Wigner 2014

Annual Report

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

Wigner RCP 2014

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Wigner RCP 2014 – Annual Report

Edited by I. Bakonyi, TS. Bíró, V. Kozma-Blázsik, A. Kmety, AJ. Lowe, B. Selmeci

Closed on 27. May, 2015

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Dear Reader,

 We have completed the third year of the Wigner Research Centre for Physics (Wigner RCP), which is one of the largest institutions of the Hungarian Academy of Sciences (MTA), representing 10% of the scientific workforce of the academic research network. In this Annual Report 2014 we display and summarize the scientific achievements we have accomplished. The year 2013 was the year of redesign, exploring new ways and new directions for the activities of the research groups and the whole institute. We can consider 2014 as a year of strengthening, when we improved and extended our activities. This Volume reports on the improvements made and their outcomes.

Firstly, the number of prestigious MTA Momentum Research Groups has been increased by one to the total number of eight. In parallel we increased the number of Wigner Research Groups to seven. These groups were selected by the Wigner scientific community 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.) A new channel has been opened in the framework of the National Brain Project ("NAP: Nemzeti Agy Program"): one more group was awarded and hosted at Wigner RCP. The research activity of this group will start at the beginning of 2015. Thus, altogether 16 out of our 40 research groups receive extraordinary or special acknowledgement (and financing) for their excellent research.

At the personal level six new MTA Bolyai scholarships, six MTA postdoc and nine MTA young researcher positions were granted in 2014 to our Institute. The MTA has continued to distribute dedicated grants for renewal of laboratories and modernization of existing research infrastructure. These supports fairly increased the research potential of Wigner RCP. Infrastructures and laboratories could apply for an SRI (Strategic Research Infrastructure) or an RRI (Registered Research Infrastructure) certificate in 2014. The NEKIFUT action was finished by the end of 2014 and certified RIs have been advertised: eight of our applicants became SRI and five applicants have received an RRI certificate, which all became Open Laboratories. 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.

Past activities and successes received their acknowledgement. Ferenc Iglói was awarded the MTA Grand Physics Prize, Gyula Tóth won the MTA Young Scientist award and Sándor Zoletnik was awarded the MTA Wigner Prize. The government of Hungary acknowledged Győző Farkas by the Széchenyi Award, Tamás Kemény and Gábor Pető by the Officer's Cross and Béla Lukács by the Knight's Cross of the Order of Merit of Hungary. Péter Lévai received the Neumann Prize of the Ministry of National Development.

New possibilities became available for us in 2014. Firstly, the opened Calls of the EU HORIZON 2020 Framework Program caused continuous excitement for most of the research groups, who prepared proposals to Brussels for collecting financial support for accomplishing their research plans. Furthermore, the Wigner RCP applied for an ERA-chair grant based on the innovation activity of our institute. In the first year of the HORIZON 2020 Program 40 proposals were submitted under the organization or the participation of the Wigner research groups. Only six proposals were awarded and, unfortunately, the ERA-chair application was also rejected. The small number of winners highlights the importance of readiness at the international level of research and the difficulty to receive acknowledgement from the EU. As the H2020 program supports industrial excellence, we increased our activities in innovation and explored industrial connections. This direction is very complicated and we need more time to discover and use real opportunities which are manageable for our Institute of basic research.

A number of important events connected to international actions occurred in 2014. CERN celebrated its 60th anniversary. Prime Minister Viktor Orbán visited CERN in January. This was the first time when a Hungarian PM visited CERN. Hungarian delegations participated in and organized many events during the year. For example, we organized a very successful CERN60 Open Weekend in Csillebérc, during which more than 700 interested participants became acquainted with Hungarian research and R&D activities at CERN. The origin of this enhanced interest can be connected to the 2013 Physics Nobel Prize for the discovery of the Higgs boson and the successful operation of the CERN@WIGNER project in the Wigner Datacenter. The Higgs discovery and the CERN60 events introduced a new focus on the construction of the High Luminosity LHC, improvement of which will open the opportunity to discover new particles and solve the mystery of dark matter and dark energy.

Space science delivered excitement also: after 20 years of preparation and 10 years of silent fly-by activity the Rosetta Mission woke up and for the first time in the history of mankind a man-made probe (Philea) has landed on a comet. In parallel, extraordinary photos were taken of the surface of an active comet. Hungarian groups from MTA Wigner RCP, MTA Energy RC and the BME University participated in this extraordinary mission. Many people followed this event with great interest in Hungary. This success story was an excellent prelude to the Hungarian entry into the European Space Agency (ESA), which occurred in February 2015.

Another milestone was the Hungarian entry into the European Spallation Source (ESS). The governmental decision opened the way for Hungarian scientists to use this extraordinary neutron source in the future. However, we first need to participate in the construction of the ESS from 2015. This construction already started in October 2014, when the foundation stone ceremony was performed in Lund with the participation of the official Hungarian Delegation. Wigner RCP is looking forward to this new opportunity, including the delivery of in-kind contributions to the construction.

These results and the extended activities of the Wigner RCP were communicated to the wider public by means of the "All Colors of Physics Bus" ("Sokszínű Fizika Busz") in 2014. This bus is filled with demonstration experiments and overseen by expert colleagues. The bus was used during weekends of Spring and Fall of 2014 to visit secondary schools and universities, giving lectures and performing experiments. These programs reached many thousands of interested young people. Thanks to the enthusiastic performances of the speakers, this outreach activity generated a wide interest both at the national and

international level. We will continue the program of the Physics Bus in 2015. In parallel we hosted dozens of visiting groups at Wigner RCP, particularly on the Girls' Day and the Wigner Open Day.

I thank all colleagues for their continuous enthusiasm and participation in the above programs, and of course for their hard work and devotion to science during this remarkable year. The year 2014 was a success for the Wigner RCP and we are looking forward to the future with great expectation. This Annual Report showcases this hard work and prove the excellence of the research activities accomplished at Wigner RCP.

Lévai Péter József

Director General

AWARDS AND PRIZES

Awards of the State of Hungary and Government of Hungary

Gy. Farkas, Széchenyi Award
T. Kemény, Officer's cross of the Order of Merit of Hungary (civil division), 2014
P. Lévai, János Neumann Prize of the Ministry of National Development
B. Lukács, Knight's cross of the Order of Merit of Hungary (civil division), 2014
G. Pető, Officer's cross of the Order of Merit of Hungary (civil division), 2014

Awards of the Hungarian Academy of Sciences

F. Iglói, Grand Physics Prize of the Hungarian Academy of Sciences
I. Kovács, Award for Young Scientists of the Hungarian Academy of Sciences, 2014
Gy. Tóth, Award for Young Scientists of the Hungarian Academy of Sciences 2014
S. Zoletnik, Jenő Wigner Prize, Hungarian Academy of Sciences, 2014
M. Csernainé, Mention of the Secretary General, Hungarian Academy of Sciences, 2014

Professional awards

K. Lengyel, Ágoston Budó Award of the Loránd Eötvös Physical Society
Z. Németh, Géza Györgyi Prize
L. Pusztai, Rezső Schmidt Prize of the Loránd Eötvös Physical Society
G. Szirmai, Pál Gombás Award of the Loránd Eötvös Physical Society

"Momentum" Program of the H.A.S., 2014

P. Dombi, 2014-2019

Bolyai János Scholarship of the H.A.S. granted in 2014

J. Asbóth, 2014-2016
A. Kiss, 2014-2016
A. László, 2014-2016
Z. Németh, 2014-2016
M. Veres, 2014-2016
V. Veszprémi, 2014-2016

KEY FIGURES AND ORGANIZATIONAL CHART

Permanent staff by profession
Total: 362

Engineers; 59; 16%   Technicians, assistants; 46; 13%

Librarians; 3; 1%

Administrative staff; 37; 10%

Scientists; 217; 60%
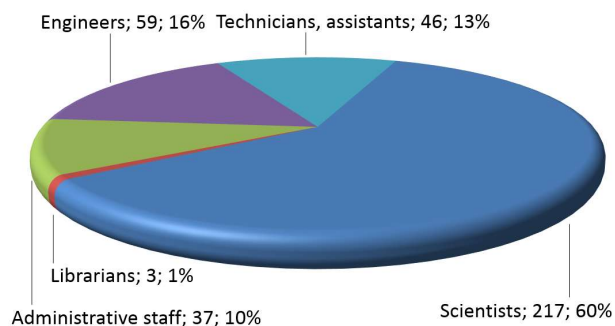
Scientists by degree/title
Total: 217

Member of the Hungarian Academy of Sciences; 4

Doctor of Sciences (Dr. Habil.); 38

University degree; 63

Ph.D.; 112
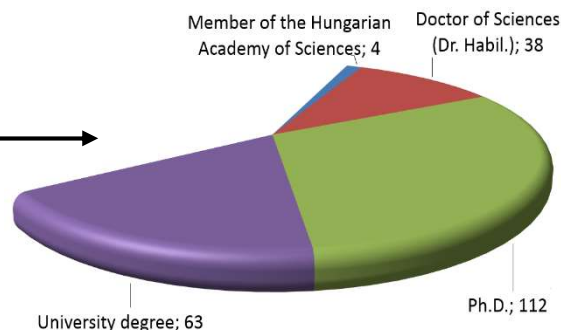
Scientists by age group
Total: 217

Age group	Count
Below 35	86
36 to 45	59
46 to 55	35
56 to 65	34
Above 65	3

Income*

National funds (NFÜ,TéT, KTIA) 4%

Others 17%

EU 20%

National Science Fund (OTKA) 5%

Hungarian Academy of Sciences 54%

Expenditure*

Others inc. travel 15%

Investments 13%

Wages and salaries 42%

Consumables 7%

Operational overhead 12%

Labour overhead 11%

*V.A.T not included.

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WIGNER RESEARCH CENTRE FOR PHYSICS — Organizational Chart (September, 2013)

DIRECTOR GENERAL

EXTERNAL ADVISORY BOARD

COUNCIL OF DIRECTORS (IT)

FORUM OF RESEARCH GROUPS

DEPUTY DIRECTOR GENERAL

Internal Control

Library

Computer Networking Centre

Wigner Datacenter

FINANCIAL DIRECTOR

Financial Department

WIGNER SCI. COUNCIL (WTT)

LEADERS' COUNCIL (VT)

RMI — 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 Lab

Mech. Workshop

SZFI — DIRECTOR

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

Technical Base

ELI Laboratory

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MOST IMPORTANT EVENTS OF THE YEAR 2014

Csilla Péntek, communication secretary

2014 was a really busy but successful year in the communication activities of the Wigner Research Centre. We appeared many times in the press and we organized some interesting events.

All Colors of Physics Roadshow. — One of the main projects was the introduction of the "All Colors of Physics Roadshow". It is an informative project consisting of three parts: presentations, experiments shows and the "All Colors of Physics Bus" itself, which serves as an interactive exhibition room for nanophysics and introducing CERN. The program is designed to attract more high-school students to natural sciences and researcher's career. In the autumn semester, we organized seven tours, three of which were in different locations of Hungary. Hundreds of interested people could participate in the programs presenting some really exciting topics in physics.

The "All Colors of Physics Bus", an experiment show, and a robot with the Wigner Logo on the roadshow.

About 25 people from the Wigner RCP researcher community participated in the project implementation and the program of the roadshow has reached nearly 2000 people.

