LW, Kooijman EE, Mann EK, Jákli A: A liquid crystal biosensor for specific detection of antigens. ***SENS BIOSENSING RES*** 8: 31-35 (2016)

12. Salili SM, Xiang J, Wang H, Li Q, Paterson DA, Storey JMD, Imrie CT, Lavrentovich OD, Sprunt SN, Gleeson JT, Jákli A: Magnetically tunable selective reflection of light by heliconical cholesterics. ***PHYS REV E*** 94:(4) 042705/1-5 (2016)

13. Tomašovičová N, Kováč J, Raikher Y, Éber N, Tóth-Katona T, Gdovinová V, Jadzyn J, Pinčák R, Kopčanský P: Biasing a ferronematic-a new way to detect weak magnetic field. ***SOFT MATTER*** 12:(26) 5780-5786 (2016)

14. Trišović N, Antanasijević J, Rogan J, Poleti D, Tóth-Katona T, Salamonczyk M, Jákli A, Fodor-Csorba K: Investigation of supramolecular architectures of bent-shaped pyridine derivatives: From a three-ring crystalline compound towards five-ring mesogens. ***NEW J CHEM*** 40:(8) 6977-6985 (2016)

Conference proceedings

15. Cvetinov M, Stojanovic M, Obadovic D, Vajda A, Fodor-Csorba K, Eber N: Broadening of mesophase temperature range induced by doping calamitic mesogen with banana-shaped mesogen. In: *Proc. 9th International Physics Conference of the Balkan-Physical-Union (BPU). Istambul, Turkey, 24-08-2015 – 27-08-2015*. *AIP CONF PROC* 1722: Paper 220008. 4 p. (2016)

16. Boukheir S, Achour ME, Oueriagli, Outzourhit A, Eber N, Costa LC: Effect of temperature and filler concentration on the electrical parameters of a dispersion of carbon nanotubes in an epoxy matrix. In: *Proc. 1st International Symposium on Dielectric Materials and Applications (ISyDMA 2016). Morocco: 04-05-2016 – 06-05-2016*. Materials Research Proceedings 1: pp. 45-48. (2016)

17. Éber N, Fekete B, Salamon P, Buka A, Krekhov A: Influence of DC voltage on the dielectric properties of nematics. In: *Proc. 1st International Symposium on Dielectric Materials and Applications (ISyDMA 2016). Morocco: 04-05-2016 – 06-05-2016*. Materials Research Proceedings 1: pp. 42-44. (2016)

S-I. Electrodeposited nanostructures

László Péter, Imre Bakonyi[E], Bertalan Jóni, Katalin Németh, Lajos Pogány[A], Sándor Zsurzsa[#]

Electrodeposited nanowires. — Ni-Co/Cu multilayered nanowires were fabricated by template-assisted nanowire growth in anodized aluminium oxid (AAO) membrane from an optimized aqueous electrolyte by using two-pulse plating. The segmented magnetic/non-magnetic nanowire structure was achieved during growth along the length of the nanowires. The electrodeposition parameters were set to obtain equal thicknesses of both kinds of layer with a repetition period of 10 nm. Structural characterization of the nanowires was carried out using SEM, TEM, HRTEM, SAED and EELS techniques in collaboration with the Universitat Autònoma de Barcelona, Spain.

These techniques yielded results confirming the multilayered structure of the nanowires. Figure 1 shows the TEM image of a single multilayered Ni-Co/Cu nanowire which was released from the AAO membrane by dissolving the template. An alternating dark and light layering sequence can be observed at the edges of the wire, both layer types having an approximate thickness of 5 nm. The diffraction pattern was measured by using SAED (see inset in Fig. 1) from the red rectangular area of the nanowire. After indexing the pattern, we found that both the magnetic and non-magnetic layers have an fcc structure. Furthermore, from the magnetic hysteresis loops measured on the nanowire array within the template in a VSM, with the magnetic field being parallel or perpendicular to the wire growth direction, we found a coercivity value of 118 Oe or 89 Oe, respectively.

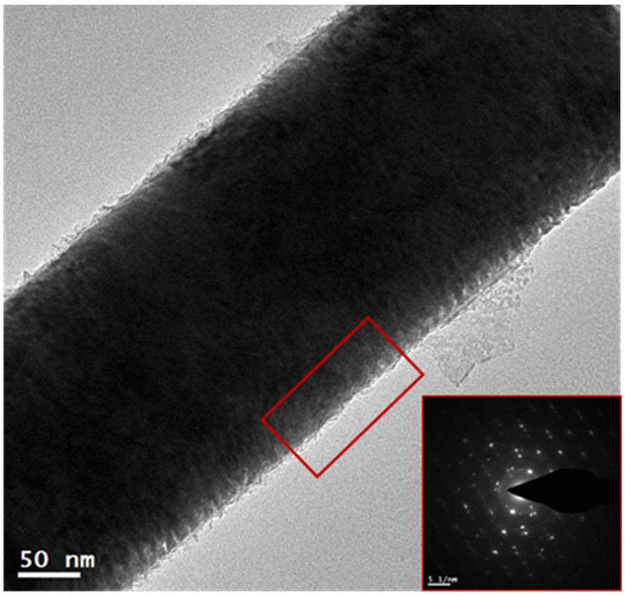

Figure 1. *TEM image of a Ni-Co/Cu multilayered single nanowire (Inset: SAED pattern of the red zone marked on the TEM image).*

Thermoelectric properties of electrodeposited multilayered nanowires. — Thermoelectric (TE) measurements have been performed on single electrodeposited nanowire samples exhibiting either the giant or the anisotropic magnetoresistance effect (GMR and AMR, respectively). The temperature-dependent (50–300 K) and magnetic field-dependent (up to 1 T) TE power factor (PF) has been determined for several Co-Ni alloy nanowires with varying Co:Ni ratios as well as for Co-Ni/Cu multilayered nanowires with various Cu layer

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[E] Professor Emeritus

[A] Associate fellow

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thicknesses, which were all synthesized via a template-assisted electrodeposition process. A systematic investigation of the resistivity as well as the Seebeck coefficient was performed for both types of nanowire samples. The TE PF was found to increase by up to 13.1 % for AMR Co-Ni alloy nanowires and by up to 52 % for GMR Co-Ni/Cu samples in an external applied magnetic field. The magnetic nanowires exhibit TE PFs that are of the same order of magnitude as TE PFs of Bi-Sb-Se-Te-based thermoelectric materials. This effect offers an opportunity to adjust the TE power output to changing loads by external magnetic fields. (These results were achieved in an international cooperation with five European partner institutes.)

Coercivity of nanoscale electrodeposited cobalt layers. — The magnetic properties and the magnetoresistance behavior were investigated for electrodeposited nanoscale Co films, Co/Cu/Co sandwiches and Co/Cu multilayers with individual Co layer thicknesses ranging from 1 nm to 20 nm. The measured saturation magnetization values supported reasonably the validity of the nominal layer thicknesses. All three types of layered structure exhibited anisotropic magnetoresistance for thick magnetic layers whereas the Co/Cu/Co sandwiches and Co/Cu multilayers with thinner magnetic layers exhibited giant magnetoresistance (GMR), the GMR magnitude being the largest for the thinnest Co layers. The decreasing values of the relative remanence and the coercive field when reducing the Co layer thickness down to below about 3 nm indicated the presence of superparamagnetic (SPM) regions in the magnetic layers which could be more firmly evidenced for these samples by a decomposition of the magnetoresistance vs. field curves into a ferromagnetic and an SPM contribution. For thicker magnetic layers, the dependence of the coercivity (H_c) on magnetic layer thickness (d) could be described for each of the layered structure types by the usual equation $H_c = H_{co} + a/d^n$ with an exponent around $n = 1$. The common value of n suggests a similar mechanism for the magnetization reversal by domain wall motion in all three structure types and hints, at the same time, at the lack of coupling between magnetic layers in the Co/Cu/Co sandwiches and Co/Cu multilayers.

Composition depth profile measurements on electrodeposited Ni-Cu/Cu multilayers. — The composition depth profile of electrodeposited Ni-Cu/Cu multilayers has been studied with Glow Discharge – Time-of-Flight Mass Spectrometry (GD-ToFMS) technique, a relatively new method that was not used before to investigate electrodeposited materials. The GD-ToFMS technique proved to be suitable to detect the layer structure and also to distinguish Ni layers with various Cu contents (8-50 at.%; see Fig. 2).

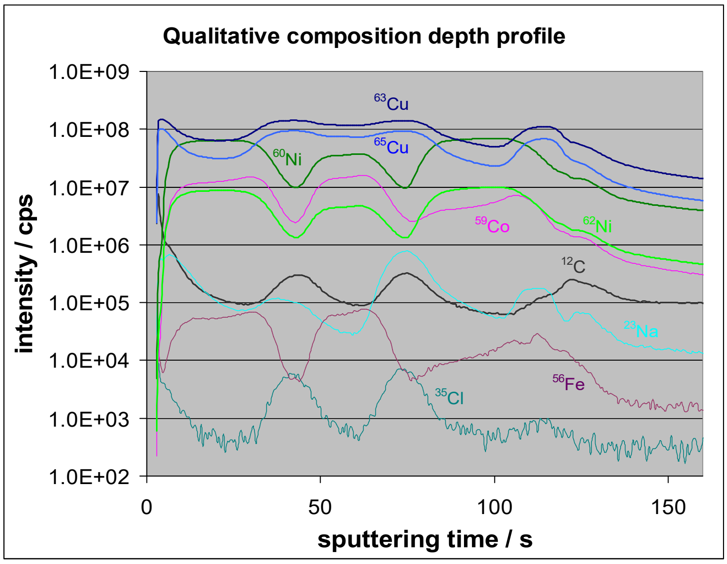

Figure 2. *Quantitative composition depth profile of an electrodeposited multilayer sample with the following nominal layer structure: Cu(20nm)/Ni-Cu-1(80nm)/Cu(80nm)/Ni-Cu-2(80nm)/Cu(80nm)/Ni-Cu-3(80nm)/Cu(20nm).*

It was found that some impurities (especially C but also Na and Cl, all originating from the components of the solution) accumulate in the Cu layer. The presence of the impurities in the Cu layer may cause a high resistivity and can yield an explanation why electrodeposited multilayers obtained from citrate baths have inferior magnetoresistance properties as opposed to nominally identical multilayers obtained from bath with no organic components. (This study was performed in co-operation with the University of Oviedo, Spain.)

Grants

OTKA K104696: Electrodeposition of special magnetic materials from non-aqueous solutions (L. Péter, 2012-2016)

International cooperation

COST Action MP1407 (17 COST and 3 non-COST countries): Electrochemical processing methodologies and corrosion protection for device and systems miniaturization: e-MINDS (Management Committee members: I. Bakonyi and L. Péter, 2015-2019)

MTA NKM-73/2016 (Hungarian-Bulgarian bilateral academic exchange project): Magnetic alloys and multilayers prepared by oscillating electrochemical reactions (Hungarian project leader: L. Péter, 2016-2018)

Publications

Articles

1. Kolonits T, Jenei P, Tóth BG, Czigány Zs, Gubicza J, Péter L, Bakonyi I: Characterization of defect structure in electrodeposited nanocrystalline Ni films. ***J ELECTROCHEM SOC*** 163: (3) D107-D114 (2016)

2. Müller C, Németh K, Vesztergom S, Pajkossy T, Jacob T: The interface between HOPG and 1-butyl-3-methyl-imidazolium hexafluorophosphate. ***PHYS CHEM CHEM PHYS*** 18: (2) 916-925 (2016)

3. Fesharaki MJ, Neuróhr K, Péter L, Révész Á, Pogány L, Molnár G, Bakonyi I: Influence of Pb additive to the spacer layer on the structure and giant magnetoresistance of electrodeposited Co/Cu multilayers. ***J ELECTROCHEM SOC*** 163: (9) D485- D492 (2016)

4. Niemann AC, Böhnert T, Michel A-K, Bäßler S, Gotsmann B, Neuróhr K, Tóth BG, Péter L, Bakonyi I, Vega V, Prida VM, Gooth J, Nielsch K: Thermoelectric power factor enhancement by spin-polarized currents - a nanowire case study. ***ADV ELECTRON MATER*** 2: (9) 1600058/1-8 (2016)

S-J. Gas discharge physics

Kinga Kutasi, Aranka Derzsi, Zoltán Donkó, Péter Hartmann, Péter Magyar[#], Pál Mezei, Károly Rózsa[A]

Gas discharge physics. – In this field, we have carried out measurements of electron transport parameters (drift velocity, longitudinal diffusion coefficient, and Townsend ionization coefficient) in different gases: argon, synthetic air, methane, deuterium as well as carbon dioxide. The experiments have been accompanied by kinetic computations based on Monte Carlo simulation of the electron transport, and solutions of the Boltzmann kinetic equation. The research on radiofrequency plasmas has focused on electronegative gases in which we have investigated the frequency dependence of the asymmetry effects, the electron power dynamics and the formation of spatial structures (“striations”). We have also addressed the origin of resonance effects in radiofrequency plasmas via particle-based simulations and developed a new, in-situ technique for the determination of secondary electron emission yields of discharge electrodes in radiofrequency plasma sources.

Strongly coupled plasmas. – In a vertically confined quasi-two-dimensional dusty plasma composed of superparamagnetic, charged dust grains and immersed in an external magnetic field B, the grains interact via both Yukawa and magnetic dipole-dipole potentials. We have analyzed the effect of the strength of the confining potential on the in-plane correlations and on the wave propagation. In addition to the in-plane compressional and transverse waves, there appears an out-of-plane transverse wave generated by the oscillation of the grains in the confining potential. The theoretical approach used the quasi-localized charge approximation paralleled by molecular dynamics simulations. The influence of an external homogeneous magnetic field on the quasilocalization of the particles in strongly coupled three-dimensional Yukawa systems was investigated via molecular dynamics computer simulations. The caging time is found to be enhanced by the magnetic field B. The anisotropic migration of the particles in the presence of magnetic field indicate a more significant increase of localization in the direction perpendicular to B, while a moderate increase is also found along the B field lines. Associating the particles’ escapes from the cages with jumps of a characteristic length, a connection is found with the diffusion process: the diffusion coefficients derived from the decay time of the directional correlation functions in both the directions perpendicular to and parallel with B are in very good agreement with respective diffusion coefficient values obtained from their usual computation based on the mean-square displacement of the particles.

Furthermore, in this field the transport (thermal conductivity) effects in strongly coupled plasmas have been investigated and quantified by molecular dynamics simulations.

High-frequency discharge systems for surface treatment. – We have determined the characteristics of the empty and loaded afterglow systems based on a flowing surface wave

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[#] Ph.D student

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microwave discharge. In this system, the discharge is generated in a 5 mm diameter tube, where due to the relatively high gas flow rate used, a pressure drop occurs along the tube. Since the surfatron used for coupling the microwave power into discharge can be moved along the tube, discharges at different pressure conditions can be generated under the same flow condition and system configuration, as illustrated in Fig. 1. Meanwhile, the length of the early-afterglow region varies with the surfatron's position, which further defines the composition of the gas entering the reactor. We have determined the effect of the surfatron position on the afterglow plasma composition entering the reactor in the case of binary and ternary mixtures. In the case of loaded systems, we determined how the pressure varies along the system when a small-diameter tube is placed into reactor and the afterglow is guided through it, and further on, how the plasma composition changes due to the pressure drops developed along the system at different flow conditions.

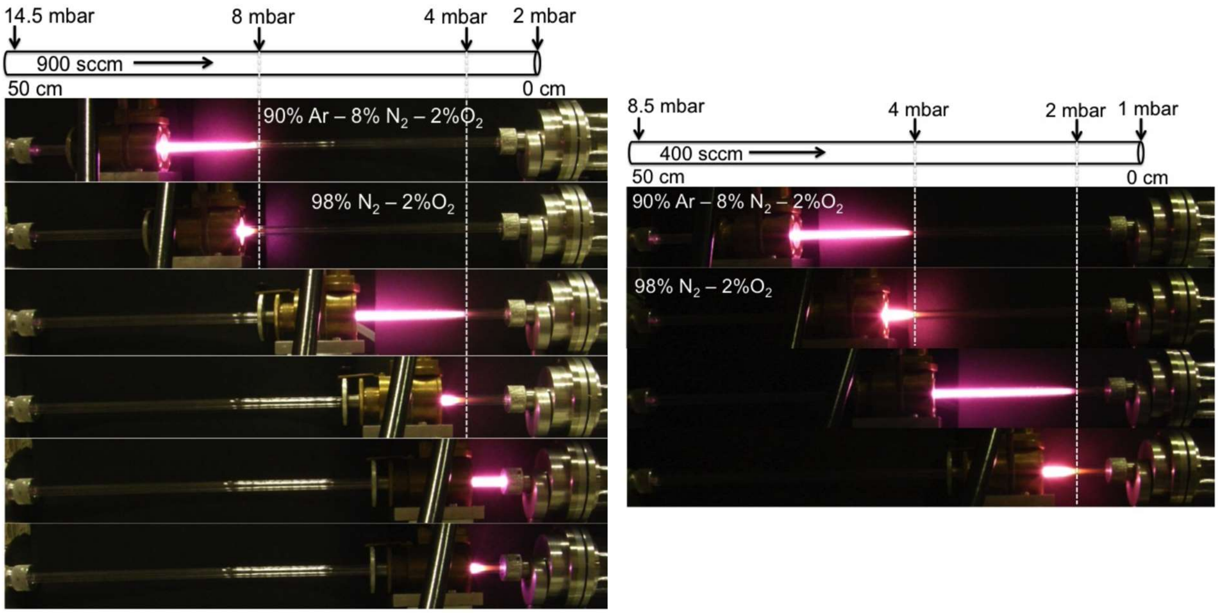

Figure 1. *Images of ternary and binary mixture discharges realized along the quartz tube at different pressures when using 900 sccm and 400 sccm gas flow rates, which yields 2 mbar and 1 mbar, respectively, in the reactor connected to the discharge tube.*

Grants:

OTKA-K-104531 High and low-frequency discharges for biomedical applications and nanostructuring (K. Kutasi 2012-2017)

OTKA K-105476 High performance modeling and simulation of low-temperature and strongly coupled plasmas (Z. Donkó, 2013-2017)

NKFIH K-119357 Non-equilibrium charged particle kinetics in ionized gases (Z. Donkó, 2016-2020)

NKFIH PD – 121033 Reactive gas discharges excited by tailored voltage waveforms (A. Derzsi, 2016-2019)

NKFIH K-115805 Complex plasmas in action (P. Hartmann, 2015-2019)

Bilateral HAS - Serbian Academy of Sciences: Interaction of non-equilibrium atmospheric pressure plasmas with model surfaces (K. Kutasi 2016-2018)

COST Action TD1208 Electrical discharges with liquids for future applications (Manager Committee Members K. Kutasi, I. Korolov 2013-2017)

International cooperation

G. J. Kalman (Boston College)

M. Bonitz (Univ. Kiel)

J. Schulze (West Virgina University, USA / Ruhr University, Bochum)

R.P. Brinkmann, T. Mussenbrock (Ruhr University, Bochum)

J.-P. Booth (Ecole Polytechnique, Paris)

Baylor University Texas

Institute of Physics Belgrade (Belgrade, Serbia), Interaction of discharge plasmas with surfaces (Zoran Lj. Petrovic, Nevena Puac)

Josef Stefan Institute Ljubljana (Ljubljana, Slovenia), Surface treatments in afterglow plasmas (Miran Mozetic)

Institut Jean Lamour Ecole des Mines Nancy (Nancy, France), Gabriel Lippmann Centre Luxembourg (Luxembourg) Elementary processes in afterglow plasmas (Thierry Belmonte, David Duday)

Publications

Articles

1. Bastykova NK, Donko Z, Kodanova SK, Ramazanov TS, Moldabekov ZA: Manipulation of dusty plasma properties via driving voltage waveform tailoring in a capacitive radiofrequency discharge. ***IEEE T PLASMA SCI*** 44:(4) 545-548 (2016). Proc. 14th Workshop on the Physics of Dusty Plasmas (WPDP). 26-05-2015 – 29-05-2015

2. Brandt S, Berger B, Schüngel E, Korolov I, Derzsi A, Bruneau B, Johnson E, Lafleur T, O'Connell D, Koepke M, Gans T, Booth J-P, Donkó Z, Schulze J: Electron power absorption dynamics in capacitive radio frequency discharges driven by tailored voltage waveforms in CF4. ***PLASMA SOURCES SCI T*** 25:(4) 045015/1-17 (2016)

3. Bruneau B, Lafleur T, Gans T, O’Connell D, Greb A, Korolov I, Derzsi A, Donkó Z, Brandt S, Schüngel E: Effect of gas properties on the dynamics of the electrical slope asymmetry effect in capacitive plasmas: comparison of Ar, H 2 and CF 4. ***PLASMA SOURCES SCI T*** 25:(1) 01LT02/1-6 (2016)

4. Bruneau B, Korolov I, Lafleur T, Gans T, O'Connell D, Greb A, Derzsi A, Donkó Z, Brandt S, Schüngel E, Schulze J, Johnson E, Booth J-P: Slope and amplitude asymmetry effects on low frequency capacitively coupled carbon tetrafluoride plasmas. ***J APPL PHYS***

119:(16) 163301/1-10 (2016)

5. Daksha M, Berger B, Schuengel E, Korolov I, Derzsi A, Koepke M, Donkó Z, Schulze J: A computationally assisted spectroscopic technique to measure secondary electron emission coefficients in radio frequency plasmas. ***J PHYS D APPL PHYS*** 49:(23) 234001/1-11 (2016)

6. Derzsi A, Lafleur T, Booth J-P, Korolov I, Donkó Z: Experimental and simulation study of a capacitively coupled oxygen discharge driven by tailored voltage waveforms. ***PLASMA SOURCES SCI T*** 25:(1) 015004/1-14 (2016)

7. Donko Z, Dyatko N: First-principles particle simulation and Boltzmann equation analysis of negative differential conductivity and transient negative mobility effects in xenon. ***EUR PHYS J D*** 70:(6) 135/1-11 (2016)

8. Dzhumagulova KN, Masheyeva RU, Ott T, Hartmann P, Ramazanov TS, Bonitz M, Donkó Z: Cage correlation and diffusion in strongly coupled three-dimensional Yukawa systems in magnetic fields. ***PHYS REV E*** 93:(6) 063209/1-7 (2016)

9. Dzhumagulova KN, Masheyeva RU, Ramazanov TS, Donkó Z: Effect of buffer gas induced friction on the caging of particles in a dusty plasma. ***CONTRIB PLASM PHYS*** 56: 215-220 (2016)

10. Gueye M, Gries T, Noël C, Migot-Choux S, Bulou S, Lecoq E, Choquet P, Kutasi K, Belmonte T: Interaction of (3-aminopropyl)triethoxysilane with pulsed Ar–O2 afterglow: application to nanoparticles synthesis. ***PLASMA CHEM PLASMA P*** 36:(4) 1031-1050 (2016)

11. Korolov I, Vass M, Bastykova NKh, Donkó Z: A scanning drift tube apparatus for spatiotemporal mapping of electron swarms. ***REV SCI INSTRUM*** 87:(6) 063102/1-7 (2016)

12. Korolov I, Vass M, Donkó Z: Scanning drift tube measurements of electron transport parameters in different gases: argon, synthetic air, methane and deuterium. ***J PHYS D*** 49:(41) 415203/1-13 (2016)

13. Korolov I, Derzsi A, Donkó Z, Schüngel E, Schulze J: The influence of electron reflection/sticking coefficients at the electrodes on plasma parameters in particle-in-cell simulations of capacitive radio-frequency plasmas. ***PLASMA SOURCES SCI T*** 25:(1) 015024/1-14 (2016)

14. Kutasi K, Noel C, Belmonte T, Guerra V: Tuning the afterglow plasma composition in Ar/N-2/O-2 mixtures: characteristics of a flowing surface-wave microwave discharge system. ***PLASMA SOURCES SCI T*** 25:(5) 055014/1-16 (2016)

15. Liu YX, Schungel E, Korolov I, Donko Z, Wang YN, Schulze J: Experimental observation and computational analysis of striations in electronegative capacitively coupled radio-frequency plasmas. ***PHYS REV LETT*** 116:(25) 255002/1-6 (2016)

16. Magyar P, Hartmann P, Kalman GJ, Golden KI, Donkó Z: Factorization of 3-point static

structure functions in 3D Yukawa liquids. ***CONTRIB PLASMA PHYS*** 56:(9) 816-829 (2016)

17. Ott T, Donkó Z, Bonitz M: The energy-autocorrelation function in magnetized and unmagnetized strongly coupled plasmas. ***CONTRIB PLASMA PHYS*** 56:(3-4) 246-252 (2016)

18. Rosenberg M, Kalman GJ, Hartmann P, Donkó Z: Waves in a quasi-two-dimensional superparamagnetic dusty plasma liquid in a trap. ***PHYS REV E*** 94:(3) 033203/1-10 (2016)

19. Schüngel E, Korolov I, Bruneau B, Derzsi A, Johnson E, O'Connell D, Gans T, Booth J-P, Donkó Z, Schulze J: Tailored voltage waveform capacitively coupled plasmas in electronegative gases: Frequency dependence of asymmetry effects. ***J PHYS J PHYS D APPL PHYS*** 49:(26) 265203/1-15 (2016)

20. Wilczek S, Trieschmann J, Eremin D, Brinkmann RP, Schulze J, Schuengel E, Derzsi A, Korolov I, Hartmann P, Donkó Z, Mussenbrock T: Kinetic interpretation of resonance phenomena in low pressure capacitively coupled radio frequency plasmas. ***PHYS PLASMAS*** 23:(6) 063514/1-9 (2016)

S-K. Liquid structure

László Pusztai, Pál Jóvári, László Kőszegi[A], György Mészáros[A], Ildikó Pethes, Szilvia Pothoczki, Erzsébet Sváb[A], László Temleitner

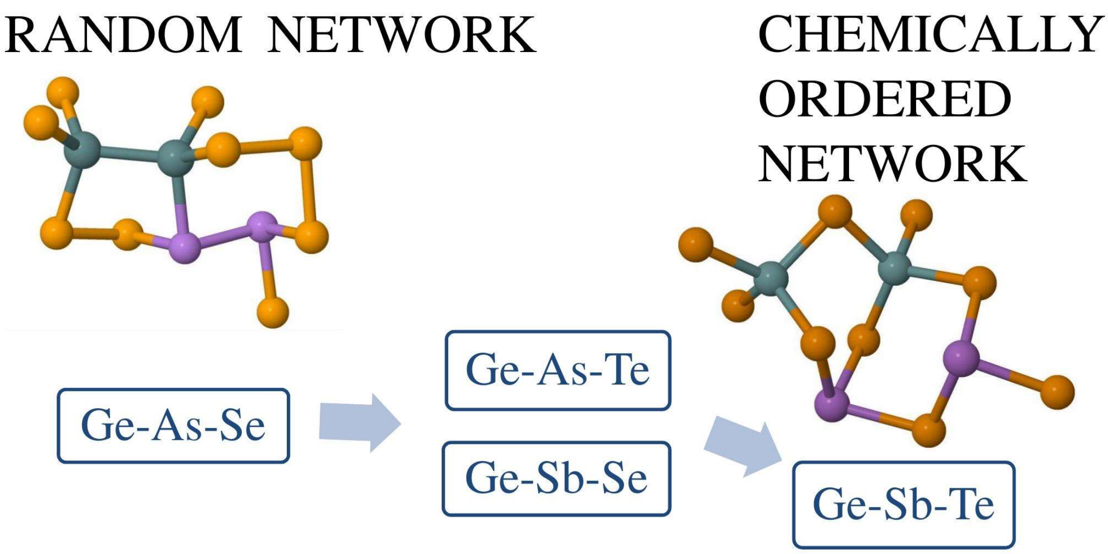

Figure 1. *Chemical ordering in ternary chalcogenide glasses increases upon substituting As*

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with Sb and Se with Te

Understanding disordered structures. — The main activity of our research group is the investigation of the microscopic structure of liquids, amorphous materials and disordered crystals. We combine experimental data, such as total scattering structure factors (TSSF) from X-ray and neutron diffraction (XRD and ND, respectively) and EXAFS spectra, with computer modeling tools, such as Reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations. As a result of such an approach, large sets (containing tens of thousands) of atomic coordinates ('particle configurations') in simulation boxes are provided that are consistent (within errors) with experimental data. These configurations are then subjected to various geometrical analyses, so that specific questions concerning the structure of a material may be answered. Below we provide some selected results from the year of 2016.

Covalent glasses. — The structure of $Ge_{20}Sb_xSe_{80-x}$ (x = 5, 15, 20) glasses was investigated by neutron and X-ray diffraction as well as EXAFS at the Ge, Sb, and Se K-edges. Large-scale structural models were obtained by fitting simultaneously the experimental data sets in the framework of the reverse Monte Carlo simulation technique. It was found that the structures of these glasses can be described mostly by the chemically ordered network model. Ge–Se and Sb–Se bonds are preferred; Se–Se bonds in the Se-poor composition (x = 20) and M–M (M = Ge, Sb) bonds in strongly Se-rich glass (x = 5) are not needed. The quality of the fits was significantly improved by introducing Ge–Ge bonding in the nearly stoichiometric composition (x = 15), showing a violation of chemical ordering. It was found that chemical short-range order of glassy chalcogenides becomes more pronounced upon substituting As with Sb and Se with Te. Ge–As–Se glasses behave as random covalent networks over a very broad composition range. Chemical short-range order and disorder coexist in both Te-rich and Te-poor Ge–As–Te glasses, whereas amorphous $Ge_{14}Sb_{29}Te_{57}$ and $Ge_{22}Sb_{22}Te_{56}$ are governed by strict chemical preferences (Fig. 1).

Molecular liquids. — Our efforts concerning the structure of *alcohol-water* liquid mixtures have been extended to aqueous solutions of *methanol* and *1-propanol*, besides those of *ethanol*. Series of MD simulations for *methanol-water* and *1-propanol-water mixtures* with 0 to 100 molar % of methanol and 1-propanol have been performed. XRD experimental data of methanol solutions could be reproduced nearly quantitatively, particularly at low and high alcohol concentrations, providing a good basis for revealing details of the atomic structure. Comparing the O — O — O angular distributions, it was shown that the H-bonded environment of water molecules is more sharply determined and is less strongly influenced by methanol concentration than the H-bonded neighborhood of methanol molecules. From detailed hydrogen bond statistical analyses, it has become apparent that as a general trend, both water and methanol molecules prefer to coordinate water molecules via H-bonding.

Metallic glasses. — The structure of $Pd_{81}Ge_{19}$ prototype metal-metalloid glass was investigated by neutron diffraction, x-ray diffraction and EXAFS at the Ge K-edge. These experimental data sets were fitted simultaneously by the RMC simulation technique. Structural information was obtained by analysing the resulting particle configurations. The cutoff distance method and the Voronoi tessellation method were used to determine the first neighbour shells of Ge and Pd atoms. It was revealed that on the average, Ge atoms are surrounded by 10.6-11 Pd atoms while the average number of Ge atoms around Ge atoms is less than 0.3. The total coordination number of Pd atoms was around 12 by the cutoff distance method and 14 by the Voronoi tessellation method. Thus, the contribution of 'distant Voronoi neighbors' to the average coordination numbers was found to be significant.

Disorder in crystals. — The pressure dependence of adsorption of argon at 77K in silicalyte-2 (MEL type) zeolite shows a substep, when the unit cell contains approximately 26-30 Ar atoms. To reveal the microscopic origin of this phenomenon, neutron powder diffraction measurements on empty, low and high Ar-loaded silicalite-2 with Ar isotopic substitution were performed, which is followed by n-RMC and Grand Canonical MC simulations. At high load, the original tetragonal symmetry of the matrix structure become distorted, the positions of argon atoms in matrix behave ordered and the atoms are linked closer to the wall of the pores in comparison with the low-load situation (Fig. 2).

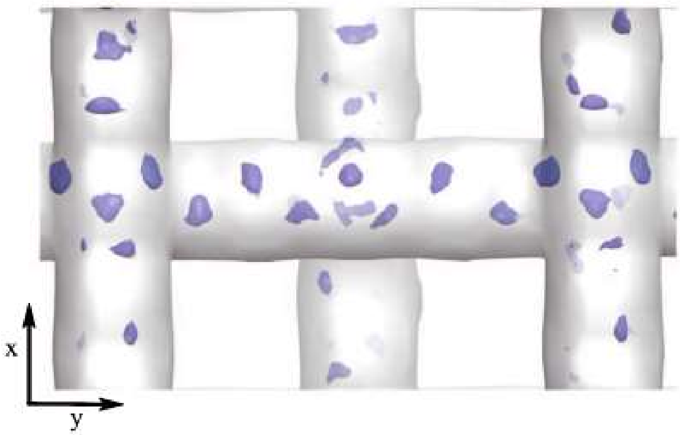

Figure 2. *Distribution of argon atoms in the channels of silicalite-2 (high-load situation)*

Grants

OTKA SNN 116198: Structure and thermodynamics of Hydrogen bonded liquids (L. Pusztai, 2016-2018)

MTA-LAS Hungarian-Latvian bilateral: X-ray Absorption Experiments for Disordered and Nanocrystalline systems: Interpereting Data via Reverse Monte Carlo Methods (L. Pusztai, 2016-2018)

TÉT_12_MX-1-2013-0003 Hungarian-Mexican bilateral (L. Pusztai, 2015-2016)

Publications

Articles

1. Babilas R, Mariola K-G, Burian A, Temleitner L: A short-range ordering in soft magnetic Fe-based metallic glasses studied by Mössbauer spectroscopy and Reverse Monte Carlo method. ***J MAGN MAGN MATER*** 406: pp. 171-178. (2016)

2. Gereben O, Pusztai L: Hydrogen bond connectivities in water-ethanol mixtures: On the influence of the H-bond definition. ***J MOL LIQ*** 220: 836-841 (2016)

3. Jóvári P, Lucas P, Yang ZY, Bureau B, Kaban I, Beuneu B, Pantalei C, Bednarčik J: On the structure of Ge–As–Te–Cu glasses. ***J NON-CRYST SOLIDS*** 433: 1-5 (2016)

4. Krezhov K, Vladikova D, Raikova G, Malakova T, Genov I, Nonova Tz, Sváb E, Fábián M: BACE0.85Y0.15O 3-δ based materials for solid oxide fuel cells: room temperature neutron diffraction study. ***RAD CONF PROC*** 1: 117-123 (2016)

5. Krezhov K, Vladikova D, Raikova G, Genov I, Malakova T, Dimitrov D, Sváb E, Fábián M: Structure study of $BaCe_{0.85}Y_{0.15}O$ (3-δ) as solid state fuel cell material. ***AIP CONF PROC*** 1722: Paper 140008/1-4 (2016). Proc. 9th International Physics Conference of the Balkan-Physical-Union (BPU). Istanbul, Turkey: 24-08-2015 – 27-08-2015

6. Méndez-Bermúdez JG, Dominguez H, Pusztai L, Guba S, Horváth B, Szalai I: Composition and temperature dependence of the dielectric constant of 1-propanol/water mixtures: Experiment and molecular dynamics simulations. ***J MOL LIQ*** 219: 354-358 (2016)

7. Pethes I, Kaban I, Stoica M, Beuneu B, Jóvári P: Chemical ordering in $Pd_{81}Ge_{19}$ metallic glass studied by reverse Monte-Carlo modelling of XRD, ND and EXAFS experimental data. ***PHYS SCRIPTA*** 91:(10) 104004/1-10 (2016)

8. Pethes I, Chahal R, Nazabal V, Prestipino C, Trapananti A, Michalik S, Jóvári P: Chemical short-range order in selenide and telluride glasses. ***J PHYS CHEM B*** 120:(34) 9204-9214 (2016)

9. Pethes I, Nazabal V, Chahal R, Bureau B, Kaban I, Belin S, Jóvári P: Local motifs in GeS_2–Ga_2S_3 glasses. ***J ALLOY COMPD*** 673: 149-157 (2016)

10. Sánchez-Gil V, Noya EG, Guil JM, Lomba E, Valencia S, Da Silva I, Pusztai L, Temleitner L: Evidence of a structural change in pure-silica MEL upon the adsorption of argon. ***J PHYS CHEM C*** 120:(4) 2260-2270. (2016)

11. Schumacher M, Weber H, Jovari P, Tsuchiya Y, Youngs TGA, Kaban I, Mazzarello R: Structural, electronic and kinetic properties of the phase-change material $Ge_2Sb_2Te_5$ in the liquid state. ***SCI REP*** 6: Paper 27434. 11 p. (2016)

12. Stunault A, Vial S, Pusztai L, Cuello GJ, Temleitner L: Structure of hydrogenous liquids: separation of coherent and incoherent cross sections using polarised neutrons. ***J PHYS CONF SER*** 711: 012003/1-5 (2016) Proc. 10th International Conference on Polarised Neutrons for Condensed MatterInvestigations (PNCMI). Sydney, Ausztrália: 2014.09.15 -2014.09.19.