Place	Visitor number (approximate)
ELTE (The Opening Ceremony)	100
Mechatronics High School	300
CERN Open Days	250
Pécs	900
Hungarian Science Festival (MTÜ)	30 (+ the visitors of the MTA EK and MTA TTK MFA)
Gyöngyös	400
	Total: 1980 / a half year

CERN 60. — As several research groups of Wigner RCP are participating in CERN projects, there was no doubt about to join the CERN 60 events. The first program was in May, at the Eötvös Loránd University, where Professor Rolf-Diether Heuer (former president of the CERN) inaugurated the "All Colors of Physics Bus" and delivered a lecture to a fully-packed auditorium.

Inauguration of the "All Colors of Physics Bus"

As the second part of the CERN 60 events series, our Research Centre organized the CERN Open Days in September. More than 200 people visited the "All Colors of Physics Bus", the Wigner Datacenter and the exhibition about the CERN research groups. They could also take a virtual tour in the Large Hadron Collider (LHC) tunnel via the online connection supported by two colleagues present in the CERN Geneva headquarter.

A lecture about the CERN and the online tour in the LHC

Open Days. — Every year we organize two open days, one in spring, and another one in autumn. The spring event is the Girls' Day, which is an interactive open day for high school girls, organized by the Association of Hungarian Women in Science. On this day, companies in the Information and Communications Technology world, research institutes and universities in different areas of natural sciences and information technology organize programs all over the country. In the Wigner RCP, girls can visit laboratories, can have a talk with young researchers and get a glimpse into the everyday life of scientists.

A very similar yearly program but for a wider audience is the Wigner Open Day, which is part of the Hungarian Science Festival (organised by the Hungarian Academy of Sciences). In 2014, approximately 200 students visited our research centre, and about 30 scientists helped the implementation of these programs.

Rosetta-mission. — One of the most important results of the year in the Wigner RCP, was the successful landing of the Philae, the lander unit of space mission Rosetta. Its central computer and data collector units were jointly developed by the Wigner RCP and the Space and Ground Facilities Ltd. The presentation of this project was done via a year-round communication ended by the live broadcast of the landing in the TIT Planetarium, Budapest, which was organized by the Wigner RCP and the Club of the Hungarian Scientific Journalists.
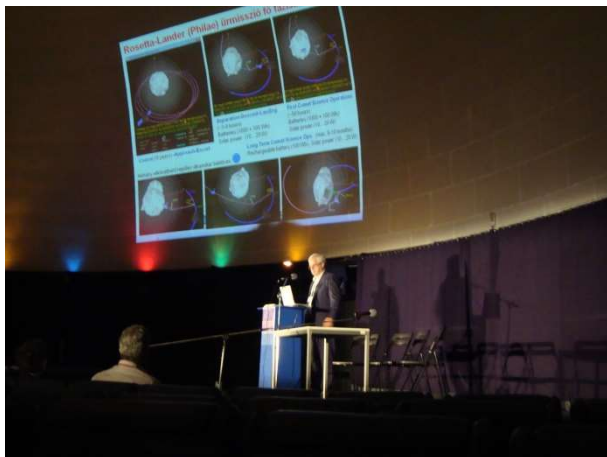
A lecture about the mission before the landing.

The Rosetta display case in the Planetarium.


The Churyumov-Gerasimenko cakes.

LANDING ON A COMET

András Balázs, Department of Space Physics and Space Technology

Some days ago I was browsing the internet and found an article about technological evolution and space research, and the "prospects" of humankind in such a context. Reading through the article and other readers' comments, in one comment I noticed a remarkable sentence: "Humankind needed 10000 years to land on a comet, but our Sun still has about 6 billion years of life left". I would not dare to assess and predict what the prospects of humankind look like on such a time scale, nevertheless the landing of Philae on the surface of a comet in 2014 was considered a significant achievement by experts and even by the public.

As for myself and my colleagues, for many years we have been directly involved with the requirements definition, hardware and software design and implementation, and the testing and validation of the central fault-tolerant on-board computer and its operating software of the Philae lander. We need time now to realize and become accustomed to a sudden new situation: the Rosetta-Philae project is not a challenge any more; it is not hard work ahead of us, but a successfully-mastered milestone behind us. Moreover, "us" in this context means not only my colleagues at Wigner FK, but also many scientists, engineers and technicians in many research institutes and countries all over Europe; in national space agencies, industrial partners and the European Space Agency as the leader and integrator of Rosetta's venture.
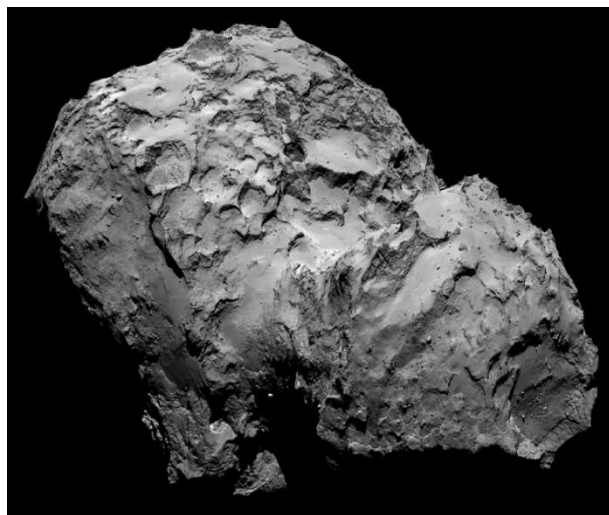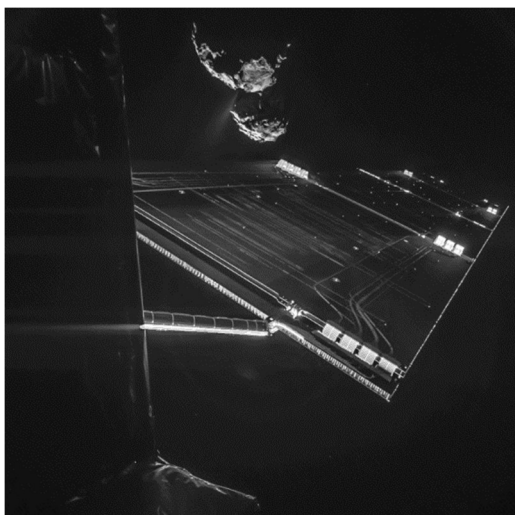
Comet CG/67P 500 million km from Earth, 18 km from the Rosetta spacecraft in the field of view of the CIVA panoramic camera aboard Philae still aboard Rosetta, and by the OSIRIS narrow angle camera (right)

On the 12th of November 2014, nearly 20 years of efforts culminated in a rare event full of excitement, concerns, hopes, and emotions: the landing of Philae on the comet CG/67P and the science performed on the surface during the 50 hours or so that corresponds to the lifetime of the probe's primary energy source. With regard to the aforementioned metaphor about the prospects of humankind: as a rule, no one and nothing can ever be absolutely perfect, and the landing of Philae was not either. Upon touching down on the surface, the lander could not attach itself to the comet due to an unexpected failure of the anchoring subsystem. Instead of staying at the initial touchdown site, the lander bounced and made one big and two further smaller bounces over the comet before finally coming to rest at an unknown location on the rocky terrain. The lander remained mechanically intact and proved to be functional even during the triple bouncing period, keeping radio contact with the Rosetta spacecraft. Afterwards, the lander was able to start its science program on the comet, which has a rotation period of 12.6 hours. Philae reported and delivered autonomously all the measured data of the scheduled experiments reliably and regularly during the radio visibility periods.

Eleven scientific experiments are accommodated aboard the Rosetta spacecraft, and a further ten scientific instruments are aboard the Philae lander: an α-p-x-ray spectrometer; an evolved gas analyser for elemental, molecular and isotopic composition; a panoramic, stereoscopic and descent camera; an infrared microscope; a comet acoustic surface and sounding experiment; a permittivity probe; a dust impact monitor; a multi-purpose sensor for surface and sub-surface science; a magnetometer; a plasma monitor; a comet nucleus sounding experiment; and a drill and sample distribution system.

Philae happened to finally land in a somewhat unfortunate orientation and some of its solar panels seem to be partially in shadow of nearby obstacles. Consequently, the illumination period of the solar panels is shorter than anticipated and the power they produce is less than expected. Under such circumstances the battery cannot be charged effectively enough. However, hope is not lost that Philae may still return to "life" in the coming months as the comet moves closer to the Sun.

The mission – one of the cornerstone missions of ESA – is of high relevance from a technological and research organisational point of view in Europe, and from the scientific point of view worldwide. In recent years, several short-term close observations delivered valuable data about other comets, as in the case in former missions to comets that performed a single, high-speed fly-by. However, the Rosetta mission is unique and provides much more than previous missions. A comet is not a passive, dead chunk of matter. As it moves closer to the Sun in its Keplerian orbit, it becomes increasingly more active. Complex physical and chemical processes take place at an increasing rate in the comet's nucleus, on its surface, in its atmosphere of gas and dust surrounding the nucleus, and in its coma and tail.

It is so far an unparalleled venture, in that a spacecraft smoothly approached a celestial body of such a small mass and size and performed many complicated manoeuvres during its 10-year journey in the Solar System. Furthermore, the Rosetta spacecraft executes additional fine manoeuvres to fly a multitude of low altitude orbits around the comet, mapping its shape and surface in detail never seen before, and will perform many observations and measurements while orbiting the comet for over a year. The Rosetta

spacecraft is richly equipped with scientific instruments delivering a wealth of new knowledge about the CG/67P comet, in addition to spectacular pictures. The Philae lander contributed significant new knowledge with measurements taken directly on the surface of the comet. As scientists interpret, analyse and evaluate the large amount of data gathered, old comet models may prove to be incorrect or need some (perhaps significant) upgrading. New methods and modelling approaches may need to be developed to explain the results of the measurements taken on the comet.

Finally let me adduce an extract from an email we sent to the Philae community:

"It was impressive how the whole community mastered the on-comet in situ conditions after the somewhat unexpected landing scenario. From touchdown, almost nothing ran as originally planned, but the lander – thanks to its robust design – survived its landing on the comet. Afterwards, all teams and individuals did their utmost through the following days and nights; scientists, subsystem teams and lander operators cooperated with each other throughout the mission to make decisions rapidly. The team spirit and commitment to provide an opportunity for all lander experiments to take data, despite the not altogether favourable conditions, was also fascinating."

The "front-end section" of Philae community

RESEARCH GRANTS AND INTERNATIONAL SCIENTIFIC COOPERATION

Valéria Kozma-Blázsik, scientific secretary

Wigner RCP researchers participate in a wide range of national and international scientific collaborations, spanning over 35 countries on different continents. These collaborations are crucial in order to achieve both the scientific goals, as well as provide a sound financial basis for the research activities of the two member institutes.

As government funding accounts for only about 50 % of financial revenue at Wigner RCP, the role of additional sources of income is becoming exceedingly important. Such additional funds come from a variety of sources: the National Fund for Basic Research (OTKA) makes up about 5%, EU cofounded national grants 17%, EU FP grants complemented by other foreign grants 18%, and the remaining 10% come from other scientific contracts.

Thanks to currently funded grants, there was still an increase in overall revenue secured during 2014 compared to the previous year. Despite this, 2014 was a tough year. Hard work was required as Wigner RCP had to balance its budget by topping up its basic government support using additional grant sources. In spite of a sharp decline in the number of newly awarded grants, the overall value of grants in the different categories listed in the previous paragraph still increased, with the notable exception of OTKA grants that of the Hungarian national fund dedicated to basic research.