13. Tscheliessnig R, Pusztai L: Proteins in solution: Fractal surfaces in solutions. ***CONDENS MATTER PHYS*** 19:(1) 13803/1-8 (2016)

Others

14. Temleitner L, Kőszegi L: Mtest diffractometer. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R, Nagy E, Rosta L, pp. 36-37 (2016)

15. Temleitner L, Pusztai L, Pothoczki Sz: Tetraéderes molekuláris folyadékok. Egyszerű anyagok, fejfájást okozó problémák (Tetrahedral molecular liquids. Simple materials, problems causing headache, in Hungarian) ***TERMÉSZET VILÁGA*** 147:(8) 346-349 (2016)

See also: S-L.1, S-L.7, S-L.11, S-L.16, S-L.17

S-L. Nanostructure research by neutron scattering

Adél Len, László Almásy, Katalin Bajnok, Margit Fábián, György Káli, Gergely Nagy, László Rosta[A], Noémi Kinga Székely, Gyula Török[A], Renáta Ünnep[#], Tamás Veres

The research group has been involved in several research projects and various user measurements performed on the neutron scattering instruments operated by the members of the Group: Small-Angle Neutron Scattering (SANS) instrument, Time-of-Flight spectrometer, Three-axis spectrometer, Reflectometer and PSD Diffractometer. Some of the results are specified below.

Estimation of out-of-plane correlation length in periodic Ni(Mo)-Ti multilayers. — Interface roughness strongly influences the reflectivity of neutron supermirrors (SM). The out-of-plane correlation of the interface roughness was studied using X-ray off-specular reflectometry in DC-sputtered periodic Ni(Mo)-Ti multilayers. Long-range roughness replication is manifested in sharp off-specular resonant diffuse scattering peaks. The finite out-of-plane correlation length leads to peak broadening. Using kinematical approach, a lower estimate of 1000, 3200 and 2800 Å out-of-plane correlation lengths was found for samples of Ni and Ti layer thickness (69, 57) Å, (96, 67) Å and (118, 85) Å, respectively. This work was made in collaboration with the Functional Nanostructures group and the Research Centre for Natural Sciences.

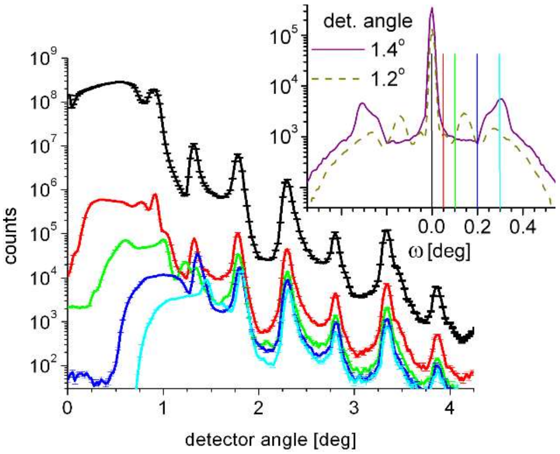

Figure 1. *Specular and off-specular X-ray $\Delta\theta$–$\Delta 2\theta$ scans (at λ = 1.54 Å) for the periodic multilayer using different offsets. The inset shows the ω-scan for detector angles 1.2° and 1.4° with the applied offset angles in the main figure.*

SANS features of thylakoid membranes of *vccn1-1* (Cl^- channel) mutant *Arabidopsis.* — The behaviour of thylakoid membranes of *vccn1-1* (Cl^- channel) mutant *Arabidopsis* plant, along with its wild types was studied by SANS. The thylakoid membranes of their leaves retained their periodic organizations: they exhibited SANS profiles with a Bragg peak at around 0.026–0.028 $Å^{-1}$. The Bragg peak of detached, infiltrated leaves from dark-adapted *vccn1-1* mutant showed a shift to higher q values as compared to the wild type. This proved to be true for the isolated thylakoid membrane from *vccn1-1* mutant: the small difference between the *vccn1-1* mutant and wild type persisted despite the shifts in the q values. These SANS measurements while showed the preservation of the regular, periodic organization of grana thylakoid membrane, revealed smaller lamellar repeat distances in *vccn1-1* mutants, indicating a somewhat

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tighter stacking and/or narrower lumen compared to the wild type – evidently due to changes in the electrostatic conditions. We also studied the differences between *vccn1-1* and wild type upon KCl and KNO_3 treatment. KCl and KNO_3 caused minor shifts in the position of Bragg peak to higher q values both in the wild type and *vccn1-1*.

Vitrification-development of glass matrices for high-level radioactive wastes. — New glassy samples suitable to retain the radionuclides, and to block access to the biosphere were successfully prepared. The atomic structure of the glasses was studied by neutron and X-ray diffraction measurements. It was established that the basic network structure consisted of tetrahedral SiO_4 units and of mixed trigonal BO_3 and tetrahedral BO_4 units which formed mixed $^{[4]}$Si-O-$^{[3]}$B, $^{[4]}$Si-O-$^{[4]}$B bond-linkages. The shortest second-neighbour distances were obtained for the Si-U and B-U pair correlation functions, indicating that U atoms could be incorporated in the matrix glass structure even when they were present with high concentration. It was shown that the stable amorphous system could incorporate maximum 40 w% high-level waste.

SANS measurements on archaeological ceramic samples from the Late Roman / Early Medieval archaeological settlement of Keszthely (Hungary) have been performed at the Yellow Submarine and FSANS instruments. A correlation between the firing temperature and the SANS curves was set up, showing that the method – as complementary to others – was suitable for analysing the high-temperature nanostructural behaviour of ceramics. No linear dependence between sizes of pores, cracks, voids and firing temperature, and no significant difference between the small-angle scattering of tempered and not tempered samples was found; however, linear dependence of exponent p (obtained from the curve fitting) on temperature was observed allowing to determine the firing temperature of the archaeological samples from Keszthely.

Polystyrene (PS) membranes modified by fullerenes and star-shaped polymers with fullerene centers (6-polystyrene-arms stars with a single C_{60}-center and double centered C_{60} fullerenes having 12 arms) were studied by SANS. The samples were saturated with D-toluene that lead to the filling of the free volume in polymers, and caused a formation of chain-like channels grouped into submicron structures. The size of a polymer segment consisting of 8 monomer units (0.3 nm) and the correlation radius of the fullerene stars (1 nm) were measured. The measurement revealed that the fullerene complex is composed of 26 segments that agrees with the functionality ($f \sim 6$) of the star/stars when its arm is composed of 4-5 segments. Data analysis using the formalism of correlation functions (Fig. 2) has revealed three structural levels, therefore the segmental size, correlation radius and the average distance between the neighboring stars were calculated. These results enabled to perform similar measurements on membranes and films modified by fullerenes and star-shaped polymers. These PS membranes are used – among others - as gas separating membranes. The filling degree was maximal for the linear polymer, and it decreased for PS with free fullerene C_{60}. In the case of a matrix composed of 6-arm polymer, the formation of fine channels having a lower total free volume was observed. Using the 12-arm stars in the matrix, the permeability became higher due to the appearance of molecular order. The simple embedding of free fullerene into PS-matrix became more homogeneous via linking the chains (van der Waals interactions). The star addition regulated the structure and migration of channels via formation of gradient regions and more pronounced short range order in the case of 12-arm stars.

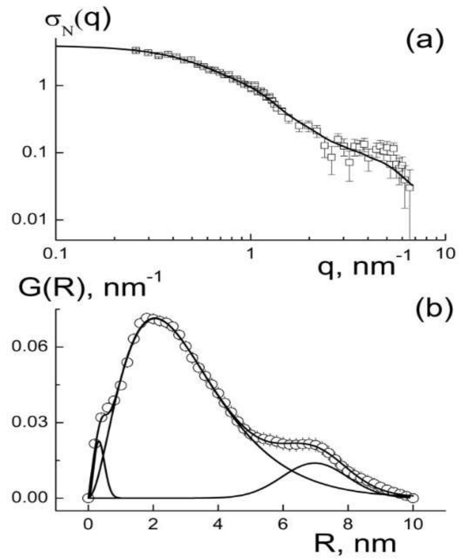


Figure 2. *The normalized coherent cross section $\sigma_N(q)$ (a) and the coherent correlation function G(R) (b). Fitting curves (a,b) and partial correlation functions (b) are shown.*

Time-of-flight neutron diffraction (TOF-ND) analysis of archaeological objects in the framework of Cultural heritage related projects – 1. Late Bronze Age defensive and offensive armors and other objects excavated from the same tomb ('Lendület' project) showed extremely homogeneous intergranular elemental distribution; the missing of texture and stress indicated that the armors were heated to high temperature together, probably during a burial rite. 2. Fragments of copper and bronze cauldrons from the Hunnic period recovered in Hungary ('Iperion') were found to be as-cast high-purity copper (with few exceptions), free from any plastic deformation. Low-bronze objects could be related to a different culture. 3. Damascus blades from the Wallace Collection ('Iperion') showed oriental distributions of the cementite grains, besides the texture and stress analyses of the ferrite phase. It was shown that high-carbon oriental blades can be divided into two groups by the methods of forging. In one type the cementite inclusions were randomly oriented while in the other the c-axis of Fe_3C crystallites were perpendicular to the plane of the blade. 4. Silver dishes related to the Seuso treasure of extremely great value can be investigated by non-destructive methods only. At first, two silver plates found in the bed of the Sava river before 1908 were studied. An earlier non-destructive elemental analysis has shown relatively strong macroscopic distribution of copper. The high-precision TOF-ND and PGAA analyses have shown that copper is homogeneously distributed in the bulk. Phase and texture analyses have been performed as well.

Grants

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

H2020-IPERION CH-2014-2015: 654028 (L. Rosta, 2015-2019)

H2020-654000, SINE2020 Science & Innovation with Neutrons in Europe in 2020 Training (L. Rosta, 2015-2019)

HAS complementary support

International cooperation

HAS Poland Academic Exchange,

HAS Romania Academic exchange, Institute of Chemistry Timisoara

TéT DST-India, Babha Atomic Research Centre, Mumbai

Publications

Articles

1. Fábián M, Sváb E, Krezhov K: Network structure with mixed bond-angle linkages in MoO_3–ZnO–B_2O_3 glasses: Neutron diffraction and reverse Monte Carlo modelling. ***J NON-CRYST SOLIDS*** 433: 6-13 (2016)

2. Petrenko VI, Avdeev MV, Bulavin LA, Almásy L, Grigoryeva NA, Aksenov VL: Effect of surfactant excess on the stability of low-polarity ferrofluids probed by small-angle neutron scattering. ***CRYSTALLOGR REP+*** 61: 121-125 (2016)

3. Putz A-M, Len A, Ianăşi C, Savii C, Almásy L: Ultrasonic preparation of mesoporous silica using pyridinium ionic liquid. ***KOREAN J CHEM ENG*** 33:(3) 749-754 (2016)

4. Pisárčik M, Pupák M, Devínsky F, Almásy L, Tian Q, Bukovský M: Urea-based gemini surfactants: Synthesis, aggregation behaviour and biological activity. ***COLLOID SURFACE A*** 497: 385-396 (2016)

5. Viani A, Sotiriadis K, Len A. Šašek P. Ševčík R: Assessment of firing conditions in old fired-clay bricks: The contribution of X-ray powder diffraction with the Rietveld method and small angle neutron scattering. ***MATER CHARACT*** 116: 33-43 (2016) doi: 10.1016/j.matchar.2016.04.003

6. Fábián M, Araczki Cs: Basic network structure of SiO 2 –B 2 O 3 –Na 2 O glasses from diffraction and reverse Monte Carlo simulation. ***PHYS SCRIPTA*** 91:(5) 054004/1-8 (2016) doi: 10.1088/0031-8949/91/5/054004

7. Fábián M, Sváb E: Formation of mixed bond-angle linkages in zinc boromolybdate glasses. ***J AM CERAM SOC*** 99:(7) 2292-2299 (2016) doi: 10.1111/jace.14233

8. Herdean A, Teardo E, Nilsson AK, Pfeil BE, Johansson ON, Ünnep R, Nagy G, Zsiros O, Dana S, Solymosi K, Garab G, Szabó I, Spetea C, Lundin B: A voltage-dependent chloride channel fine-tunes photosynthesis in plants. ***NAT COMMUN*** 7: 11654/1-11 (2016) doi: 10.1038/ncomms11654

9. Tian Q, Krakovský I, Yan G, Bai L, Liu J, Sun G, Rosta L, Chen B, Almásy L: Microstructure changes in polyester polyurethane upon thermal and humid aging. ***POLYMERS*** 8:(5) 197/1-12 (2016) doi: 10.3390/polym8050197

10. Kolokathis PD, Káli G, Jobic H, Theodorou DN: Diffusion of aromatics in silicalite-1: experimental and theoretical evidence of entropic barriers. ***J PHYS CHEM C*** 120:(38) 21410-21426 (2016) doi: 10.1021/acs.jpcc.6b05462

11. Fábián M, Sváb E, Krezhov K: Network structure of molybdate glasses by neutron and X-ray diffraction and reverse Monte Carlo modelling. ***J PHYS CONF SER*** 746:(1) 012068/1-8 (2016) doi: 10.1088/1742-6596/746/1/012068

12. Kasztovszky Zs, Káli Gy, Kis Z, Kovács I, Len A, Maróti B, Pánczél-Bajnok K, Rosta L, Szőkefalvi-Nagy Z: Applications of neutron-based and ion beam methods in Cultural Heritage research at the Budapest Neutron Centre. TECHNE SCI SERV HIST ART CIVIL

2016:(43) 70-74 (2016) http://www.ceric-eric.eu/uploads/About/CERICbrochurePFs.pdf

13. Rogante M, Rosta L: Feasibility study for neutron beam investigation of the Turin Shroud. INT J NEW TECH RES 2:(3) 86-95 (2016) https://www.ijntr.org/download_data/IJNTR02030023.pdf

Conference proceeding

14. Araczki Cs, Fábián M: Nagy aktivítású radioaktív hulladékok kondicionálása és atomi szintű szerkezetvizsgálata (Conditioning of HLW and their basic atomic structure, in Hungarian). In: Őszi Radiokémiai Napok 2016, Budapest, Ed.: Szentmiklósi László, Magyar Kémikusok Egyesülete (2016) pp. 89-90

Book, book chapters

15. Baranyi R; Nagy E; Rosta L (eds.): Progress Report on the activities at the Budapest Research Reactor. Budapest Neutron Centre, 2016, pp. 1-200

16. Fábián M, Sváb E: Atomic structure of amorphous materials studied by neutron diffraction. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R, Nagy E, Rosta L, pp. 23-25 (2016)

17. Fábián M, Sváb E: PSD - Neutron powder diffractometer with position sensitive detectors. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R, Nagy E, Rosta L pp. 34-35 (2016)

18. Zavdoveev A, Maksakova A, Pashinska E, Varyukhtin A, Len A, Füzi J, Rosta L: Sans study of nanoscale structure of low-carbon steel after rolling with shear. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 26-29 (2016)

19. Káli Gy: TOF - High resolution time-of-flight powder diffractometer. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 38-39 (2016)

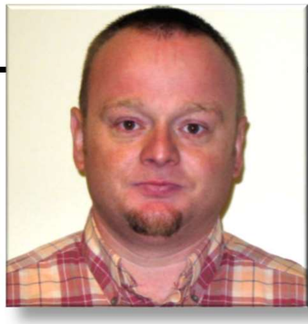
20. Almásy L, Len A, Ünnep R: YS-SANS - Small angle neutron scattering intrument yellow submarine. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 40-41 (2016)

21. Rosta L, Belgya T, Káli Gy, Kasztovszky Zs, Kis Z, Kovács I, Maróti B, Szentmiklósi L, Szőkefalvi-Nagy Z, Jambon A, Rehren T: "Beads from Heaven" - Neutron techniques reveal five-thousand-year-old iron smithing skills. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 14-18 (2016)

22. Hnatowicz V, Kasztovszky Zs, Kucera J, Macková A, Rosta L: Neutron beam analytical methods. In: *Nuclear Physics for Cultural Heritage,* eds.: Mackova A, MacGregor D, Azaiez F, Nyberg J, Piasetzky E, European Physical Society (EPS), Mulhouse (2016) pp. 23-29 doi: 10.1071/978-2-7598-2091-7_5

See also: S-K.4, S-K.5, S-M.2, S-M.7

S-M. Neutron optics



Zoltán Imre Dudás, János Füzi, Zoltán László[#], Márton Markó, Ferenc Mezei[E], Alex Szakál[#]

Neutron instrumentation development. — Members of the group accomplished the development of an energy-selective neutron imaging set-up for the investigation of the cold neutron moderator and beam extraction optics of the Budapest Research Reactor in the frame of the BrightnESS Horizon2020 project. This implied removal of a guide section, development of a dedicated chopper, detector and enforcement of shielding. The experience thus gained is employed in the design of a similar test beamline at ESS. In the frame of the same project, a multiblade solid boron converter neutron detector has been developed at ESS and thoroughly tested for efficiency and resolution on a cold neutron beamline at BNC.

The researchers of the Neutron Spectroscopy Department take part in the design of the neutron guide system of the macromolecular time-of-flight neutron diffractometer (NMX) going to be built at the European Spallation Source (ESS) in Lund, Sweden. The NMX will be the first TOF protein neutron diffractometer in the world. The source-sample distance is 157.5 m, the maximal beam size is 5 mm and the maximal needed divergence is 0.4 degree. The original guide system of NMX was simple, it had a short curved part and a straight section till the sample. Due to the decrease of the source size, this guide did not provide enough neutrons at the sample. The main difficulties of the design are the robustness of the guide system against floor movement, alignment accuracy and waviness of the mirrors, the need for decreasing the shielding cost, i.e., decreasing the number of neutrons within the guide while the intensity at the sample does not decrease, and that the neutron guide shall go out of line of sight within the first 24.5 m to avoid the fast neutrons going through the wall of the biological shielding. To solve these problems, we developed new methods for calculation of the robustness. We designed a new kind of guide system which produces a wide beam with low divergency within a short length meanwhile it goes out of the line of sight. The beam at the bunker wall has 0.1 degree divergence and its size is 4.5 cm in each direction. This beam is transported by a straight guide until the focusing part. We chose a parabolic focusing which focus the parallel beam to the sample which is also not used in the case of neutrons. This focusing solution increases the guide robustness against angular misalignment and waviness. The new solution increased the number of neutrons reaching the sample both because of the increased robustness and due to the better optimization possibilities meanwhile the total intensity in the guide decreased by one and a half order of magnitude, thus the needed shielding size decreased by a factor of two. The final decision on the guide system and also the publication of the results will be in 2017.