Concerning OTKA grants a significant decline occurred both in the number and the monetary value of funding received. While in 2013 eleven new projects were started with a total of 58.4 million HUF support, in 2014 less than half that number, only five new OTKA proposals won funding in an amount of 106.6 million HUF. While the value of the new grants seems to be higher, during the same period 5 OTKA projects were completed thus their total monetary value shrunk at first slightly from 275.5 million HUF in 2012 to 271.8 million HUF in 2013, but then more dramatically down to only 218.7 million HUF by 2014. Though the number of OTKA projects running in 2014 remained unchanged, the sharp decrease both in number of successful new proposals and in overall grant amounts received compared to the previous two years raises strong concerns for the future.

The significance of international funding lines cannot be overstated, and it is notable that the safety net that they provide is highly valued and desired by the researchers. As a consequence, Wigner RCP was among the leading research organisations among the 10 new EU countries in the Central Eastern European region in terms of attracting EU FP7 funds.

2014 was the first year of the new Horizon 2020 program period, which required a lot of preparation. Thanks to the EU proposal preparation support of H.A.S. that was offered to research institutes, researchers could actively participate in consortium building events and conferences. In 2014 one FP7 and thirty H2020 proposals were submitted. Five of them won financial support so far and three grant agreements were already signed in 2014,

among them two research infrastructure projects (COMPARE & EUROFusion), and one ICT project on Future Internet (XIFI).

European Research Council
Established by the European Commission

Final paperwork on another two funded projects (AIDA-2020 and IPERION CH) is in progress, while another eleven proposals are currently in the process of evaluation. Most of the proposals submitted are in the Excellent Science pillar. At least five researchers worked on ERC Starting and Consolidator grant projects, Marie Curie Sklodowska Actions. Unfortunately the seven FET Open projects could not be part of the winning teams. In summary of these results, the scientists working on large-scale infrastructure projects are the most successful in becoming partners in various consortiums.

WIGNER RESEARCH INFRASTRUCTURES

The Hungarian Government launched the National Research Infrastructure Survey and Roadmap (NEKIFUT) project as a part of its 2007–2013 mid-term science, technology and innovation strategy. In the frame of this project, a register of Hungarian research infrastructures (RIs[*]) of strategic importance (SRI[**]) was established. In 2014 this register was updated, moreover it was extended to include all RIs rather than SRIs only. All RIs in Hungary and, therefore, all Wigner RIs were eligible to apply for the 'registered' (RRI) or the 'strategic' (SRI) status. The proposals were evaluated and assessed by thematic working groups and the Board of the project, a process resulting in the NEKIFUT Register.

The RIs of Wigner Research Centre have been organized into laboratories. Most of the laboratories are of open access or are members of open-access networks so that they can be used by non-local researchers and companies. Wigner RIs have about 300 external users. Five Wigner RIs, three networks coordinated by the Wigner Research Centre and three further networks with Wigner RI's participation were ranked as "research infrastructures of strategic importance" title while another 13 Wigner RIs became part of the NEKIFUT Register as RRIs.

Research infrastructure of strategic importance of the Wigner Research Centre include:

— Innovative Gaseous Detector Development Laboratory
— Ion beam laboratory of Wigner Research Centre for Physics
— Non-equilibrium and Nanostructured Magnetic Materials Laboratory
— Preparation and complex study of optical single crystals
— Wigner Femtosecond Laser Laboratory
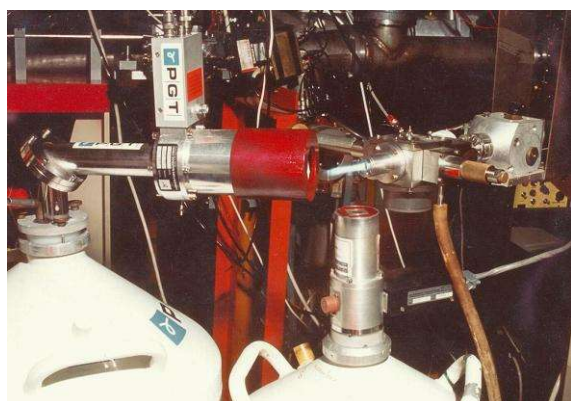
Ion beam laboratory of Wigner Research Centre for Physics

Optical Test Laboratory, part of the FEMTOLAB NEKIFUT RI

SRI networks coordinated by the Wigner Research Centre are:

— Hungarian CERN Grid Consortium
— Network of Hungarian Mössbauer Laboratories
— Optical spectroscopy network

Wigner RIs participate in the following SRI networks:

—— Budapest Neutron Centre
—— Hungarian Ion-beam Physics Platform (HIPP)
—— Hungarian Small-Angle Scattering Network

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[*] Research infrastructure (RI)

A research infrastructure within the NEKIFUT project means equipments, assemblies of equipment, banks of living and non-living material, data banks, information systems and services that are essential for scientific research activities and the dissemination of results. The related human resources form an integral part of RIs that enable the professional operation, use and services. The structure and size of the research infrastructure largely depend on the characteristics of the specific discipline and the needs of the research using the infrastructure.

[**] Research infrastructure of strategic importance (SRI)

An RI is a research infrastructure of strategic importance if all of the following criteria are met: it contributes to solving national tasks of strategic importance; it enables the carrying out of a research activity considered high level by international standards; it provides a research opportunity for more independent research groups and it is open, with equal opportunities for users if they meet the conditions set out in the publicly available regulations; its institutional, funding, management and human resources situation ensures the operation in accordance with the above mentioned criteria.

INNOVATION ACTIVITIES OF WIGNER RCP

Zsuzsanna Tandi, innovation secretary

Although Wigner RCP's primary focus is on basic research and development, we strive to apply our research results in everyday life. In 2014 we searched for different ways to increase collaboration with the industrial sector. Our new innovation strategy is based on experience gained from our contract relationships and on brainstorming with business partners.

In accordance with the strategy determined by Wigner RCP's management, we have established a number of new industrial relationships with companies whose activities are closely related to the research areas of our institutes. This enables us to organise joint market-oriented R&D projects. Numerous proposals have been submitted with the contribution of Wigner RCP. Some proposals have already received grants, while others are still waiting for the result of their evaluation. We have projects for developing real-time respiratory analysis detectors, protocol-managed workflow for medical information systems, metamaterial development for new generation aerial, muon tomography, phase-field modelling of polycrystalline and multi-phase solidification etc.

New industrial connections help support our large-scale consortial proposals. This is supported by the three open laboratories set up at the Institute for Solid State Physics and Optics. Some of their results have been used in an industrial context by companies such as Akusztika Ltd and Hoya Lens Hungary Corporation.

The Intellectual Property Rights regulations of Wigner RCP have been updated to support industrial connections, adjusting to the new code of practice of the Intellectual Property Rights of H.A.S. We have updated our non-disclosure agreement used in business negotiations. We are making efforts to support cooperation among research institutes and industrial companies.

Cooperation within the institutes and between different teams has been developed by means of seminars and discussions that were organised jointly with Zoltán Bay Applied Research Non-profit Ltd. Last year we further developed the hELIos laboratory, where in addition to laser systems based on chirped pulse amplification theory researchers performed numerous experiments related to ELI-ALPS (e.g. analysis of optimal surfaces, pump-experiments etc).

Wigner RCP joined one of the CERN-supported organisations (HepTech – leading high energy physics technologies for industrial technology transfer opportunities), and is keen to learn from the advanced Technology Transfer Office 's (TTO) experiences how to establish its own TTO.

The introduction of the CONVEX project registration system is an important result. This tool is capable of storing the project drafts in a unified form and it provides support for professional, financial, and managerial control of the project plans before their final phase. We created a database that enables us to meet the requirements of recording and saving project documentation, keeping record of the obligations connected to the projects.

OUTSTANDING RESEARCH GROUPS

MTA's "Momentum" Research Teams

The MTA's "Momentum" Program's objective 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 Hungarian Academy of Sciences (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 Groups' purpose is to provide the best research groups with support for a year. Its primary goal is to retain in science and in the Research Centre excellent young researchers who are capable of leading an independent research group. 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-B. Heavy-ion physics

Wigner research group

Gergely Gábor Barnaföldi, Dániel Berényi[#], Tamás Sándor Biró, Miklós Gyulassy, Szilveszter Miklós Harangozó[#], Miklós Horváth[#], Péter Kovács, Péter Lévai, Péter Pósfay[#], János Révai, Károly Ürmössy[#], Péter Ván, György Wolf, Miklós Zétényi
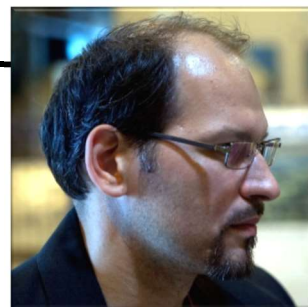
High-energy heavy-ion physics is connected to a large variety of physics disciplines. Our researches probe fundamental concepts of classical and modern thermodynamics, hydrodynamics, and quantum theory. Therefore, we have several theoretical and practical topical research directions covering a wide spectrum, 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). We have continued our theoretical investigations in the direction of high-energy physics phenomenology connected to existing and future state-of-the-art detectors. Concerning international theoretical collaborations we have established joint work with the Goethe Institute (Germany), LBNL (USA), CCNU (China), UNAM (Mexico), and ERI (Japan). We highlight below some of our major published results in details.

Perturbative and non-perturbative QCD. — Recent data from the Beam Energy Scan (BES) and dAu runs at RHIC/BNL, especially azimuthal correlations and spectra at $p_T < 2$ GeV/c, present surprising similarity of azimuthal transverse flow harmonics. These harmonics are mathematically the nth Fourier cosine coefficient extracted from *2m* particle correlation data as a function of the transverse momentum, $v_n^{2m}(p_T)$. At the LHC, pPb and PbPb collision data have challenged the belief that data can be solely interpreted in terms of a local equilibrium "perfect fluid". We reported these results at the Quark Matter 2014 conference. In parallel we published work on azimuthal harmonics associated with initial-state non-Abelian 'wave interference' effects predicted by perturbative QCD gluon bremsstrahlung and sourced by Color Scintillation Arrays (CSA) of color antennas. CSA are naturally identified with multiple projectile and target beam jets produced in inelastic pA reactions. We find a remarkable similarity between azimuthal harmonics sourced by initial-state CSA and those predicted with final-state perfect-fluid models of high-energy pA reactions. The question of which mechanism dominates in pA and AA remains open at this time.

By searching for more general properties of semiclassical fields, we have studied photon fields radiated by a single decelerated point charge. We demonstrated that the illusion of a Landau or a Bjorken flow in rapidity spectra emerges, together with a thermal effect on the transverse momentum distribution related to, but not identical with, the Unruh temperature. In a paper published in EPJ A, we analyzed the classical electromagnetic radiation of an accelerating point charge moving in a straight line trajectory. Detectable differences between our approach and spectra obtained from hydrodynamical models occur at high transverse momenta and are due to interference.

We made continued progress on the application of non-perturbative QCD methods to nuclear phenomena. In the case of non-perturbative directions: applications of the mass-gap method were continued supporting the gluon plasma equation of state.