Neutron holography. — Research on the methodology and applications of atomic resolution neutron holography has been continued. The local structure of a Sn single crystal with Cd

[#] Ph.D student

[E] Professor Emeritus

impurities was reconstructed and the distortions of the crystal structure around the impurity atom was discussed. It was found that the effect of the different interatomic potentials around the impurity atoms has to be included beside the Friedel oscillation of the conduction electrons to fit the model to the measured distortions. For the first time, 3D displacements of atoms were measured showing the tendency of the local structure changing to the white-tin phase stable at lower temperatures

Structural investigation of hybrid silica gels. — Alkyl- and aryl-substituted silica gels were synthesized and characterized using complementary physicochemical methods. The silica host materials are designed to be proper host materials, for biomolecules or organic dyes, especially enzymes or porphyrins. The influence of the type and quantity of organic moiety upon the silica support physicochemical properties were studied and correlated with the optical emission property of the in situ entrapped metalloporphyrin. In every case, the samples with substituted silica support yielded higher optical emission of the porphyrin, compared to the unsubstituted case.

Grants

TÉT_13_DST-1-2013-0017 Development and technology transfer for marketable components of cold neutron moderator and beam extraction systems at advanced neutron sources (L. Rosta, 2015-2017)

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

H2020-INFRADEV-2014-2015: 654000 – SINE2020 – World class Science and Inovation with Neutrons in Europe 2020 (MTA-EK, 2015-2019)

International cooperation

European Spallation Source, Forshcungszentrum Jülich, Institute Of Chemistry of the Romanian Academy, Paul Scherrer Institut, Niels Bohr Institute, Technical University of Denmark, École polytechnique fédérale de Lausanne.

China Academy of Sciences – Institute of High Energy Physics – China Spallation Neutron Source: Neutron scattering instrumentation development for the China Spallation Neutron Source built in Dongguan.

Publications

Articles

1. Szabó Zs, Füzi J: Implementation and identification of Preisach type hysteresis models with Everett function in closed form. ***J MAGN MAGN MATER*** 406: 251-258 (2016) doi: 10.1016/j.jmmm.2016.01.027

2. Hurtony T, Szakál A, Almásy L, Len A, Kugler S, Bonyár A, Gordon P: Characterization of the microstructure of tin-silver lead free solder. ***J ALLOY COMPD*** 672: 13-19 (2016) doi: 10.1016/j.jallcom.2016.02.177

3. Groitl F, Graf D, Birk JO, Markó M, Bartkowiak M, Filges U, Niedermayer C, Rüegg C, Rønnow HM: CAMEA - A novel multiplexing analyzer for neutron spectroscopy. ***REV***

SCI INSTRUM 87:(3) 035109/1-7 (2016) doi: 10.1063/1.4943208

4. Szakál A, Markó M, Cser L: Local distortions revealed by neutron holography in SnCd0.0026 alloy. ***PHYS REV B*** 93:(17) 174115/1-6 (2016) doi: 10.1103/PhysRevB.93.174115

5. Russina M, Kemner E, Mezei F: Intra-cage dynamics of molecular hydrogen confined in cages of two different dimensions of clathrate hydrates. ***SCI REP*** 6: 27417/1-8 (2016) doi: 10.1038/srep27417

6. Tsapatsaris N, Lechner RE, Markó M, Bordallo HN: Conceptual design of the time-of-flight backscattering spectrometer, MIRACLES, at the European Spallation Source. ***REV SCI INSTRUM*** 87:(8) 085118/1-12 (2016) doi: 10.1063/1.4961569

Book chapters

7. Füzi J, Len A: FSANS - Time-of-flight small angle neutron scattering instrument. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 42-43 (2016)

8. Veres T, Cser L: REF - Cold neutron reflectometer. Progress Report on the activities at the Budapest Research Reactor, Eds.: Baranyi R; Nagy E; Rosta L pp. 44-45 (2016)

See also: S-L.18

S-N. Laser applications and optical measurement techniques

Attila Tibor Nagy, Aladár Czitrovszky**,** Kárpát Ferencz, Zoltán György Horváth[A], Péter Jani[A], Attila Kerekes[#], Szilvia Kugler, Dániel Oszetzky, Lénárd Vámos

Aerosol drug delivery/deposition in human lungs. — An optical measurement method based on laser particle counting has been developed, which can be used as a replacement of the commonly used analytical methods. A new procedure was developed based on optical image processing for the determination of the amount of deposited particles on the catch plates of cascade impactors. We utilized this method for the investigation of the effect of the humidity on the size distribution of the inhaled drug particles.

A measurement setup was built and utilized to study the temporal development of the size distribution of the generated mist of pressurized metered dose inhalers (pMDI) which influence the spatial deposition distribution of the particles in the human airways. While the pump with the flow controller generates constant flow rate in a closed loop, the breath simulator and the mixing inlet ensures realistic breathing patterns at the pMDI device. An optical particle counter (OPC) isokinetically samples particles from the main flow providing the necessary dilution to avoid coincidence of particles in the measurement volume caused by the high concentration. Measurements were performed to determine the temporal variation of the size distribution of the aerosols generated by pMDI devices and also studied the effects of the synchronization problems commonly raised during the usage of these devices.

All of the above mentioned methods have their own advantages in terms of speed and sensitivity of the measurement. The established theoretical and experimental background and the elaborated methods and tools can be used widely not only for the investigation of aerosol drug delivery, but for studying the deposition properties of natural and toxic aerosols as well.

Study of optical properties of aerosols. — Optical aerosol instrumentation was utilized to identify the sources of aerosol contamination in the air of Budapest. The results of the size distribution and absorptivity measurements show clear correlation with weather conditions, indicating the differences between the locations in the neighbourhoods.

Optical thin-film structures consisting of nanoscale laminated layers. – We have continued our research towards the development of optical thin-film structures containing nanooptically thin layers for advanced applications in laser physics and information technology.

EXMET – Interferometric measurement methods. — The Michelson-type interferometer which was developed in the previous phase of this project was utilized for plasma

[A] Associate fellow
[#] Ph.D student

diagnostics. The properties of the plasma generated in rubidium vapors by intense femtosecond laser pulses were studied using interferometry scheme in coaxial arrangement with the ionizing laser beam (Fig. 1.). This method was found to be a useful tool for laser plasma diagnostics and may complement the absorption spectroscopy methods. It can be even utilized with laser sources that produce less intense measuring beam because of the intrinsic nature of interferometry.

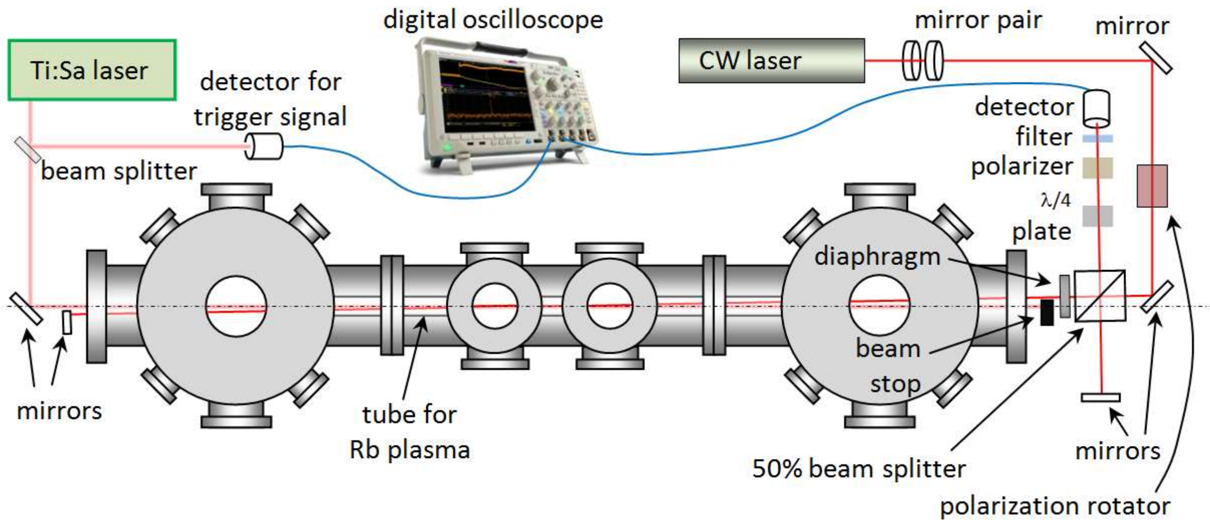


Figure 1. *Schematic measurement setup for studying the dynamics of an Rb plasma generated by ultra-short laser pulses*

Development of an imaging optical inspection device with a pinhole camera. – In cooperation with the Institute of Technical Physics and Material Sciences of Centre for Energy Research, an upgraded version of our "Imaging Optical Inspection Device With A Pinhole Camera" was developed. The aim was to increase the size of the measurable targets. It requires a significant increase of brightness of the special „point like" light source, the speed and range of precisely controlled target movement, and data processing. The unit was successfully installed in the clean-room of IISB (Erlangen, Germany). (For details see: http://www.ellipsometry.hu/)

Service laboratory for optical measurements. — We have continued the utilization of our surface profiler based on white light interferometry. We have performed aerosol measurements by optical and spectroscopic methods in the frame of academic cooperations and industrial contracts.

Grants

EAC 2011, 82013-00 European Aerosol Conference (A. Czitrovszky, 2011-2016)

EXMET 93010-15: Development of interferometric measurement methods and its applications (A. Czitrovszky, 2014- 2016)

HAS – Wigner RCP 81018-13: Infrastructural Developments, establishing a service laboratory for optical measurements (A. Czitrovszky, 2014-2015)

HION - Wigner RCP: Investigation of sampled industrial aerosols by Raman spectroscopy, optical and electron microscopy (A. Czitrovszky 2015-2016)

LASRAM - Wigner RCP: Development of medical laser systems using fibre lasers and femtoseconds pulse lasers (A. Nagy, A. Czitrovszky 2016-2018)

International cooperation

University of Vienna (Nagy Attila Tibor) – Wladyslaw Witold Szymanski, Study of optical properties of aerosols and their climate relevance with dual wavelength optical particle spectrometer

University of Vienna (Nagy Attila Tibor) – Bernadett Weinzierl, ERC A-LIFE project

Max Planck Institute of Quantum Optics (Garching, Germany) (Czitrovszky Aladár) - Ferenc Krausz, Study of ultrafast light-matter interactions.

Publications

Articles

1. Hutli E, Bonyár A, Oszetzky D, Nedeljkovic MS: Plastic deformation and modification of surface characteristics in nano and micro levels and enhancement of electric field of FCC materials using cavitaion phenomenon. ***MECH MATER*** 92: 289-298 (2016)

2. Nagy A, Czitrovszky A, Kerekes A, Veres M, Szymanski WW: Real-time determination of absorptivity of ambient particles in urban aerosol in Budapest, Hungary. ***AEROSOL AIR QUAL RES*** 16:(1) 1-10 (2016)

3. Fattahi H, Alismai A, Wang H, Brons J, Pronin O, Buberl T, Vámos L, Arisholm G, Azzeer AM, Krausz F: High-power, 1-ps, all-Yb:YAG thin-disk regenerative amplifier. ***OPT LETT*** 41:(6) 1126-1129 (2016)

4. Kerekes A, Nagy A, Veres M, Rigó I, Farkas Á, Czitrovszky A: In vitro and in silico (IVIS) flow characterization in an idealized human airway geometry using laser Doppler anemometry and computational fluid dynamics techniques. ***MEASUREMENT*** 90: 144-150 (2016)

See also: S-M.2, S-R.6

S-O. Femtosecond lasers for nonlinear microscopy

Róbert Szipőcs, Norbert Kiss#, Ádám Krolopp

Femtosecond fiber lasers for nonlinear microscopy. — During the last couple of years, we have been developing a pulsed Yb-fiber oscillator and amplifier system with a variable repetition rate in the 1 to 36 MHz range in collaboration with our industrial partner, R&D Ultrafast Laser Ltd. First we used this laser in our novel, hand-held 3D nonlinear microscope system (*FiberScope*) for applications in dermatology and nanomedicine. The laser delivers ~0.4 ps pulses at around ~1030 nm, which makes it an excellent candidate for two-photon imaging of GCaMP in neuroscience as well. GCaMP is a genetically encoded calcium indicator, and its main advantage is that it can be genetically specified for studies in living organisms. In the absence of calcium, this protein is in a poorly fluorescent state, but after Ca^{2+}-binding, it is brightly fluorescent. In Figure 1, we show 3D reconstructions of 2PE auto-fluorescence images of brain slices comprising GCaMP in its certain neurons in the "poorly fluorescent state". The high quality of the images results from the fact that our fiber laser was operated at a relatively low, ~6 MHz repetition rate.

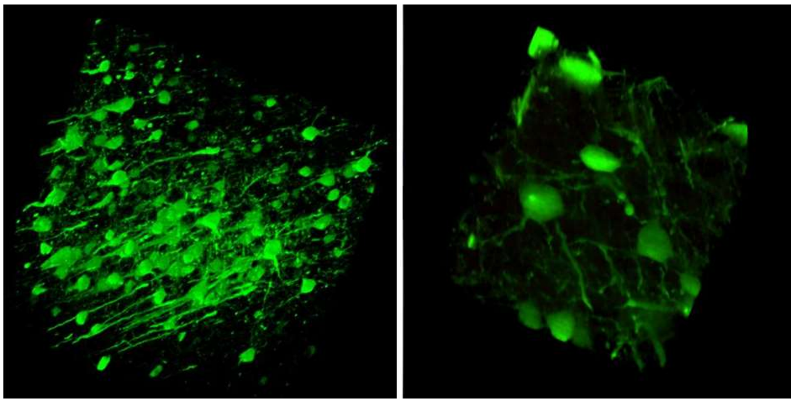


Figure 1. *2PE auto-fluorescence images of GCaMP expressing neurons excited by our mode-locked Yb-fiber laser oscillator - amplifier system operating at ~6 MHz repetition rate (central wavelength ~1030 nm, pulse duration: ~0.4 ps, average power on sample: ~14 mW). Left: 3D reconstruction of z-stack images with dimensions of 600 µm x 600 µm. Right: 3D reconstruction of z-stack images with dimensions of 50 µm x 50 µm.*

Coherent anti-Stokes Raman spectroscopy (CARS) microscopy. — Last year, CARS imaging of the CH_2 bonds of lipids was successfully used to perform a quantitative analysis of the myelin loss in a cuprizone model of sclerosis multiplex (SM) depending on the drug treatment. This year, we have aimed at label-free imaging of proteins as well as NO in living tissues, such as in murine skin or in the brain. To this end, we optimized our CARS imaging system for protein and NO detection, which required several modifications and improvement in our optics and the laser system. Note that the concentration (and hence

Ph.D student

the CARS signal) of NO is orders of magnitude smaller than that of the lipids in myelin, that is why NO imaging is a challenging task. For demonstrative purposes, we show two CARS images of murine skin recorded for “lipid” and “protein” settings (Fig. 2, left) and one CARS image of an artificial sample containing NO in a gaseous state (Fig. 2, right). In the latter experiment, NO was generated from an aqueous solvent of sodium nitroprusside (SNP) after exposing it to white light for a few tens of seconds before the imaging.

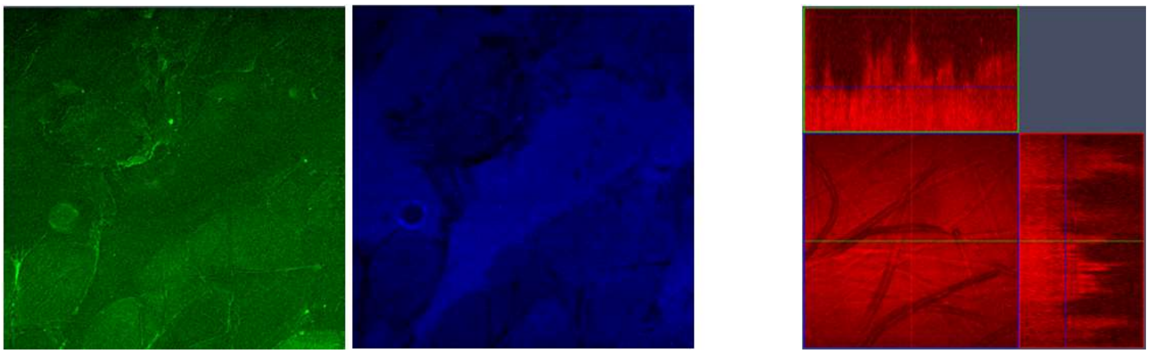


Figure 2. *Left: CARS images of the stratum corneum of murine skin for “lipid” (green) and “protein” (blue) settings. Right: CARS image of NO distribution in a SNP solvent containing artificial tissue.*

Currently, we are working on the development of more sophisticated, non-resonant background-free imaging techniques for 3D distribution detection of low-concentration molecules (e.g. NO), such as FM-CARS or our newly developed TD-CARS method.

Broadband beam steering mirrors in nonlinear microscopy. — Broadband dielectric beam steering mirrors are key components for nonlinear microscopes comprising tunable Ti:sapphire lasers. This year we characterized dispersion of a few mirror samples by spectral interferometry and showed how they affected our imaging quality. As an example, we show the measured group delay of a BB1-E03 mirror (product Thorlabs Inc.) for s- and p-polarized light (Fig. 3, up), and how it affects the pulse shape after four reflections at around a resonance wavelength (Fig. 3, down). In practice, one obtains considerably lower signal in a nonlinear microscope when the peak intensity of the optical pulses is reduced by such unexpected dispersive effects (see Fig. 3, down).