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New approaches in thermodynamics. — During our searches for the physical origin of the power-law-tailed Tsallis–Pareto distribution, we showed that certain fluctuations in particle number at fixed total energy lead exactly to a cut-power law distribution in the one-particle energy, via the induced fluctuations in the phase-space volume ratio. The temperature parameter is expressed automatically by an equipartition relation, while the q-parameter is related to the scaled variance and to the expectation value of the particle number. For the binomial distribution, q is smaller; for the negative binomial, q is larger than one. These results also represent an approximation for general particle number distributions in the reservoir up to second order in the canonical expansion. For general systems the average phase-space volume ratio expanded to second order delivers a q parameter related to the heat capacity and to the variance of the temperature. However, q differing from one leads to non-additivity of the Boltzmann–Gibbs entropy. We demonstrated that a deformed entropy, K(S), can be constructed and used for demanding additivity. This requirement leads to a second order differential equation for K(S). Finally, the generalized q-entropy formula contains the Tsallis, Rényi and Boltzmann–Gibbs–Shannon expressions as particular cases. For diverging temperature variance we obtain a novel entropy formula.

We have analyzed the role of thermodynamic principles in classical elasticity and derived that the fundamental rheological building block of local equilibrium viscoelastic solids is the so-called Kluitenberg–Verhás body. Therefore the dispersion and damping of elastic waves (for example, in seismology) can be characterized in more detail. We have also investigated an objective and weakly nonlocal extension of classical heat conduction theory, and a requirement of compatibility with kinetic theory and relativistic considerations resulted in a unified classical field theory for heat conduction beyond Fourier law, including ballistic transport.

Hadronization. — By testing our ideas and mathematical results on high-energy experimental data we demonstrated that charged pion spectra in central and peripheral PbPb collisions at 2.76 TeV energy per nucleons, colliding beam energy, obtained via perturbative quantum chromodynamics improved parton model calculations. This can be also approximated by the Tsallis distribution for transverse momenta both above and below 4 GeV/c. We have proposed a model in which hadrons produced in heavy-ion collisions stem either from 'soft' or 'hard' processes and are distributed according to the Tsallis distribution in both types of yields. We described transverse spectra parallel to the aforementioned azimuthal anisotropy (v2) of charged hadrons. We repeated our calculations for various centrality PbPb collisions analytically. Finally we obtained, that the anisotropy decreases for more central collisions.
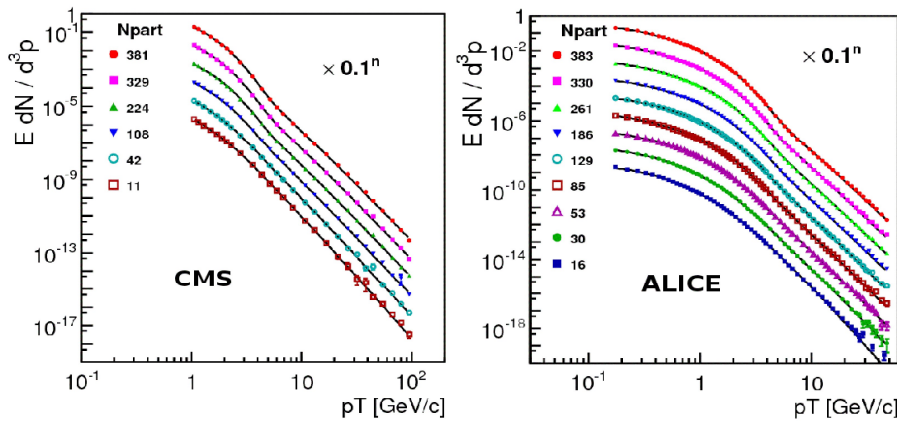

Figure 1. Soft spectra reveal a statistical power-law tail depending on the total multiplicity, while hard spectra show a constant power. (Please consider that the graphs belong to different axis divisions.)

Hadrons at low energy. — The phase diagram of the strongly interacting matter is a heavily-studied field both theoretically and experimentally. Our aim is to develop a model which reproduces the vacuum phenomenology in Quantum Chromo Dynamics (QCD). We developed an effective model, which is an extension of the usual SU(3) linear sigma model, that contains a low energy multiplet for every hadronic particle type. These multiplets are a scalar nonet, a pseudoscalar nonet, a vector nonet, an axial vector nonet, a baryon octet, and a baryon decuplet. We calculated the tree-level baryon masses and possible two-body decuplet decays. The baryon masses are generated through spontaneous symmetry breaking. These calculated quantities are used to determine the model parameters through a multi-parametric minimization process, which compares the calculated physical quantities with their experimental values. We found that the calculated quantities are in good agreement with the experimental data. We apply this model to investigate the chiral phase transition with additional constituent quarks and Polyakov loops. We determine the parameters of the Lagrangian at zero temperature in a hybrid approach, where we treat the mesons at tree-level, while the constituent quarks at 1-loop level. We assume two nonzero scalar condensates and together with the Polyakov loop variables we determine their temperature dependence according to the 1-loop level field equations. We found that only with the identification of the low mass scalar as the f 0 meson is a reasonable phase transition temperature allowed.

Identified hadron spectra with ALICE. — We coordinate the Hungarian contribution to CERN's largest heavy-ion experiment, ALICE, where the main research direction is the analysis of the identified hadron spectra. Our group participates in the High Momentum Particle Identification Detector (HMPID) of the ALICE detector, which aims to measure pion, kaon and proton spectra on a track-by-track basis up to 4.5 GeV/c. Our group participated in the data analysis of the identified spectra and the pion-to-proton ratio. In parallel to this, the ageing test of the HMPID CsI photo-cathode has been performed in addition. Since the ALICE TPC is able to measure the identified spectra we analysed the data measured in pp and pA in collaboration with the Mexican UNAM group. Within the collaboration we signed 21 peer-reviewed high-impact papers, a further 9 conference proceedings, and we presented 6 posters.

In addition to data analysis, our group plays an important role in the following ALICE upgrade work: the proposal for the Very High Momenta Particle Identification Detector (VHMPID), the ALICE TPC upgrade jointly with the Wigner's Innovative Particle Detector Development "Lendület" group, and the ALICE Offline & Online (O2) Upgrade Project together with the Wigner DAQ Laboratory and Wigner GPU Laboratory.

Education, PR and future. — Connected to our group we had 4 PhD and 5 MSc students of which G. Bíró, Sz. Karsai, and R. Kovács participated in young researcher's projects and submitted their Scientific Students' Association (TDK) thesis as well. The following group members participated as guest editors: T. S. Biró as editor-in-chief in EPJ A Hadrons and Nuclei, and guest editor of the Wigner Yearbook 2014, G. G. Barnaföldi as editor YouResAstro 2014 conference proceedings, P. Lévai, T. S. Biró, G. G. Barnaföldi as editors of the Proceedings of the "Wigner 111 Colourful & Deep International Symposium".

Group members actively participated in the following workshop and conference organizations: "ISOTDAQ 2014" at MTA Wigner RCP; "The Future of Many-Core Computing in Science: GPU Day 2014" at MTA Wigner RCP; "Zagreb – Budapest Meetup 2014 for ALICE" in Zagreb, Croatia; "Wigner – CCNU Mini Workshop 2014", at MTA Wigner RCP; "10th International Workshop on High-pT Physics in the RHIC/LHC Era", in Nantes, France; "7th FIKUT: Workshop of Young Researchers in

Astronomy and Astrophysics 2014" at MTA Wigner RCP; "Sigma Phi 2014 Conference" in Rhodes, Greece.

Furthermore, group members participated in PR activities such as the Colorful Physics Bus of the Wigner Institute, the "AtomCsill" series of the Eötvös Loránd Physical Society and Eötvös University, "Girls' Day 2014" at MTA Wigner RCP, the Budapest Science Meetup, and several media appearances in internet news articles, in radio programmes, film, and on television.

Grants

OTKA NK 77816: Theoretical and experimental investigation of high energy particle production in the CERN LHC ALICE experiment (P. Lévai, 2009-2014)

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

OTKA K 71989: Nuclear matter in extreme condition at FAIR (GSI Darmstadt) accelerator (Gy. Wolf, 2008-2013)

OTKA K81161: Experimental and theoretical investigation of heat conduction (Consortium leader: P. Ván, 2010-2014)

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

OTKA K109462: Theoretical investigations of the strongly interacting matter produced at FAIR (CBM, PANDA) and NICA (Dubna) (Gy. Wolf, 2012-2016)

MTA SNK-66 2013: Thermal and mechanical phenomena in media with multiscale microstructure (P.Ván and J.Engelbrecht, 2013-2015, Estonian-Hungarian academic collaboration project)

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)

ESTONIAN – HUNGARIAN academic exchange, Grant no. SNK-66/2013 (Hungarian leader: P. Ván, Estonian leader: J. Engelbrecht).

CHINESE – HUNGARIAN TéT Grant No TET_12_CN_D0524D1E (P. Lévai, 2013-2015).

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

CERN ALICE VHMPID upgrade project, G.G. Barnaföldi (Wigner group leader, 2012-2014)

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

Earthquake Research Institute, (Tokyo, Japan), Thermodynamics of rate- and state dependent friction (T. Hatano).

RHIC, Brookhaven National Laboratory (K. Ürmössy, 2013-2014)

Long term visitor

Mitsui Noa (P. Ván, 1 year), Anja Habersetzer (Gy. Wolf 3 months), Kamel Ourabah (T.S. Biró, 3 weeks)

Ben-Wei Zhang, LongGang Pang, Shen Keming (P. Lévai, 1 month).

Publications

Articles

1. Acconcia TV, et al. incl. Agócs AG, Barnaföldi GG, Bencédi G, Bencze G, Berényi D, Boldizsár L, Futó E, Hamar G, Kovács L, Lévai P, Molnár L, Oláh L, Pochybová S (50 authors): VHMPID RICH prototype using pressurized C_4F_8O radiator gas and VUV photon detector. **NUCL INSTRUM METH A,** 767: pp. 50-60. (2014)

2. Berényi D, Varró S, Lévai P, Skokov VV: Describing pair production in inhomogeneous external fields with the Dirac-Heisenberg-Wigner formalism. **EPJ WEB CONF,** 78: Paper 03001. 4 p. (2014)

3. Berezovski A, Engelbrecht J, Ván P: Weakly nonlocal thermoelasticity for microstructured solids: microdeformation and microtemperature. **ARCH APPL MECH,** 84:(9-11) pp. 1249-1261. (2014)

4. Betz B, Gyulassy M: Constraints on the path-length dependence of jet quenching in nuclear collisions at RHIC and LHC. **J HIGH ENERGY PHYS,** 2014:(8) Paper 090. 24 p. (2014)

5. Biró TS, Jakovác A: QCD above Tc: Hadrons, partons, and the continuum. **PHYS REV D,** 90:(9) Paper 094029. 13 p. (2014)

6. Biró TS, Szendi Z, Schram Z: Quarks, flow and temperature in spectra. **J PHYS-CONF SER,** 509: Paper 012027. 8 p. (2014)

7. Biró TS, Szendi Zs, Schram Zs: Illusory flow in radiation from accelerating charge. **EUR PHYS J A,** 50:(3) Paper 60. 7 p. (2014)

8. Biró TS, Ván P: Classical and quantum parts in Madelung variables: Splitting the source term of the Einstein equation into classical and quantum parts. **EPJ WEB CONF,** 78: Paper 02003. (2014)

9. Biró TS, Barnaföldi GG, Ván P, Ürmössy K: Statistical power law due to reservoir fluctuations and the universal thermostat Independence principle. **ENTROPY,** 16:(12) pp. 6497-6514. (2014)

10. Biró TS, Barnaföldi GG, Ván P: New entropy formula with fluctuating reservoir. **PHYSICA A,** 417: pp. 215-220. (2014)

11. Cimmelli VA, Jou D, Ruggeri T, Ván P: Entropy principle and recent results in non-equilibrium theories. **ENTROPY,** 16:(3) pp. 1756-1807. (2014)

12. Gogokhia V: SU(3) Color Gauge Invariance and the Jaffe-Witten Mass Gap in QCD. **J**

MATH SCI, 197:(6) pp. 761-769. (2014)

13. Gyulassy M, Levai P, Vitev I, Biró TS: Initial-state bremsstrahlung versus final-state hydrodynamic sources of azimuthal harmonics in p + A at RHIC and LHC. **NUCL PHYS A,** 931: pp. 943-948. (2014)

14. Gyulassy M, Levai P, Vitev I, Biró TS: Non-Abelian bremsstrahlung and azimuthal asymmetries in high energy p+A reactions. **PHYS REV D,** 90:(5) Paper 054025. 16 p. (2014)

15. Horváth M, Biró TS: Multicomponent modified Boltzmann equation and thermalization. *EUR PHYS J PLUS* 129:(8) Paper 165. 9 p. (2014)

16. Kopy NK, Čadež A, Lévai P: Few memories of Yakov Zeldovich. **NONL PHEN COMPL SYST,** 17:(4) pp. 467-470. (2014)

17. Kovacs P, Lukacs A, Varoczy J, Wolf Gy, Zetenyi M: Baryon octet and decuplet phenomenology in a three-flavor extended linear sigma model. **PHYS REV D,** 89: Paper 054004. 11 p. (2014)

18. Kovács P, Wolf G: Zero temperature properties of mesons and baryons from an extended linear sigma-model. **J PHYS-CONF SER,** 503:(1) Paper 012035. 5 p. (2014)

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23 Shevchenko NV, Révai J: Faddeev calculations of the K̄ NN system with a chirally motivated K̄ N interaction. I. Low-energy K-d scattering and antikaonic deuterium. *PHYS REV C,* 90:(3) Paper 034003. 15 p. (2014)

24. Topor Pop V, Gyulassy M, Barrette J, Gale C, Petrovici M: Open charm production in p + p and Pb + Pb collisions at the CERN Large Hadron Collider. **J PHYS G NUCL PARTIC,** 41: Paper 115101. 34 p. (2014)

25. Ván P, Berezovski A, Papenfuss C: Thermodynamic approach to generalized continua. **CONTINUUM MECH THERM,** 26:(3) pp. 403-420. (2014)

26. Ván P, Biró TS: Thermodynamics and flow-frames for dissipative relativistic fluids. **AIP CONF PROC** (Mexico City, Mexico: 09. 09 2013.- 09. 13. 2013.), 1578: pp. 114-121. (2014)

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28. Xu J, Buzzatti A, <u>Gyulassy M</u>: Azimuthal jet flavor tomography with CUJET2.0 of nuclear collisions at RHIC and LHC. **J HIGH ENERGY PHYS,** 2014:(8) Paper 063. 87 p. (2014)

29. Xu JC, Buzzatti A, <u>Gyulassy M</u>: The tricky azimuthal dependence of jet quenching at RHIC and LHC via CUJET2.0. **NUCL PHYS A,** 932: pp. 128-133. (2014)

See also: R-I.4, R-P. (Aladi, Földes)

ALICE Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2014, here we list only a short selection of appearances in journals with the highest impact factor.

1. Abelev B et al. incl. <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [947 authors]: Measurement of prompt D-meson production in p-Pb collisions at $\sqrt{s_{NN}}$ =5.02TeV. **PHYS REV LETT**, 113:(23) Paper 232301. 11 p. (2014)

2. Abelev B et al. incl. <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [950 authors]: Exclusive J/ψ Photoproduction off Protons in Ultraperipheral p-Pb Collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. **PHYS REV LETT**, 113:(23) Paper 232504. 11 p. (2014)

3. Abelev B et al. incl. <u>Agócs AG</u>, <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [943 authors] : J/psi production and nuclear effects in p-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. **J HIGH ENERGY PHYS**, 2014:(2) Paper 073. 26 p. (2014)

4. Abelev B et al. incl. <u>Agócs AG</u>, <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [948 authors]: Measurement of charged jet suppression in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. **J HIGH ENERGY PHYS**, 2014:(3) Paper 013. 38 p. (2014)

5. Abelev B et al. incl. <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [945 authors]:Suppression of ψ(2S) production in p-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. **J HIGH ENERGY PHYS**, 2014:(12) Paper 73. 20 p. (2014)

6. Abelev B et al. incl. <u>Agócs AG</u>, <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [942 authors] : Multi-strange baryon production at mid-rapidity in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. **PHYS LETT B**, 728: pp. 216-227. (2014)

7. Abelev B et al. incl. <u>Agócs AG</u>, <u>Barnaföldi GG</u>, <u>Bencédi Gy</u>, <u>Berényi D</u>, <u>Boldizsár L</u>, <u>Dénes E</u>, <u>Hamar G</u>, <u>Kiss G</u>, <u>Lévai P</u>, <u>Molnár L</u>, <u>Oláh L</u>, <u>Pochybova S</u> [941 authors] : Multiplicity dependence of pion, kaon, proton and lambda production in p-Pb collisions at $\sqrt{s_{NN}}$ =

5.02 TeV. **PHYS LETT B**, 728: pp. 25-38. (2014)

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9. Abelev B et al. incl. Agócs AG, Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [948 authors] : Centrality, rapidity and transverse momentum dependence of J/ψ suppression in Pb-Pb collisions at $\sqrt{s_{NN}}$ =2.76 TeV. **PHYS LETT B**, 734: pp. 314-327. (2014)

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12. Adam J, et al. incl. Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [946 authors]: Beauty production in pp collisions at $\sqrt{s}$ = 2.76 TeV measured via semi-electronic decays. **PHYS LETT B**, 738: pp. 97-108. (2014)

13. Abelev B et al. incl. Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [945 authors]: Transverse momentum dependence of inclusive primary charged-particle production in p–Pb collisions at $\sqrt{s_{NN}}$=5.02 TeV. **EUR PHYS J C**, 74:(9) Paper 3054. 10 p. (2014)

14. Abelev B et al. incl. Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [928 authors]: Measurement of quarkonium production at forward rapidity in collisions at $\sqrt{s}$ = 7 TeV. **EUR PHYS J C**, 74: Paper 2974. 24 p. (2014)

15. Abelev B et al. incl. Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [943 authors]: Neutral pion production at midrapidity in pp and Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV **EUR PHYS J C**, 74:(10) Paper 3108. 20 p. (2014)

16. Abelev B et al. incl. Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [957 authors]: Event-by-event mean p(T) fluctuations in pp and Pb-Pb collisions at the LHC. **EUR PHYS J C**, 74:(10) Paper 3077. 15 p. (2014)

17. Abelev B et al. incl. Agócs AG, Barnaföldi GG, Bencédi Gy, Berényi D, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Molnár L, Oláh L, Pochybova S [948 authors]: Two- and three-pion quantum statistics correlations in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV at the

CERN Large Hadron Collider. **PHYS REV C**, 89:(2) Paper 024911. 29 p. (2014)

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See also: R-I (CBM Collaboration)

R-C. Gravitational Physics

Wigner research group

Gergely Debreczeni, Dániel Barta[#], Máté Ferenc Egri-Nagy, István Rácz, Mátyás Vasúth

The Gravitational Physics Research Group of Wigner RCP of the HAS conducts research on various fields including theoretical field theory, numerical and post-Newtonian general relativity calculations, experimental gravitational wave data analysis and fundamental research in algorithm optimization and many-core computer science. The progress and results of last year are summarized below.

Experimental gravitational wave data analysis. — During the year of 2014 the Virgo gravitational wave detector has gone through critical hardware upgrades to increase the sensitivity of the instrument. As such, no new data have been taken. The main activity of the collaboration and of our group was to prepare for the next data taking period, for the operation of the Advanced Virgo detector. As the result of the intense preparatory work, the analysis groups reached a quite high level of maturity in terms of operational and pipeline readiness. The main contribution from our group to this work was the coordination of the algorithmic and computational aspects of this effort. G. Debreczeni acted as the chair of the Virgo VDASC group co-chair of LVCComputing group and as the Computing Coordinator of the Virgo Collaboration. Scientific results and works can be summarized as follows:

1. The Wigner Virgo Group was working on the development of an algorithm (the 'GWorecast' pipeline – see Figure 1) which is, for the first time ever in history of gravitational wave research, able to predict the approximate time and sky location of a compact binary neutron star coalescence event by observing only the early inspiral part of the waves emitted. The applicability of this algorithms will be of utmost important in increasing the confidence level of gravitational wave events associated with gamma ray bursts**.**
2. By exploiting operational level concurrency of the algorithms involved, we managed to increase the sensitivity of the so-called Polynomial search pipeline which looks for the continuous gravitation wave signals emitted by compact binary sources. The outcome of this work was that we managed to extend the volume of the Universe that can be observed by gravitational wave detectors**.**
3. Significant progress has been achieved in the development of the search pipeline of continuously rotating, isolated neutron stars**.**

Reduced basis representations of gravitational waveform templates. — A large number of predicted waveform templates are used by data analysis of targeted search techniques for merging binary black hole sources based upon matched filtering. Waveforms for inspiralling binaries are parametrized by a set of intrinsic physical quantities that result in an eight-dimensional parameter space. The high dimensionality makes gravitational wave searches,

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parameter estimation, and modeling prohibitively expensive and computationally infeasible with most methods. To address these issues, the construction of high-accuracy reduced-basis representations that determines a relatively small set of the most relevant waveforms is essential.
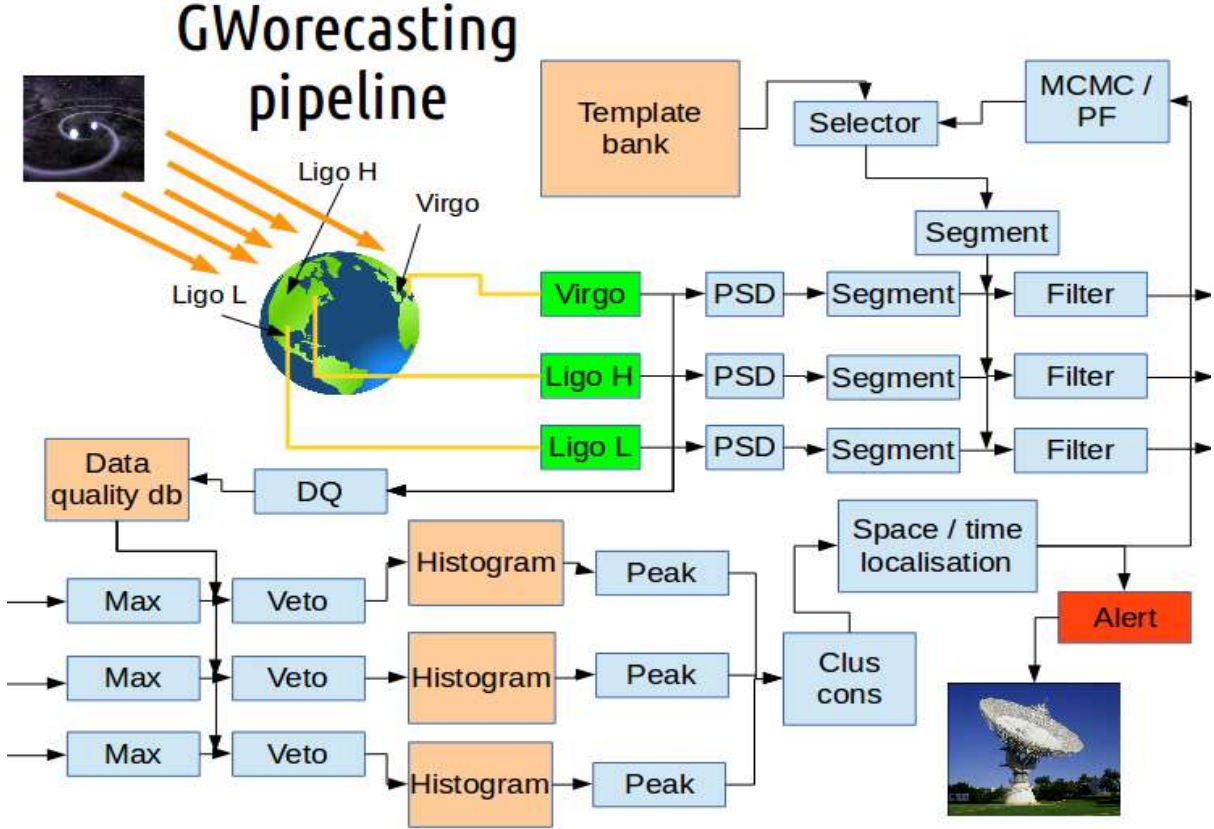