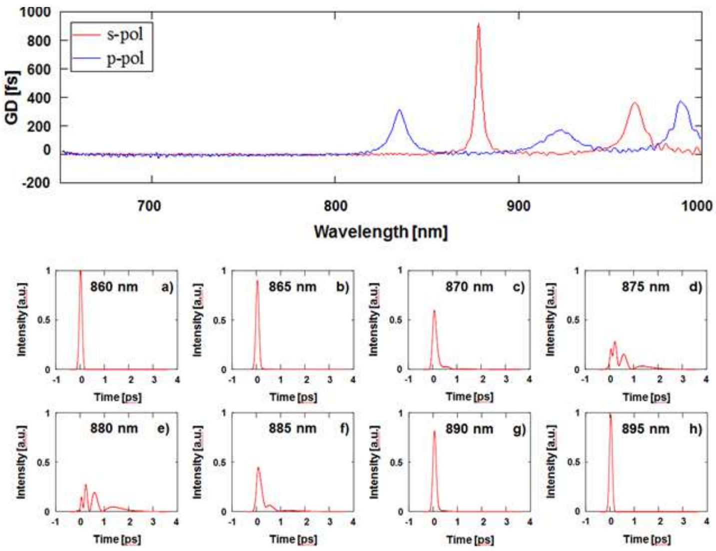


Figure 3. *Up: Measured group-delay vs. wavelength functions of an ultra-broadband dielectric mirror (two reflection, AOI: 45 degrees, Thorlabs Inc. BB1-E03). Down: Calculated intensity vs. time functions of transform limited 130 fs pulses being reflected on the same dielectric mirrors for s-polarized light at 45 degrees of AOI at different central wavelenghts.*

Grants

KTIA_13_NAP-A-I/16 National Brain Research Program, - Neuronal myelinization and nitric-oxide dynamics studied by CARS microscopy (R. Szipőcs, 2014-2017)

Publications

Articles

1. Krolopp Á, Csákányi A, Haluszka D, Csáti D, Vass L, Kolonics A, Wikonkál N, Szipőcs R: Handheld nonlinear microscope system comprising a 2 MHz repetition rate, modelocked YB-fiber laser for in vivo biomedical imaging. ***BIOMED OPT EXPRESS*** 7:(9) 3531-3542 (2016) doi: 10.1364/BOE.7.003531

2. Haluszka D, Lőrincz K, Kiss N, Szipőcs R, Kuroli E, Gyöngyösi N, Wikonkál NM: Diet-induced obesity skin changes monitored by in vivo SHG and ex vivo CARS microscopy. BIOMED OPT EXPRESS 7:(11) 4480-4489 (2016) doi: 10.1364/BOE.7.004480

Conference proceedings

3. Grósz T, Kovács AP, Szipőcs R: Ultra-broadband dielectric beam steering mirrors for in vivo nonlinear microscopy: how mirror performance affects imaging quality and laser safety issues? In: *Proc. Optical Interference Coatings 2016, 19–24 June 2016, Tucson, Arizona, United States*, OSA Washington, 2016, JTu3A.55 3 pages doi: 10.1364/OIC.2016.TB.5

4. Szipőcs R, Krolopp Á, Csákányi A, Haluszka D, Vass L, Wikonkál N: FiberScope: an optical fiber laser based, handheld 3D nonlinear microscope system for in vivo diagnostic applications in dermatology and nanomedicine. In: Proc. Biomedical Optics 2016 25 April 2016 - 28 April 2016, Fort Lauderdale, Florida, USA. OSA Washington, 2016, JTu3A.55 3 pages doi: 10.1364/CANCER.2016.JTu3A.55

S-Q. Crystal physics

László Kovács, László Bencs, Gábor Corradi[A], Gabriella Dravecz, István Földvári[A], Ivett Hajdara, Nikoletta Laczai[#], Krisztián Lengyel, Gábor Mandula, Ágnes Péter[A], Katalin Polgár[A], Zsuzsanna Szaller, Éva Tichy-Rács[#]

Crystal growth of niobates and borates. – Stoichiometric $LiNbO_3$ (sLN) crystals doped with 1-2 at% rare-earth ions (Sm^{3+}, Nd^{3+}, Yb^{3+}) have been grown by the Czochralski and the high-temperature top-seeded solution growth (HTTSSG) methods for IR spectroscopic experiments. An extra large prism (Fig. 1) has been prepared for tilted-front pumping ultra-short THz pulse generation using an sLN:Mg crystal grown by a semi-continuous feeding HTTSSG technique with a Mg-dopant concentration slightly above the photorefractive threshold. $Li_6Y_{0.99}Pr_{0.01}(BO_3)_3$ (LYB:Pr) and β-barium borate (BBO) crystals have also been grown for spectroscopic and nonlinear optical applications.

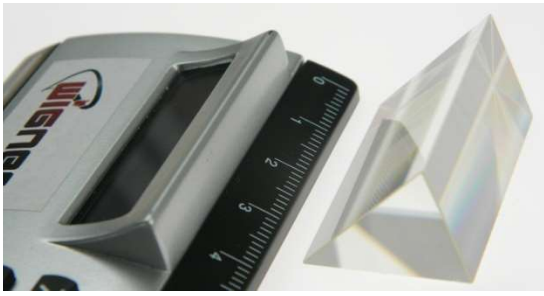


***Figure 1**. Mg-doped stoichiometric $LiNbO_3$ crystal prism prepared for high-intensity THz pulse generation.*

Characterization of polaronic distortion in $LiNbO_3$. — Polarization around trapped charges in oxides is assumed to be strongly confined but up to now experimental data on the distortion were lacking. We used a molecular probe ($OH^–$ ions) to determine the displacements of nearest-neighbour ions around $O^–$ small polarons in $LiNbO_3$ crystals created by *p*s pump pulses in the blue region. Some of the holes were temporarily trapped at oxygens in the direct vicinity of impurity $OH^–$ ions which could be detected by the absorption of probe pulses in the infrared as a transient 3 cm^{-1} redshift of the stretcing vibration frequency of part of the $OH^–$ ions. The vibration was described by a Morse potential, the adjacent polaron by point-charge potential changes caused by the trapped charge and its shifted neighbours, both modifying the Morse potential. Assuming a ~12% increase of the nearest Nb^{5+} neighbour distance from the trapping site (Fig. 2), agreement with the experimental redshift and earlier expectations could be achieved. On the other hand, assuming only a trapped hole without polaronic halo was found to result in a blueshift of the $OH^–$ frequency, contradicting experiment.

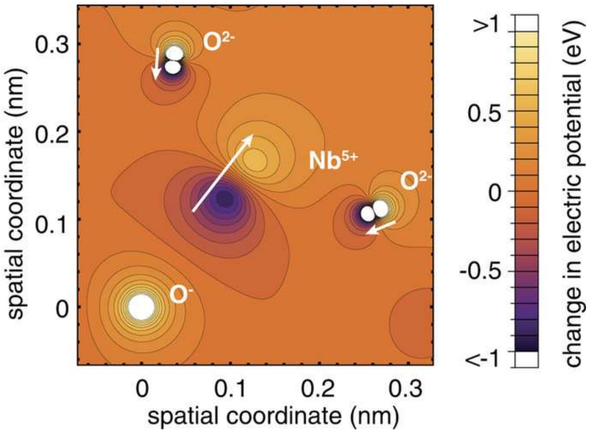


***Figure 2**. Electrostatic potential changes due to hole polaron trapping (in the origin), enlarged arrows indicating the polaronic displacements of neighbouring lattice ions.*

Spectroscopy of lithium yttrium orthoborate ($Li_6Y(BO_3)_3$, LYB) single crystals. – The electronic dipole orientation of the transition of Yb^{3+} ion pairs in 20 mol% Yb-doped LYB was shown to be parallel to the chain of rare-earth sites in the crystal lattice using high-resolution infrared absorption spectroscopy. Luminescence emission generated by coherent pair excitation has been successfully demonstrated by applying a high-intensity laser source. It was shown by SIESTA quantum-chemical calculations that the incorporation of Yb^{3+} ion pairs at nearest neighbour Y sites is energetically more favourable than for larger Yb-Yb distances. The spin-Hamiltonian tensors of isolated Yb^{3+} centres in LYB have been derived from angular dependent EPR spectra measured for 1 mol% Yb.

Using saturation spectroscopy in LYB:Er at 8 K the homogeneous linewidth, the population relaxation kinetics, and the magnetic-field-induced splitting of the spectral holes for the $^4I_{11/2}$ – $^4I_{13/2}$ – $^4I_{15/2}$ transitions of Er^{3+} ions have been determined. The sensitivity of the spectral hole distances to the external magnetic field intensity is ~20% lower in LYB:Er than found earlier in $LiNbO_3$:Er. The same splitting and sensitivity was also confirmed by using high resolution FTIR absorption spectroscopy for a magnetic induction of 120 mT.

Analytical methods for environmental and advanced materials. – Airborne particulate matter (PM) over two rural roads of Piên (South Brazil), paved with ultramafic rocks, was analysed with EPMA, XRF and XRD to characterize elemental composition and crystallinity. Single-particle compositions indicated a few percentages of serpentine and amphibole in PM. The deposition efficiency of chrysotile in two principal segments of the human respiratory system was estimated using a lung deposition model. Almost half of the inhaled particles deposited in the respiratory system. Asbestos depositions were significant (~25 %) in lower airways, even under rest situation and nose breathing.

Interaction between bovine serum albumin (BSA) and silicon carbide (SiC), investigated in nanocrystals by fluorescence spectroscopic and simulation methods, was found to be both dynamic and static. A new model was applied to describe the dynamic quenching effect with huge bimolecular quenching constants. The average binding distance between BSA and SiC was derived from the fitted model parameters and Förster's theory. Computer simulation of molecular docking identified a possible docking site of SiC in the surrounding of the tryptophan-134 residues of BSA.

High-resolution continuum-source graphite furnace atomic absorption spectrometry (HR-CS-GFAAS) methods were developed for the determination of the Al contaminant and the main component Si in SiC nanocrystals with a size-distribution of 1–8 nm dispersed in non-aqueous solution. Similar procedures starting from solid samples were optimized for the vaporization/atomization processes of Mg, evaporating lithium niobate optical single crystals doped with various amounts of Mg.

Grants

OTKA K101819: Design, fabrication and analysis of luminescent silicon carbide nanocrystals for in vivo biomarker applications (Á. Gali, participants: L. Bencs, G. Dravecz, 2012-2016)

International cooperation

Tartu University (Estonia), Spectroscopy of doped borate crystals for quantum optics and dosimetry (G. Corradi, participants: L. Kovács, K. Lengyel and É. Tichy-Rács)

Osnabrück University (Germany), Small polarons in luminescent $LiNbO_3$: From bulk to nanocrystals (Zs. Kis, participants: G. Corradi, I. Hajdara, L. Kovács, K. Lengyel, G. Mandula, L. Oláh, Zs. Szaller)

Paderborn University (Germany), Paramagnetic resonance spectroscopy of rare earth doped oxide crystals (G. Corradi)

Publications

Articles

1. Dravecz G, Bencs L, Beke D, Gali A: Determination of silicon and aluminum in silicon carbide nanocrystals by high-resolution continuum source graphite furnace atomic absorption spectrometry. ***TALANTA*** 147: 271-275 (2016) doi: 10.1016/j.talanta.2015.09.067

2. Laczai N, Kovács L, Péter Á, Bencs L: Solid sampling determination of lithium and sodium additives in microsamples of yttrium oxyorthosilicate by high-resolution continuum source graphite furnace atomic absorption spectrometry. ***SPECTROCHIM ACTA B*** 117: 8-15 (2016) doi: 10.1016/j.sab.2015.12.008

3. Lengyel K, Beregi E, Földvári I, Corradi G, Kovács L, Solarz P, Ryba-Romanowski W: Effect of symmetry reduction on the electronic transitions in polytypic GdAl3(BO3)4:Eu:Tb crystals. ***OPT MATER*** 53: 30-33 (2016) doi: 10.1016/j.optmat.2016.01.011

4. Mandula G, Kis Zs, Kovács L, Szaller Zs, Krampf A: Site selective measurement of relaxation properties at 980nm in Er^{3+} doped congruent and stoichiometric lithium niobate crystals. **APPL PHYS B-LASERS O** 122:(4) UNSP 72/1-8 (2016) doi: 10.1007/s00340-016-6341-z

5. Unferdorben M, Buzády A, Hebling J, Kiss K, Hajdara I, Kovács L, Péter Á, Pálfalvi L: Index of refraction and absorption coefficient spectra of paratellurite in the terahertz region. ***J INFRARED MILLIM TE*** 37: 703-709 (2016) doi: 10.1007/s10762-016-0261-1

6. Romet I, Aleksanyan E, Brik MG, Corradi G, Kotlov A, Nagirnyi V, Polgár K: Recombination luminescence of Cu and/or Ag doped lithium tetraborate single crystals. ***J LUMIN*** 177: 9-16 (2016) doi: 10.1016/j.jlumin.2016.04.014

7. Bridges F, Mackeen C, Kovács L: No difference in local structure about a Zn dopant for congruent and stoichiometric $LiNbO_3$. ***PHYS REV B*** 94:(1) 014101/1-5 (2016) doi: 10.1103/PhysRevB.94.014101

8. Ajtony Z, Laczai N, Dravecz G, Szoboszlai N, Marosi Á, Marlok B, Streli C, Bencs L: Fast and direct screening of copper in micro-volumes of distilled alcoholic beverages by high-resolution continuum source graphite furnace atomic absorption spectrometry. ***FOOD CHEM*** 213: 799-805 (2016) doi: 10.1016/j.foodchem.2016.06.090

9. Dravecz G, Laczai N, Hajdara I, Bencs L: Solid sampling determination of magnesium in lithium niobate crystals by graphite furnace atomic absorption spectrometry. ***SPECTROCHIM ACTA B*** 126: 1-5 (2016) doi: 10.1016/j.sab.2016.10.008

10. Freytag F, Corradi G, Imlau M: Atomic insight to lattice distortions caused by carrier self-trapping in oxide materials. ***SCI REP*** 6: 36929/1-7 (2016) doi: 10.1038/srep36929

11. Godoi RHM, Goncalves SJ, Sayama C, Polezer G, Neto JMR, Alfoldy B, Van Grieken R, Riedi CA, Yamamoto CI, Godoi AFL, Bencs L: Health implications of atmospheric aerosols from asbestos-bearing road pavements traditionally used in Southern Brazil. ***ENVIRON SCI POLLUT R*** 23:(24) 25180-25190 (2016) doi: 10.1007/s11356-016-7586-0

Article in Hungarian

12. Buzády A, Tóth Gy, Unferdorben M, Hebling J, Oláh L, Hajdara I, Kovács L, Mező E, Lemli B, Kunsági-Máté S, Pálfalvi L: Dielektromos jellemzők meghatározása a THz-es frekvenciatartományban (Determination of dielectric parameters in THz frequency region, in Hungarian). ***FIZIKAI SZEMLE*** 66:(12) 413-417 (2016)

Book chapter

13. Földvári I, Péter Á, Sujan GK: Bi_2TeO_5: growth and properties. In: Reference Module in Materials Science and Materials Engineering. Ed.: Saleem Hashmi, Elsevier, Oxford, pp. 512-515 (2016) doi: 10.1016/B978-0-12-803581-8.02394-8

WIGNER DATACENTER

Gábor Pető, Kármen Almási, Balázs Bagó, Péter Bányai, Ferenc Cseh, Artúr Dummel, Andrea Gál, Szabolcs Hernáth, Péter Horváth, Zoltán Kárpáti, Ferenc Kis, Ildikó Kovács, Miklós Madurovicz, Dezső Mihalovics, Imre Molnár, Zoltán Nagy, Szilvia Rácz, János Sajben, Domokos Szabó, Péter Szabó, Zoltán Szeleczky, Balázs Szentiványi, Gábor Szentiványi, Endre Tóth, Viktor Tóth, Ágnes Vona

The main mission of the Wigner Datacenter: acquisition and application of world-class ICT competencies and technologies; provision of sustainable, efficient and superior datacenter services to support the CERN Tier-0 and other international and domestic cutting-edge research, including direct support to the Wigner RCP and other H.A.S. research centres. Independent participation – in a sustainable way and playing a decisive role – in international and domestic research, development and innovation (R & D & I) projects that require high level, extensive IT background.

The Wigner Datacenter's (WDC) provides IT services mostly for the academic sphere. The complex, high availability infrastructure provides 1.200 m^2 white space for 3.6 MW IT load on a targeted 1.5 Power Usage Effectiveness (PUE) and is operated with a group of 25 people.

The Wigner Datacenter provides 3 different service levels based on the idea of the diversification. In frame of pure infrastructure lease for governmental purposes the National Information and Communication Services Ltd. has been the client of the Datacenter for more than 3 years. In this relationship the Datacenter's availability for 2016 is 100.00%.

In 3 IT rooms the Wigner Datacenter provides enhanced hosting services for the European Organization for Nuclear Research (CERN) to serve a significant ratio of the Tier-0 level demand of the Organization. In 2016 the availability of Wigner Datacenter in connection with this contract is 100.00%: the services provided by WDC were complied fully with the extremely rigorous SLA (Service Level Agreement) defined by CERN. In order to satisfy CERN's high expectations, the 3-people group of WDC's IT technicians has made more than 850 interventions not including the installations, cabling and network detection tasks. Although the Datacenter is interconnected with CERN's IT rooms in Geneva by two 100 Gb links, the preparatory works of a 3rd 100 Gb link were lunched in 2016.

The most value-added service of the Wigner Datacenter is providing cloud services of the academic sphere mostly in Hungary. WDC's IT engineer group consist of 5 people which is responsible for the development and IT operation of the cloud infrastructure. Meanwhile in frame of the Wigner Cloud, WDC provides IaaS exclusively for projects within Wigner RCP, the MTA Cloud operated jointly with MTA SZTAKI is open to the whole Hungarian scientific community. During the development of its whole Openstack based cloud infrastructure, the team of the Wigner Datacenter could strongly rely on the knowledge and experience originated from CERN in frame of a successful knowledge transfer.

The goal of Wigner Datacenter is not only to maintain the co-operation with CERN and serve the IT needs of the Hungarian academic sphere, but it also wishes to participate in several

R&D&I projects. To comply with this role, Wigner Datacenter complements its basic cloud services with a significant tape storage capacity and focuses on strategic level on the issue of IT security.

WIGNER GPU LABORATORY

G.G. Barnaföldi[1], D. Berényi[#1], G Bíró[#1], G. Debreczeni[A], Sz.M. Harangozó[#], M.F. Nagy-Egri[#]

The aim of the Wigner GPU Laboratory is to provide support for any fields in science in sense of parallel computing techniques, especially for faster numerical calculations in gravitational and high-energy physics, astronomy, astrophysics, material sciences, and detector simulations. We have started with GPU technologies in 2009, but later our aim was improved to any kind of parallel computing technology. Today, many- and multi-core, GPU, FPGA, Xeon Phi technologies are all available in the laboratory. Beside the academic environment and other institutes, we have connections to industrial partners as well.