Figure 1. *Schematic flow diagram of the GWorecast algorithm. The goal of the pipeline is to predict the expected arrival time and sky location of the high-amplitude part of gravitational waves and associated gamma ray bursts. Having that information in time, it is possible to trigger collaborating electromagnetic telescopes, thus increase detection confidence by coincident observations.*

Waveform (2.5PN):

$$h_\times(\phi) = -\frac{\mu m \cos\Theta}{a(1-e^2)D_L}$$
$$\times \left[(5e\sin\phi + 4\sin2\phi + e\sin3\phi)\cos2\gamma - (5e\cos\phi + 4\cos2\phi + e\cos3\phi + 2e^2)\sin2\gamma\right],$$

$$h_+(\phi) = -\frac{\mu m(1+\cos^2\Theta)}{a(1-e^2)D_L}\left[\left(\frac{5e}{2}\cos\phi + 2\cos2\phi\right.\right.$$
$$+ \frac{e}{2}\cos3\phi + e^2\right)\cos2\gamma + \left(\frac{5e}{2}\sin\phi + 2\sin2\phi$$
$$\left.+ \frac{e}{2}\sin3\phi\right)\sin2\gamma + (e\cos\phi + e^2)\frac{\sin^2\Theta}{1+\cos^2\Theta}\right]$$
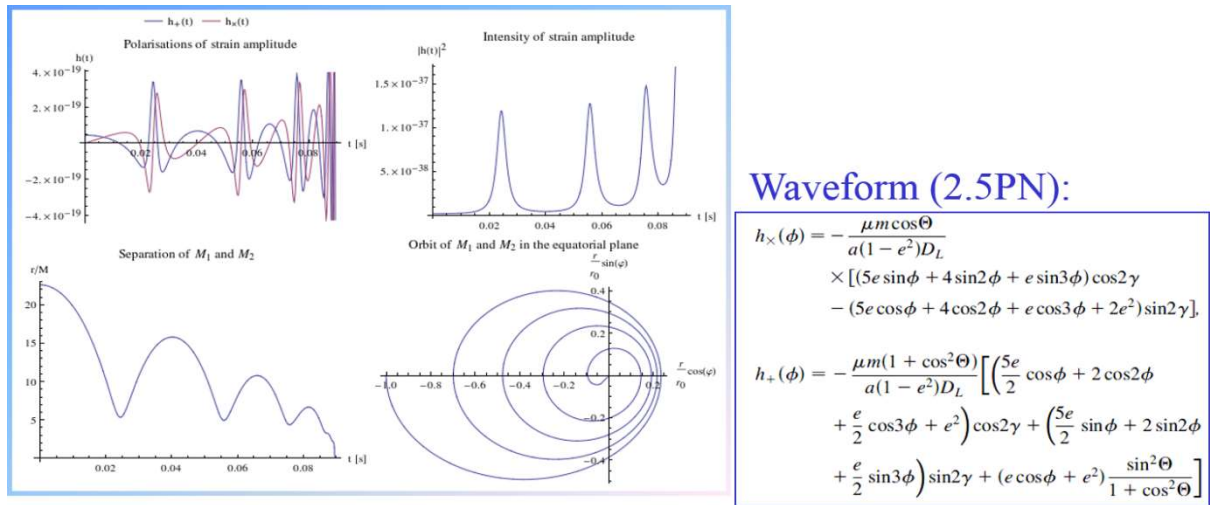
Figure 2. *Numerical integration of the evolution of the orbit and radiated gravitational waves.*

Our goal has been to develop interpolation techniques in the parameter space of waveforms: with a projection to a lower base, this allows one to significantly reduce the number of templates used and the computational demands for the search for signals. Thus the resulted reduction where the eccentricity is about to play the main role will prove to be just as significant as it has been shown in the case of spin. We would like to efficiently compress and accurately represent the space of waveforms for non-precessing binary black hole inspirals, which constitutes eight-dimensional parameter space. It is expected that the resultant reduction where the eccentricity plays the main role will prove to be just as significant as it has been shown in the case of spin.

We have reached a major stage by completing the following steps:

a.) generated a set of TaylorT4-expanded input waveforms that covers the multi-dimensional parameter space domain
b.) developed fast Fourier transforms (FFTs) of the time-domain via discrete sampling of the interpolating functions and by transformation of samples into the frequency domain
c.) defined frequency grids separately for amplitudes and phases over the multi-dimensional parameter space
d.) computed reduced bases for the amplitudes and phases with the SVD
e.) interpolated over the parameter space
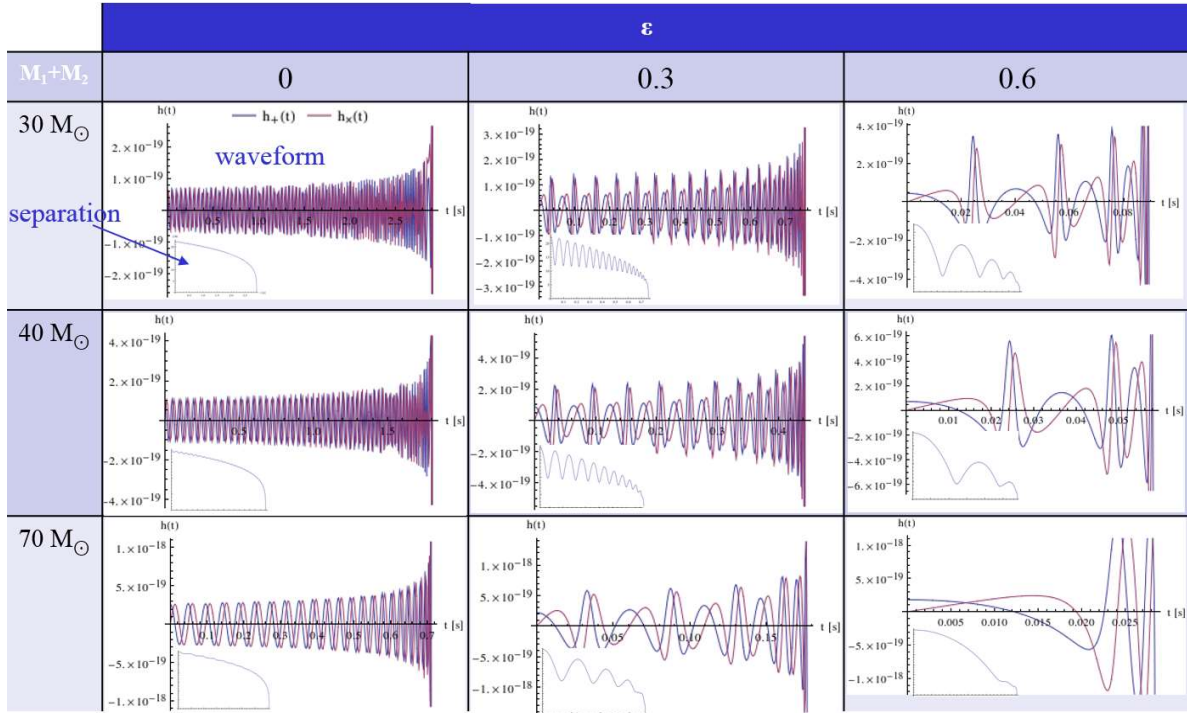f.) assembled the frequency domain surrogate model

Figure 3. *Basis waveforms of different stellar mass and eccentricity are stored in a waveform-databank. Graphical representation of waveforms in the time-domain.*

Hyperbolic capture of compact binary systems. — The coalescence of compact binary systems with high orbital eccentricity is among the significant sources of gravitational

waves. With completion of advanced gravitational wave detectors the detection of these sources is expected within the next few years.

The orbital evolution of inspiralling compact binaries can be conveniently described by the post-Newtonian (PN) approximation. In this weak field approach the gravitational potential and source velocities are considered as small parameters and the motion of the binary is approximated well by perturbed Keplerian orbits. The leading order contributions to the evolution of binaries on open orbits, moreover the energy flux, and the total energy emitted in GWs and the quadrupole contribution to the waveform during the hyperbolic interaction are well described in the literature. Moreover, there exists estimates on the expected rate of hyperbolic encounters in globular clusters and the Galactic Center. Waveforms of the multipole amplitudes for bound and unbound orbits, even the emitted energy and the energy spectrum are also presented.

In our work we have extended the description of binary systems up to the 1.5PN order, with the inclusion of the 1PN and spin-orbit (SO) contributions. Based on the radial motion of the system the conserved quantities characterizing the orbital evolution have been analyzed. Moreover, a suitable parametrization valid for all three types of binary orbits (that is, elliptic, parabolic and hyperbolic) is also introduced. These results allow us to express the radiative change of the energy and angular momentum in terms of the conserved quantities.

Is the Bianchi identity always hyperbolic? — We consider n + 1 dimensional smooth Riemannian and Lorentzian spaces satisfying Einstein's equations. The base manifold is assumed to be smoothly foliated by a one-parameter family of hypersurfaces. In both cases—likewise it is usually done in the Lorentzian case—Einstein's equations may be split into 'Hamiltonian' and 'momentum' constraints and a 'reduced' set of field equations. It is shown that regardless of whether the primary space is Riemannian or Lorentzian, whenever the foliating hypersurfaces are Riemannian the 'Hamiltonian' and 'momentum' type expressions are subject to a subsidiary first order symmetric hyperbolic system. Since this subsidiary system is linear and homogeneous in the 'Hamiltonian' and 'momentum' type expressions, the hyperbolicity of the system implies that in both cases the solutions to the 'reduced' set of field equations are also solutions to the full set of equations provided that the constraints hold on one of the hypersurfaces foliating the base manifold.

Grants and international cooperation
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R-F. Holographic quantum field theory

"Momentum" research team

Zoltán Bajnok, János Balog, Árpád Hegedűs, László Holló[#], Minkyoo Kim, József Konczer[#], Gábor Pusztai, Gábor Zsolt Tóth

Subtitle: On solving the simplest holographic correspondence.

Holography connects gravity in a d+1 dimensional curved space to a strongly-coupled d-dimensional gauge theory living on the boundary of this space. This correspondence is a duality in the sense that quantum gravity is mapped to perturbative gauge theory, while strongly coupled gauge theory to classical gravity, see Figure 1.
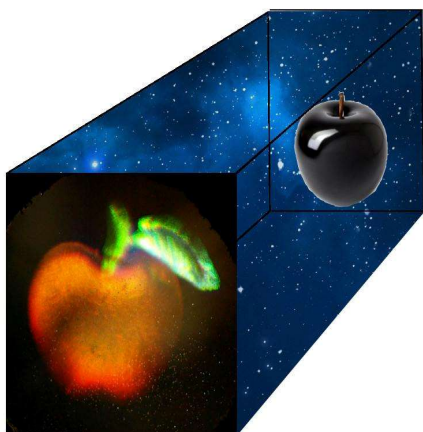

Figure 1. *Shematic figure of the holography, which connects gravity in d+1 dimensions to gauge theory living on the d-dimensional boundary of this space. The colorful holograms of the gravitational objects interact* via their "colors". The strong *chromodynamical interaction of the hologram at the boundary is equivalent to the classical gravitat*ional interaction in the bulk.

The simplest holography connects string theory (including gravity) on anti de Sitter space to the four-dimensional (4D) maximally supersymmetric gauge theory. As the four-dimensional supersymmetric gauge theory is conformal, it is completely determined in terms of its scaling dimensions and three-point couplings.

This simplest holography is described by an integrable two-dimensional quantum field theory, which provides a solid basis for our research. The scaling dimensions correspond to the energy spectrum of this integrable model, while the three-point functions to form factors of certain defect creating operators.

The general strategy to solve integrable field theories is the bootstrap method, the starting point of which is the S-matrix bootstrap. The scattering matrix, which connects asymptotic initial and final states, is determined from its restrictive functional equations (such as unitarity and crossing symmetry) supplemented by additional analytical information. The next step is the form-factor bootstrap, in which matrix elements of local operators between asymptotic states are computed using their analyticity properties originating from the already-computed S-matrix. In the third step these form factors are used to build up the correlation functions via their spectral representation and describe the theory completely off mass shell in infinite volume.

The determination of the finite volume solution is considerably more difficult. In the spectral problem this can be achieved by systematically taking into account the finite size effects due

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to the scatterings of particles. The leading finite size effect of a multiparticle state comes from the quantization of momenta which is dictated by the scattering matrix. It incorporates all polynomial corrections in the inverse of the volume. In addition, there are exponentially small (Lüscher) corrections and their leading contributions come from the polarization of the sea of virtual particles. For small volumes, these effects become dominant and one needs to perform a resummation of the virtual corrections, which sometimes can be carried out in the form of nonlinear integral equations.

The analogous program for the form factors in finite volume is still in its infancy, although it follows essentially the same conceptual steps. The polynomial finite-size corrections in the inverse of the volume are taken into account by changing the normalization of states and restricting the momenta to satisfy the quantization condition. The exponentially small corrections and their possible resummation, however, have been only conjectured for diagonal form factors.

In the simplest holographic duality we are interested not only in the spectral problem of the corresponding integrable two dimensional QFT but we also would like to determine the finite volume form factors of certain defect creating operators.

String theory on the AdS$_5 \times$S^5 background is integrable and its spectrum is conjectured to be in one-to-one correspondence with the anomalous dimensions of gauge-invariant operators in the maximally supersymmetric 4D gauge theory. In the implementation of the bootstrap program the spectral part is basically completed: the scattering matrix has been calculated and the model is solved in infinite volume. In finite volume the leading polynomial finite size corrections were described by the Beisert-Staudacher equations and the leading Lüscher correction of multiparticle states was developed by us and successfully applied for the simplest operators. We also managed to write a finite number of coupled nonlinear integral equations to describe the ground state and some excited-state energies. Recently a very elegant formulation of the finite volume spectral problem has been achieved by the so-called quantum spectral curve method. These are finite coupled equations, which relate the jump of the appearing functions to each other, and has been conjectured for certain special states and sectors of the theory.

Recently we extended the exact description of the spectrum for other sectors of the theory. Specifically, we analyzed two very interesting physical problems: the exact description of the quark anti-quark potential and the tachyonic instability of the brane anti-brane system.

For the quark anti-quark potential we proposed a novel formulation in terms of a system of coupled integral equations, which allowed a systematic weak coupling expansion. We expanded our equations to next-to-leading order and tested the results against direct two-loop gauge theory computations. We found complete agreement.

We also developed a complete description of the brane anti-brane system both in terms of a gauge theory and an integrable model. This enabled us to study tachyons in string theory, which are non-perturbative objects signalling instabilities.

As the spectral problem is conceptually completed, we started to analyze the application of the form-factor bootstrap program to the holographic duality. During the investigation we

observed that there are two kinematically complementary domains of the three-point functions of the conformal invariant maximally supersymmetric gauge theory.

In the first case one of the operators does not carry any charge on the sphere and the three-point function is related to a diagonal finite volume matrix element of a local operator. We started to develop a programme to calculate these matrix elements via diagonal finite volume form factors valid for any 't Hooft coupling neglecting vacuum polarization effects. As a starting point, we investigated the strong coupling limit of these matrix elements which we mapped to classical form factors of the analogous and well-known sine-Gordon quantum field theory. We conjectured that the diagonal form factors of any local operator can be obtained by averaging the operator for the moduli space of classical solutions. We checked this conjecture thoroughly both in infinite and finite volumes.

In the other (and complementary) kinematical domain all the operators have some charge on the sphere. We found that the three point functions do not correspond to form factors of local operators on the world-sheet, rather they correspond to form factors of a defect/boundary-creating operator. In order to gain intuition and new techniques, we developed a form factor bootstrap for such operators in simple integrable toys models and calculated their leading finite-size effects.

Grants
OTKA K 81461: Two dimensional quantum field theories and their applications (Z. Bajnok 2010-2015)

OTKA K 83267: Relativistic particle systems (J. Balog 2011-2015)

OTKA K 109312: Holographic solution to measure theories (Á. Hegedűs 2013-2015)

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

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

International cooperation
MTA Hungarian-Japanese bilateral: Integrability in gauge gravity duality and strong coupling dynamics of gauge theory; Kyoto, Tokyo and Tsukuba (Z. Bajnok, 2013-2014)

TÉT French-Hungarian bilateral: Application of spin chains and super strings to study fundamental interactions: the integrability side of the AdS/CFT correspondence; Paris Saclay and ENS (J. Balog, 2013-2014)

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

Hungarian-Korean-Polish collaboration: On the Gauge-string duality, Seoul, Krakow (Z. Bajnok 2013-2014)

Long term visitors
Ines Aniceto, Lisbon University-31 (Z. Bajnok, 2014.03.02)

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R-G. Computational systems neuroscience

 "Momentum" research team

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

The nervous system provides support for animals in efficient decision making in a variable and often ambiguous environment. Furthermore, research in recent years has shown that these decisions are close to optimal. A key prerequisite to achieve such optimality is that the necessary computations can be performed by the nervous system. In order to identify these computations our research in 2014 took two different paths: 1. we have extended our previous analysis on the link between optimal computations and stochastic neural responses; 2. we have developed a theoretical framework for the role of episodic memory in the integration of novel memories with previous knowledge.

The role of the non-deterministic nature of neural responses is a long-standing puzzle in neuroscience: while the efficiency of the nervous system is undoubted and is hard to reproduce, the working of the individual computational elements, the neurones, is apparently affected by a strong stochastic component. This stochasticity has been ignored by classical theories of the nervous system and was treated as uncontrolled noise. We have formulated a framework in which the stochasticity is not merely the product of a random process but it reflects the inherent uncertainty of the nervous system that arises naturally when interpreting our noisy and ambiguous environment. A key consequence of the framework is that the variability of the neural response distribution is systematically changing with changing stimulus attributes. More specifically, if the uncertainty of the inferences change, concomitant changes in response variability and response correlation is predicted. The proposed scenario is a natural extension of the theory on sensory coding: while the earlier approach aimed at characterising the first moment, the mean, of the neural response distribution, our theory can interpret the stimulus dependence of neural variability and covariability as well. Furthermore, the proposed computational framework is capable of characterising and predicting the structure of the whole response distribution complete with higher-order moments. Inspired by these specific predictions, we systematically revisited the range of studies available in the literature that aimed at characterising response variability and covariability beyond mean responses. Predictions of the theory showed a remarkable match with neurophysiological data. Furthermore, by analysing a publicly available data set, we have demonstrated that relationship between various forms of neural activity correlations (noise, signal, and spontaneous correlations) can be interpreted as a consequence of the same computational principles. These results help us to shed light onto hitherto unaccountable response variability and therefore make possible a deeper understanding of the neural code which ultimately might lead to better characterisation of the principles for designing brain machine interfaces.

One of the most exceptional capacities of the brain is its ability to acquire new knowledge.

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This capacity has been extensively studied by psychology and neuroscience, which led to insight how the nervous system refreshes its representation of the environment; the internal model of the external world. Refreshing the internal model is only one of the challenges the nervous system is faced with: the accumulation of knowledge requires eventual revision of the model itself, that is, the structure of the model needs to be refreshed. This is particularly true for novel environments where contingencies learned earlier are not necessarily valid any longer. Normative theories of learning distinguish between two markedly different approaches: during on-line learning, incoming data is integrated directly into the model reflecting the properties of the environment; while during batch learning data is accumulated first and learning is performed on a large chunk of the data set. The former approach is attractive since it does not necessitate the storage of a large body of data (it requires little capacity for an intermediate storage), but while this method is well suited for refreshing model parameters, using it for updating the model structure is plagued by fundamental problems. Batch learning solves the problem of model structure updates but it comes with the price of excessive temporary storage requirements, which is prohibitive for the nervous system when applying the method in memory processes. In order to find a solution for the constraints of on-line and batch learning methods during internal model updates, we have formulated a theory that provides a principled and statistically optimal framework. A particularly attractive aspect of this framework is that it is characterised by features of a specific, well-known form of memory, the episodic memory. It necessitates the retention of a limited set of data and is designed to forget data points in an optimised manner. This approach provides a normative background for an account on why the nervous system has developed separate memory systems for episodic and semantic memories. A further promise of the theory is that we will be able to predict or even avoid the characteristic systematic failures of the memory.

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R-H. Hadron physics

Wigner research group

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Quarks and gluons. — Particle physics is our attempt to understand the basic constituents of our world. What is it made of? What are the interactions between the building blocks of matter? Symmetries and gauge theories provide a coherent framework for the electromagnetic, weak, and strong interactions. The last of these, the strong force, acts between quarks and gluons and is described by the theory of quantum chromodynamics (QCD). In most circumstances, it is difficult to perform accurate calculations with QCD because the theory is strongly coupled and consequently has a nonperturbative nature. Results from the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory, later reinforced by those from the Large Hadron Collider (LHC) at CERN, showed unexpected phenomena: suppression of hadrons with high transverse momentum (p_T), and weakening of back-to-back jet correlations. These results indicated that quark matter does not behave as a quasi-ideal state of free quarks and gluons, but as an almost perfect dense fluid.