Academic projects of the Wigner GPU Laboratory — A first fully GPU-based PDE-solver programme code was developed applying the spectral method. This can be used for simulating the time dependence of Wigner-functions in 3+1 D. A program code for the data analysis of the LIGO/Virgo data was written and achieved 5-10 times faster analysis compared to the original MathLab code. GPGPU techniques in Boltzmann transport model were also investigated. We are investigating the application of structural recursive schemes in automatized parallelization on CPU and on GPU platforms. Visualization for general relativity calculations on GPUs. We also take part in the GridRipper code development for gravitational-wave simualtion and detection. We also started a joint scientific work with the international VIRGO/LIGO gravitational collaboration for inestigation of the possibilities of fast, GPU-based gravitational-wave analysis technologies. Development of HIJING++ a parallel heavy-ion Monte Carlo Generator is under progress. A machine-learning code for the ALICE jet analysis is written to obtain separation of quark/gluon jets.

Accepted project proposals – The Laboratory is working on a project-basis and provide hardware/software support for the above scientific directions. Starting from 2016 we introduced the Wigner GPU Lab fellowship, which provides resources for the local computing facilities. Recently we have 11 different ongoing scientific projects, where the laboratory provides resources and techno-scientific support.

Industrial partners – This year two partnership were established: (1) We started with the Lombiq Ltd. a fruitful joint projects, getting closer science and industry. Our first collaborative efforts will be around , the tool that converts .NET software into specialized hardware, making it a lot faster and consume a lot less power. We'll test Hastlayer with highly parallelized computations of scientific models. (2) We proposed a new gene technology with Genevillage Ltd. for tumor recognition in cancer research. We also joined the Khronos Group, D. Berényi and M.F. Nagy-Egri become the advisory members.

Education, PR and future. — Connected to our group are 4 BSc and 4 MSc students.

Visitors

[1] Members also in R-B.

[#] Ph.D student

János Sztakovics (01.03–31.08.2016); Gábor Marschalkó (01.03-30.09.2016); Tamás Hajdú (01.03-31.08.2016); László Ábel Somlai (01.04–01.07.2016); Balázs Kacskovics (01.04–31.12.2016); János Endre Maróti (01.04–01.07.2016).

THE RESEARCH LIBRARY

Anikó Kutnyánszky, Szabolcs Bálint, Andrea Harsányi, Emese Szabó, Ilona Verle

The library's main task is to provide information resources and materials for the research centres and institutes of the Hungarian Academy of Sciences (HAS). Although it is jointly financed by all of the user institutes, it is developed and managed by the Wigner Research Centre.

On 31 December 2016 the stock of the library consisted of 61399 print monographs and conference proceedings, 65 electronic books with remote access, 41158 periodical issues and 40893 research reports. From the 93 newly acquired print books that were added to the collection 52 were purchased, 40 were donated and 1 item was meant for provisional deposit.

In 2016 we had a subscription for 36 print periodical titles and the issues of 7 additional titles were donated to the library. 195 electronic journals with full-text access were available for the researchers via individual subscriptions, and the library also had access to as many as 13094 online periodicals in the scientific databases sponsored by the Electronic Information Service National Programme. Two new titles were subscribed for: Radiation Research in print and online from the beginning of the year while access to the online version of Nature Photonics became available on the campus in July.

The library has its own website, where direct links are provided to the subscription-based and open access e-journals. Besides, the website serves the readers with updates on library services and the online resources, as well as information on events, free trial periods or new subscriptions and acquisitions. According to the records, the website was visited 28112 times during the year, including the number of queries in the online catalogue.

From the library stock 295 print items (books, journal issues and reports) were borrowed and the due date of 804 items was renewed by the registered users on the campus. In addition, 392 user requests were fulfilled in electronic format by the library staff downloading the online versions of articles or scanning printed materials.

Within inter-library loan services 86 library items were provided to our registered users and we successfully completed 89 document requests made by other libraries and external partners. In 2016 we had a network of 37 partner institutes in Hungary and abroad.

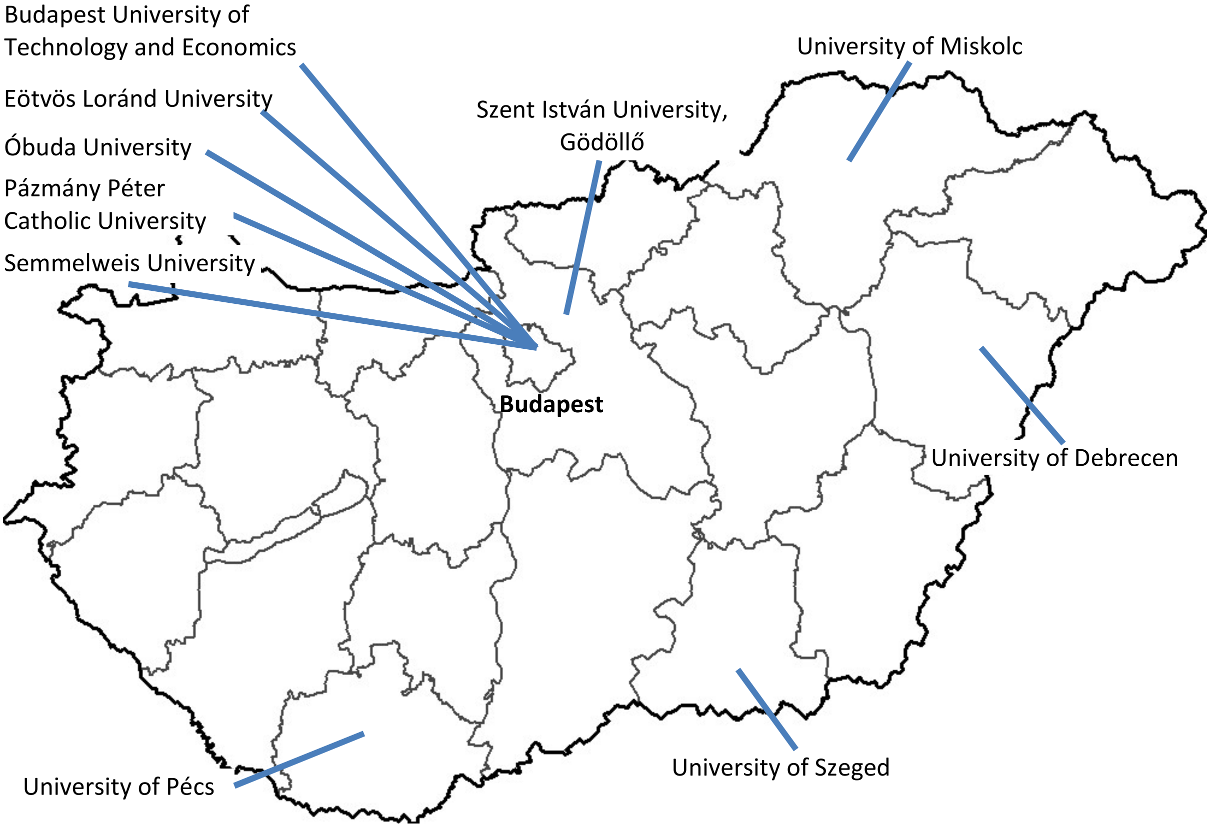
Starting with the revision of non-circulating and reference materials in the previous year, inventory was continued in 2016. The revision of the circulating books in three storages was carried out between January and November. A total of 5349 copies were sorted out from the collection, which means 8% of the total book stock. 335 of these copies were donated to other libraries, museums or archives while the rest of the sorted out materials were offered and made freely available to the employees of the institutes on the campus. Checking the stock of periodicals and the research reports published by our institute is scheduled to take part in 2017.

We went on with retrospective conversion, adding 882 records of the old stock to the online catalogue. 85 records of the new acquisitions were also created and added to the catalogue.

Members of the library team participated in 19 professional events and conferences. Like in 2015, a training session was held again in September 2016 for 15 participants to introduce young researchers to the library services, especially to the use of online resources and scientific databases.

SUPPLEMENTARY DATA

Education



Graduate and post-graduate courses

Eötvös Loránd University, Budapest

- Algebraic Bethe Ansatz and its applications (F. Woynarovich)
- Algebraic field theory I-II. (P. Vecsernyés)
- Cognitive neuroscience (L. Négyessy)
- Computational neuroscience (Z. Somogyvári)
- Conformal field theory (Z. Bajnok)
- Electrodeposition of metals (L. Péter)
- Introduction to cognitive science (P. Érdi)
- Introduction to general relativity (M. Vasúth)
- Introduction to gravitational theory and high-energy physics (G.G. Barnaföldi, M. Vasúth)
- Investigation of the inner structure of compact stars (G.G. Barnaföldi)
- Macromolecules (S. Pekker, ELTE)
- Many-body problem I-II. (G. Szirmai)
- Materials science in chemistry (L. Rosta)
- Mathematical models of the nervous system (G. Orbán)
- Nanophase metals (I. Bakonyi)
- Neural computation (BSCS[2], M. Bányai)
- Neuroinformatics (Z.Somogyvári)

[2] Budapest Semester in Cognitive Science

- Neutron physics (M. Márton)
- Nuclear solid-sate physics I-II (D.L. Nagy)
- Open quantum systems (L. Diósi)
- Optics and relativity theory (D. Varga)
- Pattern formation in complex systems (Á. Buka and T. Börzsönyi)
- Physics of jets (P. Lévai)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Physics of low temperature plasma (Z. Donkó)
- Probability theory 1-2 (M. Kornyik)
- Selected topics in experimental high-energy physics (D. Varga, F. Siklér, A.J. Zsigmond)
- Solid state physics (J. Sólyom)
- Solid state physics (MSc compulsory, I. Tüttő)
- Solid state research I-II (I. Tüttő)
- Statistical learning in the nervous system (M. Bányai, M.E. Gáspár, D.G. Nagy, G. Orbán)
- Statistical models of brain function (BSCS[1], G. Orbán)
- Superconductivity (I. Tüttő)
- The phase-structure of the strongly interacting matter (P. Lévai)
- The physics of the solar system (K. Szegő)
- Topological insulators 2. (J. Asbóth)

Budapest University of Technology and Economics

- Chapters from experimental high temperature plasma physics (G. Kocsis, T. Szepesi)
- Coherent control of quantum systems (Zs. Kis)
- Inertial confinement fusion (single lecture within the course “Introduction to the fusion plasma physics” by G. Pokol, I. Földes)
- Infrared and Raman spectroscopy (K. Kamarás)
- Interacting spin-systems in real materials (K. Penc)
- Introduction to fusion plasma physics. (S. Zoletnik)
- Introduction to theoretical plasma physics (A. Bencze)
- Introductory physics (A. Csóré)
- Ion beam analysis, part of the course Experimental methods in materials science (E. Szilágyi)
- Magnetohydrodynamics in low dimensional systems (A. Bencze)
- Mechanics I. (A. Virosztek)
- Modeling higher level brain activity (BME, Bányai, Gáspár, Nagy, Orbán)
- Modern solid state physics (A. Virosztek)
- Neutron and synchrotron radiation for condensed matter studies (L. Temleitner, L. Pusztai)
- Neutron physics (M. Márton)
- Physics of low temperature plasma (Z. Donkó)
- Quantum entanglement theory (Sz. Szalay)
- Theoretical solid state physics (A. Virosztek)
- Theory of magnetism II. (A. Virosztek)
- Spectroscopy and the structure of matter (K. Kamarás)
- Superconductivity (G. Kriza)

- Variational methods in the basic laws of physics (T.S. Biró)

Semmelweis University, Budapest

- Neocortex: from structure to function (L. Négyessy)
- Neuroelectricity (Z. Somogyvári)
- Neuroinformatics (L. Négyessy, L. Zalányi, F. Bazsó, Z. Somogyvári, M. Bányai)

Óbuda University, Budapest

- Chemistry and Physics of Polymers (S. Pekker)

Szent István University Gödöllő

- Biophysik für Tiermediziener (I.F. Barna)

University of Debrecen

- Particle Physics 1 and 2 (D. Horváth)
- Structure and Experimental Test of the Standard Model 1 and 2 (D. Horváth)

University of Pécs

- Complex examinations and methods of historical and modern curriculum of building materials - PhD lecture (A. Len)
- Control systems (J. Füzi)
- Digital control (J. Füzi)
- Electronics (J. Füzi)
- Linear algebra (I. Márton)
- Mechanics III (Dynamics) (A. Len)
- Numerical methods (P. Ádám)
- Open quantum systems (P. Ádám)
- Probability theory (B. Nagy)
- Probability theory (P. Ádám)
- Quantum information with quantum optics I-II. (T. Kiss)
- Resonant matter-light interaction (P. Ádám)
- Statistical physics (K. Szlachányi)
- Theoretical mechanics (K. Szlachányi)
- Theoretical physics III. (P. Ádám)

University of Szeged

- Analytical mechanics (L. Fehér)
- Applications of statistical physics (F. Iglói)
- Introduction to statistical physics (F. Iglói)
- Introduction to the physics of laser plasmas (I. Földes)
- Linear algebra for physicist (L. Fehér)
- Linear spaces and operators (B.G. Pusztai)
- Nuclear and particle physics 2 (L. Fehér)
- Statistical physics (F. Iglói)

- Symmetries in physics (L. Fehér)

University of Veterinary Medicine, Budapest

- Biophyics (Z. Szőkefalvi-Nagy, both in Hungarian and in English, two courses)

Laboratory practices and seminars

Eötvös Loránd University, Budapest

- Cyclotrons (A. Német)
- Elemental analysis by particle-induced X-rays emission (PIXE), extended practice for physics student (I. Kovács)
- Experiments on liquid crystals (Á. Buka, N. Éber, P. Salamon)
- Graphical processors for scientific applications (D. Berényi and M.F. Nagy-Egri)
- Laboratory course in general chemistry (G. Bazsó)
- Laboratory course in inorganic chemistry (G. Bazsó)
- Laboratory practice in solid state physics and materials science (M. Bokor)
- Magnetohydrodynamic waves, part of the course “Advanced physics laboratory” (A. Opitz)
- Materials science in chemistry Laboratory practice (L. Rosta)
- Modern physics laboratory (P. Udvarhelyi)
- NMR and Cherenkov photometry, nuclear analitics laboratory (P. Pósfay)
- Nuclear techniques for elemental analysis (RBS and ERDA), extended practice for physics student (E. Kótai, E. Szilágyi)
- Particle and nuclear physics detectors laboratory (G. Hamar, D. Varga)
- Raman spectroscopy, part of the course Laboratory practice in biophysics (M. Veres)
- The theory of C++ programming (G. Biró, Sz.M. Harangozó)

Budapest University of Technology and Economics

- Beam emission spectroscopy summer school (D. Dunai, S. Zoletnik, A. Bencze, G. Anda)
- Engineering thermodynamics 2 (R. Kovács)
- Laboratory practice (M.A. Kedves, B. Ráczkevi)
- Neutron scattering laboratory (D. Merkel)
- Infrared and Raman spectroscopy (K. Kamarás)
- Project laboratory (D. Beke)
- Thermodynamics and Heat Transfer (R. Kovács)
- Thermal physics (P. Ván)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)

University of Pécs

- Control systems (J. Füzi)
- Mathematical methods in physics IV. (P. Ádám)
- Mechanics III (Dynamics) seminar (A. Len)
- Modern physics 1 (practice) (M. Pocsai)
- Modern physics 2 (practice) (M. Pocsai)

- Statistical physics exercices (K. Szlachányi)
- Theoretical mechanics exercices (K. Szlachányi)

Semmelweis University, Budapest

- Education of medical technicians (Z. Horváth)

University of Szeged

- Analytical mechanics exercises (L. Fehér)
- Physics and biophysics laboratory practice (Zs. Kovács)
- Physics calculus for informatics engineers (Zs. Kovács)
- Physics practice for 3rd year BSc students (I. Földes)
- Statistical physics (G. Roósz)
- Symmetries in physics exercices (L. Fehér)
- Summer practice in the HILL laboratory, high intensity laser-plasma interactions (I. Földes)

Diploma works

Eötvös Loránd University, Budapest

- A. Balogh, Analyzation of gravitational waves from black hole binaries captured from open orbits (MSc, supervisor: M. Vasúth)
- Z. Bedőházi, Carrier-envelope phase changes upon ultrashort pulse propagation in dispersive media (BSc, supervisors: P. Dombi and V. Csajbók)
- D. Datz, Near-field infrared nanospectroscopy (MSc, supervisor: K. Kamarás)
- B. Hetényi, Optomechanical multistability in elasctic structures (BSc, supervisor: J. Asbóth)
- G. Kasza, Investigation of direct photon spectra and hydrodynamics modelling of high-energy heavy-ion collisions (MSc, supervisor: T. Csörgő)
- M. Lájer, A nonperturbative investigation of the 1+1 dimensional $\phi 4$ model by HIlbert space truncation (MSc, supervisor: Z. Bajnok)
- Á. Marsai, Electrodeposition of manganese-nickel alloys from methanol (BSc, supervisor: L. Péter)
- I. Nagy, Electrolytic preparation of porous aluminium oxide membranes and study of their transport properties (BSc, supervisor: L. Péter)
- B. Soós, Synchronizability and robustness of the large scale anatomical network of the Cerebral Cortex (BSc, supervisor: L. Négyessy)
- O. Surányi, Study of central exclusive processes at the CERN-CMS experiment (MSc, supervisor: F. Siklér)
- Á. Takács, Investigation of the hadronization in the non-extensive statistical approach (Supervisors: G.G. Barnaföldi and G. Papp)
- A. Timár, Properties of the diamagnetic cavity of comet 67P/Churyumov-Gerasimenko based on Rosetta measurements, (MSc, supervisor: Z. Németh)
- P. Udvarhelyi, Theoretical study of nitrogen-vacancy center near the diamond surface (MSc, supervisor: Á. Gali)

Budapest University of Technology and Economics

- Cs. Araczki, Conditioning of radioactive waste (MSc, supervisor: M. Fábián)
- D. Ágner, Temperature dependent dynamics of solid-state proteins as mirrored by their wide-line NMR spectra. (BSc, supervisors: M. Bokor and F. Simon)
- G. Balassa, Multiple scattering in high-energy geavy-ion collisions (Supervisor Gy. Wolf)
- A. Csóré, Investigation of paramagnetic point defects with quantum simulation in silicon carbide (MSc, supervisor: Ádám Gali, BME
- F. Földi, Structure study of obsidian type basalt samples (BSC, supervisor: M. Fábián)
- K. Horváth, Photostability of silicon carbide nanoclusters (BSc, supervisor: Á. Gali)
- P. Horváth, Redesigning a high temperature and high pressure measuring cell (MSC, supervisors: P. Zwierczyk and M. Fábián)
- B.A. Fekete, Patterns excited by superposition of dc and low frequency ac electric voltages in nematic liquid crystals. (MSc, supervisor N. Éber)
- Z. Herceg, Surface modification of PTFE by non-equilibrium plasma for grafting of molecules (BSc, supervisor: K. Kutasi)
- A. Késmárki, Functionalization of PMMA by cold plasma for grafting of macromolecules (BSc, supervisor: K. Kutasi)
- D. Lucsányi, Thick GEM simulations and Diamond detector development for the TOTEM experiment (MSc, supervisor: J. Sziklai)
- G. Németh: Investigation of nanostructures by near-field infrared spectroscopy (MSc, supervisor: K. Kamarás)
- Á. Schranz, Analysis of elements for low power, 850 nm, free space optical connections (MSc, supervisor: Zs. Kis)
- Zs. Szendi, Classical electrodynamics and hydrodynamics (MSc, supervisors T.S. Biró and G. Takács)
- J. Venczeli, Analysing stimuli-dependence of visual cerebral neural response-statistics (MSc, supervisor: M. Bányai)

Óbuda University, Budapest

- Á. Krolopp, Positioning the objective of the FiberScope nonlinear scanning microscope by the use of stepping motors and digital I/O signals (BSc, supervisor: R. Szipőcs)

University of Debrecen

- Á. Hunyadi, The efficiency analysis of the CMS pixel detector (MSc, supervisor: V. Veszprémi)

University of Pécs

- D. Jakab, Phases of of the low-energy Hubbard model on honeycomb lattice (Supervisor G. Szirmai)
- I. Kálmán, Optimization of periodic one photon sources by multiplexing (MSc, supervisor: P. Ádám)

University of Vienna

- F. Gesser, Normative model of episodic memory (Supervisor: G. Orbán)

Ph.D students

Eötvös Loránd University, Budapest

- K. Bajnok, 5-7th Century Pottery Production in Transdanubia (Supervisors L. Rosta, T. Vida and Gy. Szakmány)
- P. Balla, Optical properties of magnetic materials (Supervisor: K. Penc
- D. Barta, Dispersion of gravitational waves in interstellar media (Supervisor: M. Vasúth)
- Gy. Bencédi, Identification of high-momentum particles with the ALICE detector at the LHC (Supervisor: P. Lévai)
- G. Bíró, Investigation of particle production in high-energy heavy-ion collisions (Supervisors: G.G. Barnaföldi and G. Papp)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor: G. Kocsis)
- G. Csire, Quasiparticle spectrum of superconducting heterostructures (Supervisor: B. Ujfalussy)
- K.Z. Csukás, Initial value formulation of general relativity (Supervisor: I. Rácz)
- D. Datz, Chemical modification and near-field infrared microscopy of two-dimensional materials (Co-supervisor: Á. Pekker)
- A. Dombi, Quantum dynamics of atomic motion in multimode optical resonator fields (Supervisor P. Domokos)
- M. Dósa, Space weather at the inner planets (Supervisor: G. Erdős)
- T. Gombor, Holography and the gauge gravity duality, (supervisor: Z. Bajnok)
- Sz.M. Harangozó, High-momentum nuclear effects in heavy-ion collisions at CERN LHC (Supervisors: G.G. Barnaföldi and G. Papp)
- G. Homa, Quantum information and irreversibility (Supervisor: L. Diósi)
- M. Horváth, Statistical and thermodynamical studies of the strongly interacting matter (Supervisors A. Jakovác and T.S. Biró).
- Sz. Karsai, Investigation of the strongly-interacting matter in compact stars (Supervisors G.G. Barnaföldi and E. Forgács-Dajka)
- J. Konczer, Integrable methods in the AdS/CFT correspondence, (Supervisors: Z. Bajnok, Á. Hegedűs)
- B. Korbuly, Phase-field modeling of complex polycrystalline patterns (Supervisor: L. Gránásy)
- G. Kónya, Many-body physics in cavity QED (Supervisor P. Domokos)
- N. Laczai, Preparation and study of polycrystalline scintillator materials (Supervisor: L. Bencs)
- M. Lájer, Investigation of the string field theory vertex and boundary extensions of holographic dualities (Supervisors: Z. Bajnok and L. Palla)
- P. Magyar, Response functions and collective excitations of strongly coupled plasmas (Supervisor: Z. Donkó)
- K. Márton, Ultrarelativistic hadron-nucleus collisions at the CERN SPS (Supervisors: A. Laszlo and D. Varga)
- D.G. Nagy, Normative model of episodical memory (Supervisor: G. Orbán)
- M.F. Nagy-Egri, Numerical solutions of Einstein equations (Supervisor: I. Rácz)
- É. Oláh, Particle physics teaching in secondary school (within the Teacher's PhD program of ELTE, supervisors: D. Horváth and D. Varga)

- L. Oláh, Research and development of particle detectors for muon tomography and the ALICE experiment (Supervisors: G.G. Barnaföldi and D. Varga)
- P. Pósfay, Functional renormalization group method for the description of compact stars (Supervisors: G.G. Barnaföldi and A. Jakovác)
- L. Rátkai, Dynamics of crystalline self-organization within continuum theory (Supervisor: T. Pusztai)
- D. Réfy, H-mode pedestal studies with beam emission spectroscopy diagnostics (Supervisor: S. Zoletnik)
- Zs. Szendi, Hydrodynamical behavior of radiation fields (Supervisors: T.S. Biró and A. Jakovác)
- É. Tichy-Rács, Synthesis, crystallization and spectroscopic investigation of rare-earth alkali borate scintillator materials (Supervisor: K. Lengyel)
- A. Timár, Solar wind effects around a comet - investigations based on Rosetta measurements, (Supervisor: Z. Németh)
- B. Török, Learning of temporal processes (Supervisor: G. Orbán)
- M. Timár: The investigation of strongly correlated systems with renormalization methods and the approximation of high dimensional spaces with tensor factorization procedures (Supervisors Ö. Legeza, G. Barcza, ELTE)
- P. Udvarhelyi, Ab initio study of solid state quantum bits for quantum application and sensing (Supervisor: Á. Gali)
- Á. Vida, Mechanical properties of high-entropy alloys (Supervisor: L. Varga)
- A.J. Zsigmond, Measurement of Z boson production in heavy-ion collisions with the CMS detector at the LHC (Supervisors F. Siklér and G.I. Veres)
- S. Zsurzsa, Preparation and study of nanowires (supervisor: I. Bakonyi)

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- Cs. Araczki, Vitrification and structural study of high level waste produced by spent fuel reprocessing (Supervisor: M. Fábián)
- D. Beke, Synthesis and analysis of silicon carbide based nanoclusters (Supervisor: Á. Gali)
- D.R. Cserpán, Estimation of input signals based on multielectrode array measurements, (Supervisor: Z. Somogyvári)
- A. Csóré, Investigation of paramagnetic point defects in silicon carbide with quantum mechanical simulations (Supervisor: Á. Gali)
- Gy. Károlyházy, Controlled generation of point defects in silicon carbide (Supervisor: Á. Gali)
- R. Kovács, Heat conduction beyond Fourier: theories and experiments (Supervisor: P. Ván)
- M. Lampert, Turbulent and zonal flow studies in fusion plasmas (Supervisor: S. Zoletnik)
- D. Lucsányi (Supervisor: T. Csörgő)
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- G. Németh, Near-field infrared spectroscopy on two-dimensional systems (supervisor: K. Kamarás)
- F. Podmaniczky, Dynamics of solidification, pattern and defect formation in phase-field crystal theories (Supervisor: L. Gránásy)

- B. Somogyi, Semiconductor biomarkers for biological imaging: A first principles study (Supervisor: Á. Gali)
- A. Szakál, Investigation of Application Possibilities of Atomic Resolution Neutron Holography (Supervisor: L. Cser)
- T. Szarvas, Wave Propagation and Modelling of Quantum Optical Processes in Structured Dielectrics (supervisor: Zs. Kis)
- G. Thiering, Theoretical study of point defects in diamond (Supervisor: Á. Gali)
- T. Veres, Investigation of Thin Layers for Neutron Optical Applications by Neutron Reflecto-metry (Supervisor L. Cser)

Linköping University, Sweden

- V. Ivády, Investigation of point defects for quantum bit applications (Supervisor: Á. Gali)

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- D. Földes, Preparation and characterisation of new metal-organic frameworks (Supervisors: É. Kováts and S. Pekker)

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- S. Arceiz Casas: EPR characterization of crystal defects for quantum optical applications (Co-supervisor: G. Corradi)

Pázmány Péter Catholic University, Budapest

- B. Jákly, Neuromorphic robotic control based on spatio-temporal motion analysis (Co-supervisor: L. Négyessy)

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- Zs. Benkő, Causality analysis of cortical dynamical interactions based on multichannel electrode measurements (Supervisor: Z. Somogyvári)
- N. Kiss: The effects of UV-light radiation on the physiological and pathological processes of the skin, on tumour development and its control mechanisms (Supervisors: N. Wikonkál and R. Szipőcs)

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- T. Baross, The application of the Hot Isostatic Pressing (HIP) welding for fusion reactor conditions (Supervisor: G. Veres)

University of Debrecen

- Á. Hunyadi, Search for supersymmetric particles with the CMS detector at the LHC (Supervisor: V. Veszprémi)
- J. Karancsi, Search for new particles with the CMS detector at the LHC (Co-supervisor: V. Veszprémi)

University of Lund, Sweden

- A. Ster (Supervisors: B.Lörstad, L. Lönnblad and T. Csörgő)

University of Pécs

- M. Aladi, High harmonics generation from gases and clusters (Supervisor I. Földes)
- R. Bolla, Investigation of the structure of noble gas clusters from gas jets (Supervisor I. Földes)
- B. Bódi, Optimization of high harmonic generation (Supervisor: P. Dombi)
- F. Bódog, Optimization of Periodic One Photon Sources (supervisor: P. Ádám)
- V. Csajbók, Inducing ultrafast currents in dielectrics (Supervisor: P. Dombi)
- D. Jakab: Exotic phases and quantum phase transitions in many-body systems (Supervisor Z. Zimborás)
- A. Kerekes, Development and application of optical measurement methods for the investigation of the deposition of aerosols in the human airways (Supervisor: A. Nagy)
- P. Körber, Evidence of the effectiveness of masonry injections in order to install building sealings. Experimental research on bricks and masonry mortars with Scanning Electron Microscope in comparison with conventional detection methods. (Supervisors: A. Len and E.Sz. Zoltán)
- I. Márton, Ultrafast photoemission from plasmonics structures (Supervisor: P. Dombi)
- E. Molnár, Preparation of Nonclassical States by Coherent Superpositions (supervisor: P. Ádám)
- G. Mogyorósi, Preparation of Nonclassical States with Propagating Waves (supervisor: P. Ádám)
- B. Nagy, Controlling photoelectrons on the nanoscale with plasmonic nanoparticles (Supervisor: P. Dombi)
- M. Pocsai, Homogeneous rubidium plasma generation for novel particle accelerators (Supervisor: I. Barna)
- P. Sinkovicz, Simulation of quantum lattice models with ultracold gases (Supervisor G. Szirmai)
- Á. Varga, Maximal Information Quantum Measurement (supervisor: P. Ádám, J. Bergou)
- K. Varga-Umbrich: Study of coherent excitation and ionization of alkali atoms by strong laser pulses. (Supervisor M.A. Kedves)

University of Szeged

- T.F. Görbe, Integrable many-body systems of Calogero-Ruijsenaars type (Supervisor: L. Fehér)
- Zs. Kovács, Investigation of ions from the Coulomb explosion of clusters and from the TNSA acceleration of thin solid targets (Supervisor I. Földes)
- G. Roósz, Nonequilibrium relaxation in closed quantum systems (Supervisor: F. Iglói)
- H.M. Tóháti, Optical spectroscopy of carbon nanotube-based hybrid materials (Supervisor K. Kamarás)

Dissertations

Ph.D

G. Bazsó, Structural investigation of biomolecules by matrix isolation and laser techniques experiment (Supervisor: Gy. Tarczay), 151p, Eötvös Loránd University, 2016

B. Botka, Optical and Raman spectroscopy of carbon nanotube-based hybrid materials (Co-supervisor K. Kamarás) 120p, Budapest University of Technology and Economics, 2016,

D. Haluszka: Assessing the application possibilities in dermatology and potential risks of pulsed lasers used in nonlinear microscopy (Supervisors: N. Wikonkál and R. Szipőcs) 86p, University of Szeged, 2016

L. Holló, Integrable form factor program and its applications (Supervisor: Z. Bajnok) 137p, Eötvös Loránd University, 2016

M. Horváth, Statistical and thermodynamical studies of the strongly interacting matter (Supervisors: A. Jakovác and T.S. Biró) 106p, Eötvös Loránd University, 2016 (arXiv:1605.08619).

V. Ivády, Development of theoretical approaches for post-silicon information processing (Supervisor: A. Gali), 209p, Linköping University, Sweden, 2016

A. Kerekes, Development and application of optical measurement methods for the investigation of the deposition of aerosols in the human airways (Supervisor: A. Nagy) 105p, University of Pécs, 2016

J.Z. Nagy, Development of on-board data acquisition system and on-board communication system for space research equipment for research measurements in environment of the Earth, 83p, University of Óbuda, 2016

K. Németh, Chemical modification and optical spectroscopy of single-walled carbon nanotubes (Supervisor K. Kamarás) 96p, Pannon University, 2016

P. Sinkovicz, Study of the ordered phase in the fcc lattice and determination of the recurrence time in open system dynamics (Supervisor G. Szirmai) 149p, University of Pécs, 2016

A.J. Zsigmond, Measurement of Z boson production in heavy-ion collisions with the CMS detector at the LHC (Supervisors: F. Siklér and G.I. Veres), 127p, Eötvös Loránd University, 2016

D.Sc

E. Somfai, Numerical modelling of statistical physical systems far from thermal equilibrium 110p, 2016

Memberships

L. Almási	— Member of the Editorial Board of New Frontiers in Chemistry Journal (Timisoara, Romania)
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- Chairman of the Zimányi Foundation for Physics,
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- Member, International Advisory Committee, WPCF 2013 Conference, Acireale, Italy
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- Principal Investigator, PHENIX - Hungary sub-collaboration (2003-2013)
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— Editorial Advisory Board member of Journal of Non-Equilibrium Thermodynamics, de Gruyter
— Secretary of the Society for the Unity of Science and Technology
— Member of the REPS (Roland Eötvös Physical Society)
— Honorary member of the International Association of Physics Students,
— Corresponding member of the Accademia Peloritana dei Pericolanti (Classe di Scienze Fisiche, Matematiche e Naturali).

T. Vámi
— CMS Young Scientist Comitee vice-president

P. Vecsernyés
— Member of the Particle Physics Committee of the H.A.S.

G. Veres
— Member of the Hungarian Microscopy Society
— Member of the Hungarian Aerosol Society
— Governing Board Member of the European Joint Undertaking for ITER and the development of Fusion Energy

V.Veszprémi
— Member of the CMS Phase 1 Pixel Upgrade Management Board
— Member of the CMS Phase 2 Tracker Upgrade Management Board
— Member of the CMS Tracker Institutional Board
— Member of the CMS Tracker Management Board (ex officio)

I. Vincze
— Member of the Council of Doctors at the Hungarian Academy of Sciences

G.Vizi
— Board member of the MANT (Hungarian Astronautical Society)

Gy. Wolf
— Hungarian representative of the NuPECC EU FP7 HadronPhysics2, HadronPhysics3, HadronPhysicsHorizon, GSI FAIR, CBM, JRA Thuric, Toric, and Meson-Net projects.
— Leader of the PANS,
— President of the NEFIM
— Member of the NICA
— President of the of the Nuclear Physics Board, Eötvös Loránd Physical Society
— Secretary of the Nulcear Physics Board of the Hungarian Academy of Sciences
— Representative in Physics Department of the Hungarian Academy of

Sciences

Z. Zimborás — Member of the Editorial Board of Frontiers in Quantum Computing (Nature Publishing Group)

S. Zoletnik — Eurofusion General Assembly
— Eurofusion General Assembly Bureau
— International Tokamak Physics Activity Diagnostics Topical Group
— International Board of Advisors of the Institute of Plasma Physics of CAS

Conferences

Quantitative and functional aspects of associational cortical connections. Symposium at the IBRO WORKSHOP BUDAPEST, January 21-22, 2016 — The Symposium presented new results on the structural and functional connectivity of the brain on higher organization level. The approaches included quantitative anatomical results as well as new mathematical analytical tools, to reveal relation between structure and function and theoretical models that aim the understanding of organization of the cortical connectome.

10th Central European Training School on Neutron Techniques, Budapest, 2-6 May 2016. — The school gave an insight into the neutron scattering and imaging techniques and their applications for studies on structure and dynamics of condensed matter. During 5 days the participants could take advantage of 15 hours of theoretical lectures and participate to 15 hours of practical work at the neutron spectrometers and instruments located at the Budapest Research Reactor. 31 graduate and post-graduate students, young researchers participated at the training, the majority of them coming from the Central European region, however participants from other European and non-European countries were present, too.

Gravitational Waves: Astrophysical and Geophysical Perspectives, Wigner RCP, Hungarian Academy of Sciences, 5 May 2016, 80 participants. — Seminar overviewing the Hungarian contributions to the discovery of gravitational waves. It was organized by the Particle Physics Committee of the Hungarian Academy of Sciences connected to the General Assembly of the Academy with an audience of about 80 people. The whole programme of the mini-symposium including 8 talks have been video-recorded.

4th Work Meeting on Quantum Optics & Information, 6-7 May 2016 Regional Centre of the Hungarian Academy of Sciences at Pécs, approx. 42 participants. — The aim of this mini workshop was to bring together scientists in this field mainly from Hungary, but also including participants from Germany, Czech Republic, Slovakia and Portugal. We organized this workshop series based on our collaboration with the quantum information research group led by Mátyás Koniorczyk at the University of Pécs, inviting also our international collaborators and guests.

Workshop "6th GPU Day, The Future of Many-Core Computing in Science", 2-3 June 2016, Wigner RCP, Budapest, Hungary. — The "GPU Day" series has been organized by the Wigner GPU Laboratory for the 6th times in this year. The two-day workshop interconnects scientists, programmers, and parallel-computing experts from all over the world. This year we had 80 participants and visitors from US, Poland, Spain, Ukraine. Several commercial companies visited the event from Hungary and abroad.

Conference on Magneto-mechanical properties of functional materials, 1-4 June, 2016 Mátrafüred. — This small workshop was to get together material scientists from Hungary and Sweden. 38 people attended, and took place in Mátrafüred. This conference takes place regularly, but not periodically. It helped to uphold the existing collaboration between the involved scientists.

Conference 24th Low-x Meeting, Gyöngyös, June 6-11, 2016. — The 24th Low-x Meeting was organized jointly by Wigner RCP, ELTE, Budapest and KRF Gyöngyös. The conference took place in Gyöngyös, on the conference tour we visited Eger and Tokaj. The 5 days meeting attracted 58 participants from Asia, Europe, and North America. The web-page is at https://indico.cern.ch/event/472823.

Conference 2nd EUROfusion FuseCOM meeting, 28-30 June 2016, Budapest. — The meeting was organized by the Pellet and Video Diagnostics Group and took place in the Margaret Island. Around 25 fusion communication persons were attending this event from all over Europe. The meeting's aim was to share communication experience with each other, learn new tools developed by EUROfusion Communications Office and attend science communication trainings.

Conference: International Conference on Scientific and Statistical Database Management – SSDBM2016, 18-20 July, Margitsziget, Budapest, Hungary. — The annual SSDBM conference is an international forum for scholarly discourse on designing, building, analyzing and evaluating scientific and statistical data management systems and applications. This event brought together leading scientific domain experts, practitioners, application developers and users to exchange cutting-edge insights and experiences, and to inspire future research directions. The conference featured a rich program of research presentations, invited speakers, panel sessions, and demonstrations of research prototypes and industrial systems that capture the ever-increasing interdependence between data management, statistical methods, and scientific research and applications.

Beam Emission Spectroscopy Summer School, Budapest, 28.08- 3.09. 2016. — The 1st BES summer school was organized by the BES research group on the last week of August 2016 in collaboration with the Budapest University of Technology and Economics. 16 students attended the event half of them are from various European laboratories. Student groups were organized to work on experimental data of various tokamaks where fluctuations BES diagnostics are operated in collaboration with the Hungarian team. Most of these diagnostics were designed and built by the tutors of this summer school, so both theoretical and technical insight could be be given. The studied physics phenomena included fast transient events as well as plasma turbulence, where the BES diagnostics have unique capabilities.

Neural and Cognitive Architectures Workshop '16, 30 September, 2016 Budapest.

CAS – CERN Accelerator School, 2-14 October 2016, Budapest, Hotel Helia, 123 participants. — The CERN Accelerator School holds training courses on accelerator physics and associated technologies for physicists, engineers, technicians and students throughout the year. The courses take place in different member states of CERN and consist of a programme of lectures and tutorials spread over a period of one or two weeks. Participants are welcome from member states of CERN and other countries world-wide.

Workshop "MMLH2016", 5 October 2016. — The annual meeting of the Network of the Hungarian Mössbauer Laboratories was held in the form of a one day workshop. It had three foreign participants, one co-operating partner from Germany and the director and the secretary of the Mössbauer Effect Data Center from China. The workshop took place at the KFKI Campus and was attended by approx. 30 scientists.

Conference "100 éves az Általános Relativiáselmélet" (The 100th anniversary of the Theory of General Relativity, in Hungarian), 09 Nov 2016, Budapest, Hungary (30

participants). — This national conference was organized as a commemoration to the 100th anniversary of General Relativity. The conference took place at National University of Public Service, and was devoted to all aspects of GR.

CERN Hungarian Teachers Programme 2006-2016. "Celebration of Hungarian Science, 2016" at Sapientia College of Theology, Budapest, 12 Nov. 2016, more than 100 participants. — The conference was attended by more than 100 Hungarian physics teachers and representatives of the organizing and sponsoring bodies including the Roland Eötvös Physical Society, CERN, the Hungarian Academy of Sciences and the Wigner Physics Research Centre, with international videoconferencing. The past and future of the Programme were reviewed in 14 talks.

Workshop "Lectures on Modern Scientific Programming", 14-16 November 2016, Wigner FK, Budapest, Hungary. — This international workshop of the Wigner GPU Laboratory is dedicated to widen our knowledge and practice on parallel computing in science. The seminar-series-like event started from the basics of computing and informational technologies, then moved to basic and parallel programming techniques for physicists. We had 40 registered participants mostly from the Hungarian and abroad universities.

Conference "Zimányi Winter School on Heavy Ion Physics", December 5-9, 2016. — The 16^{th} Zimányi School was organized as a joint scientific meeting of Wigner RCP and ELTE University. The conference took place in building III of Wigner RCP and on one day we visited the ELTE University. The Ortvay Colloqium of Roy Lacey (SUNY Stony Brook) was jointly organized with ELTE. The 5 days meeting attracted 68 participants from Europe and US, including 28 students. We have formed a Zimányi International Advisory Committee from the core high level participants and the winners of the Zimanyi Medal to advise us and to secure the future prosperity of this conferece series. The web-page is at http://zimanyischool.kfki.hu/16

Wigner Colloquia

In the fall of 2014 we have started to organize a series of Wigner Colloquia, inviting international experts to deliver talks on fresh and interesting research topics to the entire community of our research centre. We also have dispatched a modest financial background to support this activity by occasionally reimbursing travel costs to and accomodation costs in Budapest for the invited speakers.

The concept of this series is to offer to our researchers a possibility to meet colleagues from external institutions who work on hot topics and able to present their favorite research to a wide audience of physicists, working both in experiment and theory in fields ranging from high energy particle physics via nuclear and plasma physics to material and life science related problems. We restrict our invitations in number to a few per semiannual blocks.

Wigner Colloquia in 2016

https://indico.kfki.hu/category/42/

09-02-2016 Prof. Petra Rudolf (University of Groningen): See atoms move in real time: ultrafast electron diffraction

22-03-2016 Prof. Gerard 't Hooft (Universiteit Utrecht): Black holes and elementary particle physics

05-04-2016 Prof. Jonathan Selinger (Kent State University): Understanding Higgs through Liquid Crystals, and Understanding Liquid Crystals through Higgs

19-04-2016 Prof. Gergely Zimányi (The University of California): Materials Physics in the Sunlight

29-04-2016 Prof. Maciej Lewenstein(ICFO): Random states for robust quantum metrology

24-05-2016 Prof. Gordon Baym (University of Illinois at Urbana-Champaign): Inside Neutron Stars

20-09-2016 Prof. Alois Loidl (Institut für Physik, Universität Augsburg): Skyrmion with ferroelectric polarization.

04-10-2016 Prof. Jeroen van den Brink (Institute for Theoretical Solid State Physics, IFW Dresden): Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

25-10-2016 Prof. Lars Andersson (Albert Einstein Institute): Geometry of Black Hole Spacetimes

Seminars

Weekly meetings of the Budapest and Debrecen Compact Muon Solenoid (CMS) groups:
http://www.grid.kfki.hu/twiki/bin/view/CMS/WeeklyBudapestDebrecenMeetings

Talks for the annual Zimányi School:
https://indico.cern.ch/event/464154/other-view

Wigner RCP RMI Seminars

Theoretical physics seminars
http://indico.kfki.hu/category/28/

25-01-2016	Z. Kunszt (ETH, Zürich): Events implying resonance at 750 GeV at LHC in the spectrum of di-photon endstates
26-02-2016	M. Lajer (ELTE): Truncated Hilbert Space Approach for the 1+1D phi^4 Theory
11-03-2016	Gy. Bencédi (Wigner): Multiplicity dependence of pion, kaon and proton production at large transverse momentum in pPb collisions at sqrt(s_NN)=5.02 TeV at ALICE
25-03-2016	M. Vasúth (Wigner): Direct detection of gravitational waves
01-04-2016	Ze-fang Jiang (Central China University): Hydrodynamical estimation of initial energy density for pp collision at CERN-LHC energies
06-05-2016	M. Kőfaragó (University of Utrecht, CERN ALICE): Modification of the near-side jet peak at √NN}}}=2.76$ TeV Pb--Pb collisions measured by the ALICE detector
10-06-2016	Z. Zimborás (Freie Universität Berlin): Surface laws in field theories and many-body systems
04-07-2016	A. Sfondrini (ETH Zürich): The AdS3/CFT2 correspondence and integrability
08-07-2016	K. Sakai (Meiji Gakuin University, Yokohama, Japan): BPS index and 4d N=2 superconformal field theories
08-07-2016	R. Pisarski (BNL, Brookhaven): Matrix model for the chiral phase transition
05-08-2016	P. Andersen (Purdue University): Numerical Explorations of the Lattice Loop Equations
12-08-2016	J.-M. Le Goff (CERN): The vision and concepts modus operandi of the Collaboration Spotting project
15-08-2016	M. Damodaran (Purdue University, USA): From fluid to particles: A study of phase space distributions

19-09-2016 T. Fényes: Baryon spectroscopy – 2016

23-09-2016 O. Evnin (Chula University, Bangkok and Solvay Institutes, Brussels): Weak fields and effective integrability in AdS

06-10-2016 Jean-Marie Le Goff (CERN) - Seminar

07-10-2016 M. Bejger (N. Copernicus Astronomical Center, Warsaw, Poland): Observational implications of dense matter phase transitions for the rotational evolution of neutron stars

11-11-2016 A. Frenkel (Wigner): The Salecker-Wigner quantum clock model

02-12-2016 C. Wu (Wigner): Nonconformal generalization of the fluid/gravity correspondence and its applications to RHIC physics

09-12-2016 K. Ito (Tokyo Institute of Technology): ODE/IM correspondence and the Argyres-Douglas theory

20-12-2016 B. Cole (Columbia Univ. New York): The LHC heavy ion program as seen from and with ATLAS

Wigner RCP SZFI Seminars

http://www.szfki.hu/seminar

05-01-2016 N. Shannon (Okinawa Institute of Science and Technology): Electromagnetism on Ice : from quantum spin ice to protons in water ice

12-01-2016 L. Pusztai (Wigner): Structure of liquids consisting of tetrahedrical molecules: what have we learned in 80 years?

17-01-2016 L. Temleitner (Wigner): Structural study of disordered systems by diffraction: from liquids with hydrogen to disordered crystalline phases

19-01-2016 M. Kormos (BME Theoretical Physics): Non-equilibrium dynamics of one dimensional quantum systems

26-01-2016 R. Szipőcs (Wigner): Development of a 3D CARS microscopy measuring system (Applied Research Prize of the Wigner RCP SZFI, 2015)

02-02-2016 K. Tőkési (MTA ATOMKI): Classical trajectory Monte Carlo method – real-time observation of quantum physics phenomena

11-02-2016 B. Botka (Wigner): Optical and Raman Spectroscopy of Carbon Nanotube - Based Hybrid Materials

16-02-2016 L. Pusztai (Wigner): Introduction and general installation of Liquid Structure group

16-02-2016 P. Jóvári (Wigner): Short range order in CuZr-based metallic glasses (work summary)

23-02-2016 L. Temleitner (Wigner): Structural disorder in crystals

23-02-2016 Sz. Pothoczki (Wigner): The necessity of applying molecular dynamic simulations for determining the structure of molecular liquids

23-02-2016 I. Pethes (Wigner): Applying Reverse Monte Carlo method for structural examination of covalent glasses

25-02-2016 A. Kerekes (Wigner): Development and application of optical measuring methods for examining pulmonary deposition of aerosols (in-house thesis defence)

01-03-2016 P. Magyar (Wigner): Linear and quadratic static response functions and structure functions of strongly coupled plasmas (work summary)

08-03-2016 N. Éber (Wigner): Patterns created by asymmetric strain in liquid crystals

29-03-2016 K. Gillemot (Wigner): Shear-induced segregation of dry granular particles with different friction coefficients

19-04-2016 J. Romhányi Judit (Max Planck Institute for Solid State Research, Stuttgart): Multiboson theory for the magnetoelectric helimagnet Cu_2OSeO_3

26-04-2016 S. Zsurzsa (Wigner): Electrochemical deposition of nanostructures, investigation of their magnetic and transport properties (work summary)

29-04-2016 A. Sanpera (Autonomous University of Barcelona): Quantum metrology in thermal states

ort proper V. Ayadi (Wigner): Coherence and quantum-classical correspondance in ultrafast atom-laser interaction (work summary)

03-05-2016 B. Bódi (Wigner): Attosecond control in atomic systems (work summary)

10-05-2016 P. Salamon (Wigner): Magnetic control of flexoelectric domains in a nematic fluid (work summary)

10-05-2016 Á. Pekker (Wigner): Spectroscopy of molecules loaded into nanotubes (work summary)

17-05-2016 Gy. Faigel (Wigner): Experimental solution of the phase problem in diffraction

19-05-2016 F. Podmaniczky (Wigner): Exotic nucleation methods in the Phase Field Crystal model (work summary)

24-05-2016 Z. Néda (Babes-Bolyai University, Cluj): Kinetic roughening at the triple line of a receding liquid layer

26-05-2016 N. Laczai (Wigner): Preparation and study of polycrystalline scintillator materials (in-house thesis defence)

26-05-2016 P. Sinkovicz (Wigner): Study of the ordered phase in the fcc lattice and determination of the recurrence time in open system dynamics (in-house thesis defence)

31-05-2016 O. Kálmán (Wigner): Magnetomechanical coupling of ultracold atoms and nanoconductors and determination of the magnetic noise by detecting atoms (work summary)

31-05-2016 I. Hagymási (Wigner): Topological phases and phase transitions in Anderson and Kondo lattice models (work summary)

02-06-2016 P. Rácz (Wigner): Ultrafast plasmonic photoemission in mid-infrared (work summary)

07-06-2016 K. Németh (Wigner): Investigation of interfaces and metal deposition by electrochemical methods (work summary)

07-06-2016 I. Hajdara (Wigner): Spectroscopic investigations on niobate single crystals (work summary)

09-06-2016 A. Dombi (Wigner): Bistability Effects in the Strong Coupling Regime of Cavity and Circuit Quantum Electrodynamics (in-house thesis defence)

13-06-2016 D. Boese (Graz University, Dept of Chemistry): Intermolecular Interactions: Surfaces, Molecules and Molecular Crystals

14-06-2016 S.E. Saddow (University of South Florida, USA): Silicon Carbide Biotechnology

14-06-2016 R. Ünnep (Wigner): The ultrastructure and flexibility of thylakoid membranes in different photosynthetic organisms as revealed by small angle neutron scattering (in-house thesis defence)

21-06-2016 S. Pekker (Wigner): From benzene to graphene: electron structure of polycyclic aromatic hydrocarbons and trigonal carbon allotropes

28-06-2016 G. Thiering (Wigner): Identification of oxygen point defects by ab-initio simulation methods in a diamond crystal (work summary)

30-06-2016 M. Kornyik (Eötvös Loránd University): Random matices and their eigenvalues

05-07-2016 A. Jákli (Kent State University, Chemical Physics): Stability and dynamics of liquid crystal filaments

12-07-2016 D. Lorenc (International Laser Centre, Bratislava): Tunable THz-emission from laser induced plasma and more

19-07-2016 J.L. Musfeldt (Department of Chemistry, University of Tennessee, USA):

Magnetoelectric coupling through the spin flop transition in Ni_3TeO_6

02-08-2016 N. Német (Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand): Manipulating the Squeezing Properties of a Degenerate Parametric Amplifier with Coherent, Time-Delayed Feedback

09-08-2016 K. Kono (RIKEN CEMS): Transport measurement of electron bubbles trapped under the surface of topological superfluid ^{3}He

30-08-2016 L. Himics (Wigner): Formation and spectral characterisation of luminescence centers in nanodiamond (in-house thesis defence)

06-09-2016 S. Varró (Wigner): Wigner functions for optical phase and photon number

13-09-2016 A. Vukics (Wigner): Is there a superradiant phase transition?

20-09-2016 Gy. Tarczay (Eötvös Loránd University): Chemistry and physics in reactive and inert matrices

04-10-2016 B. Kocsis (Eötvös Loránd University): Phase transitions in astrophysical liquid crystals

06-10-2016 T. Rakovszky (Max Planck Institute for the Physics of Complex Systems, Dresden): Quantum quenches in Ising field theory

11-10-2016 F. Iglói and J. Asbóth (Wigner): How does topology enter solid state physics? The 2016 Nobel prize in physics

18-10-2016 P. Claudin (Ecole Supérieure de Physique et Chimie Industrielles): Rheology of granular flows and suspensions

25-10-2016 D. Beke (Wigner): Fabrication and characterization of silicon carbide nanoclusters (in-house thesis defence)

03-11-2016 I. Nándori (Atomki, DTE): BKT phase transition and the functional renormalization group method

08-11-2016 K. Tompa (Wigner): „Bonding and release”: Molecular interactions in proteins

10-11-2016 A. Gilyén (CWI Amsterdam): On preparing ground states of gapped Hamiltonians: An efficient Quantum Lovász Local Lemma

15-11-2016 M. Csanád Máté (Eötvös Loránd University): Femtoscopy, or quantum statistical correlations in high energy physics

15-11-2016 A. Valli (National Research Councill, Istituto Officina dei Materiali (CNR-IOM), and SISSA): Many-body effects in the electronic and transport properties of pi-conjugated nanostructures: from benzene to graphene nanoflakes

22-11-2016 A. Pályi (Budapest University of Tecnolgy and Economics): Donor-based spin qubits in silicon

29-11-2016 G. Csire (Wigner): Quasi-particle spectra of superconducting heterostructures (in-house thesis defence)

30-11-2016 H. Fattahi (Max Planck Institute for Quantum Optics, Garching): Ultrabroadband pulses for attosecond pulse generation and Raman spectroscopy

06-12-2016 R. Stannarius (Dept. of Nonlinear Phenomena, Otto von Guericke Uni Magdeburg): Defect Interactions in Anisotropic Fluids

13-12-2016 K. Kamarás and S. Pekker (Wigner): Molecular motors: The 2016 Nobel prize in Chemistry

20-12-2016 A. Kuzmin (Institute of Solid State Physics, University of Latvia): X-ray absorption spectroscopy: when theory meets experiment