Our research group studies collisions of nucleons and nuclei, performs basic and advanced measurements, and tests theoretical ideas. We participate in several complementary experiments (ALICE and CMS), both in data-taking and physics analysis. In the past year our research group concentrated mostly on the analysis of pPb data recorded at LHC at $\sqrt{s_{NN}}$ = 5.02 TeV energy per nucleon pair. The large amount of collected data allowed us to perform the studies proposed at the beginning of the year.

Size and shape of the created system in pPb collisions. — Measurements of the correlation between hadrons emitted in high-energy collisions of nucleons and nuclei can be used to study the spatial extent and shape of the created system. The characteristic radii and the homogeneity lengths of the particle-emitting source can be extracted with reasonable precision. We have studied the characteristics of the one-, two-, and three-dimensional two-particle correlation functions in various center-of-mass energy pp, pPb, and peripheral PbPb collisions as a function of the transverse pair momentum k_T and of the charged-particle multiplicity N_{tracks} of the event. Charged pions and kaons at low p_T and in laboratory pseudorapidity $|\eta| < 1$ were identified via their energy loss in the silicon tracker. The correlation functions were corrected for the Coulomb interaction between particles. The contributions from other, correlated particle emissions (mini-jets, multi-body resonance decays) were also subtracted. The obtained distributions could be fit by an exponential parametrization in the relative momentum of the particle pair, both in one- and multi-dimensions.

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The extracted exponential radii for pions increase with increasing N_{tracks} for all systems and center-of-mass energies studied, for one, two, and three dimensions alike. Their values are in the range 1–5 fm, reaching their highest values for very high multiplicity pPb and for similar multiplicity PbPb collisions. The N_{tracks} dependence of longitudinal (R_l) and transverse radii (R_t) is similar for pp and pPb in all k_T bins, and that similarity also applies to peripheral PbPb if $k_T > 0.4$ GeV/c. In general there is an ordering for the radii: $R_l > R_t$, thus the pp and pPb source is elongated in the beam direction. In the case of peripheral PbPb the source is quite symmetric, and shows a slightly different N_{tracks} dependence. The most visible divergence between pp, pPb, and PbPb is seen in the so-called "out" radius (R_o) that could indicate the differing lifetime of the created systems in those collisions.
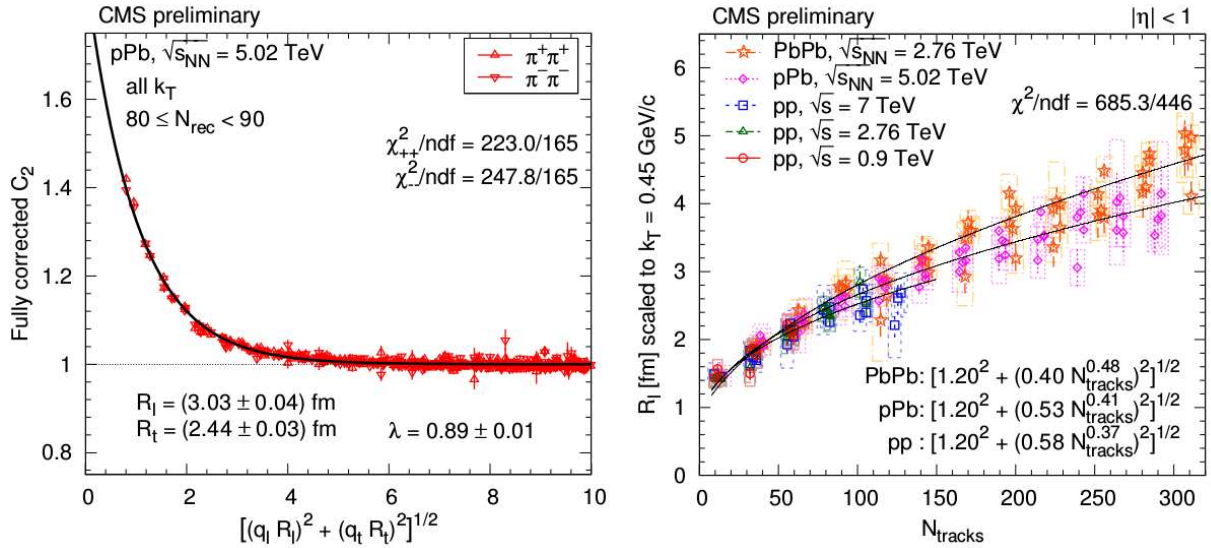

Figure 1. Left: The like-sign correlation function of pions (red triangles) corrected for Coulomb interaction and cluster contribution (mini-jets and multi-body resonance decays) as a function of the combined momentum, in a selected N_{rec} bins for all k_T. The solid curve indicates a fit with the exponential Bose-Einstein parametrization. Right: The longitudinal radius R_l as a function of N_{tracks} scaled to $k_T = 0.45$ GeV/c with help of a parametrization.

The kaon radii also show some increase with N_{tracks}, although its magnitude is smaller than that for pions. Longer-lived resonances and rescattering may play a role here. The pion radii decrease with increasing k_T. The dependence of the radii on the multiplicity and k_T factorizes and in some cases appears to be less sensitive to the type of the colliding system and center-of-mass energy. The similarities observed in the N_{tracks} dependence may point to a common critical hadron density in pp, pPb, and peripheral PbPb collisions, since the present correlation technique measures the characteristic size of the system near the time of the last interactions.

Spectra of high p_T charged hadrons in pPb collisions. — We have measured the charged-particle spectra in pPb collisions in the transverse momentum range of $0.4 < p_T < 120$ GeV/c for center-of-mass pseudorapidities up to $|\eta_{CM}| = 1.8$. The forward-backward yield asymmetry has been measured as a function of p_T for three bins in η_{CM}. At $p_T < 10$ GeV/c, the charged-particle production is enhanced in the direction of the Pb beam, in qualitative agreement with nuclear shadowing expectations. The nuclear modification factor at mid-

rapidity, relative to a reference spectrum interpolated from pp measurements at lower and higher collision energies, rises above unity at high p_T reaching an R_{pPb} value of 1.3–1.4 at $p_T \geq$ 40 GeV/c. The observed enhancement is larger than expected from next-to-leading order (NLO) perturbative QCD predictions that include anti-shadowing effects in the nuclear parton distribution functions (nPDFs) in this kinematic range.
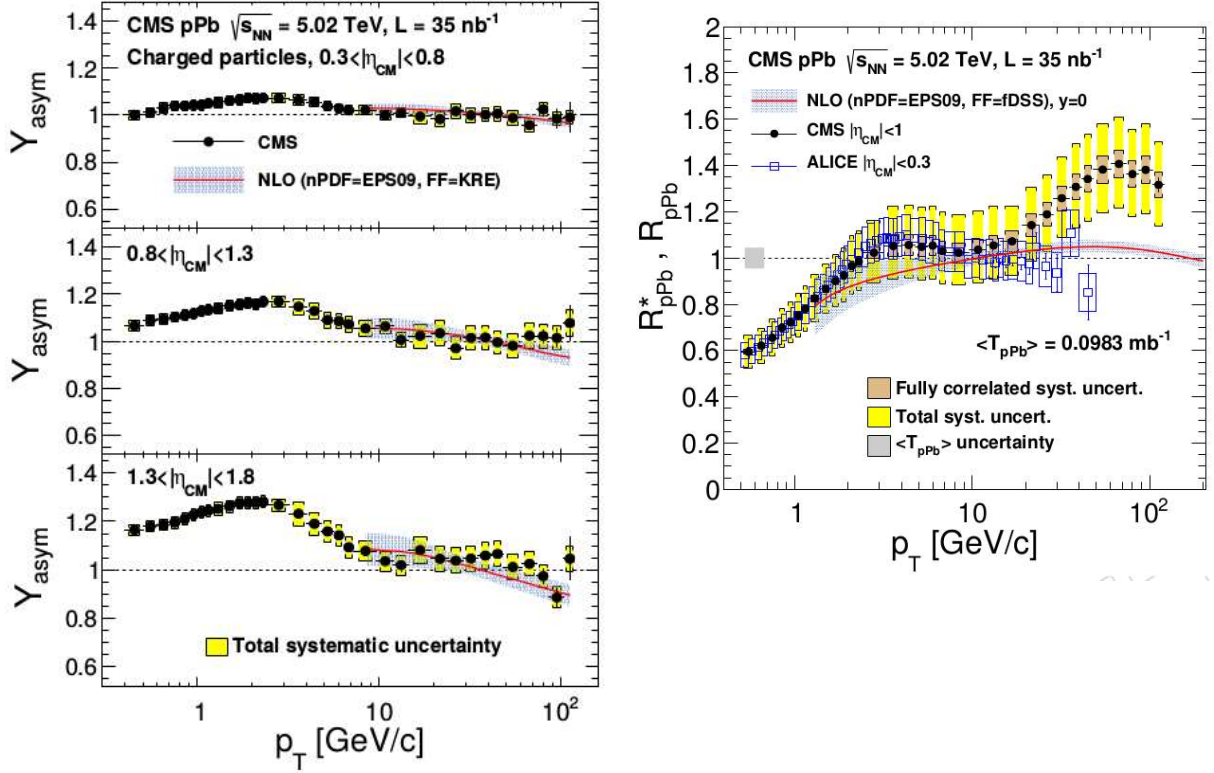

Figure 2. Left: *Charged-particle forward-backward yield asymmetry as a function of p_T for three $|\eta_{CM}|$ intervals. The asymmetry is computed as the charged-particle yields in the direction of the Pb beam divided by those of the proton beam.* **Right:** *Charged-particle nuclear modification factors measured by CMS in $|\eta_{CM}| < 1$ (filled circles), and by ALICE in $|\eta_{CM}| < 0.3$ (open squares), are compared to a theoretical prediction.*

The fact that the nuclear modification factor is below unity for $p_T < 2$ GeV/c is anticipated since particle production in this region is dominated by softer scattering processes that are not expected to scale with the nuclear thickness function. In the intermediate p_T range (2–5 GeV/c), no significant deviation from unity is found in the R_{pPb} ratio. There are several prior measurements that suggest an interplay of multiple effects in this p_T region. At lower collision energies, an enhancement ("Cronin effect") has been observed that is larger for baryons than for mesons, and is stronger in the more central collisions. This enhancement has been attributed to a combination of initial-state multiple scattering effects, causing momentum broadening, and hadronization through parton recombination (a final-state effect) invoked to accommodate baryon/meson differences. Recent results from pPb collisions at $\sqrt{s_{NN}} = 5.02$ TeV and from dAu collisions at $\sqrt{s_{NN}} = 200$ GeV suggest that collective effects may also play a role in the intermediate-p_T region. Most theoretical models do not predict a Cronin enhancement in this p_T range at LHC energies as the effect of initial-state multiple scattering is compensated by nPDF shadowing.

The observed rise of the nuclear modification factor up to $R_{pPb} \approx 1.3$–1.4 at high p_T, albeit with large uncertainty, is much stronger than expected theoretically. None of the available theoretical models predict enhancements beyond $R_{pPb} \approx 1.1$ at high p_T. In particular, although the p_T range corresponds to parton momentum fractions $0.02 \leq x \leq 0.2$, which coincides with the region where parton anti-shadowing effects are expected, none of the nPDFs obtained from global fits to nuclear data predict enhancements beyond 10% at the large virtualities of relevance here. We also show the measurement of the ALICE Collaboration, which is performed in a narrower pseudorapidity range than the CMS one, and uses a different method to obtain the pp reference spectrum based on ALICE pp data measured at $\sqrt{s}$ = 7 TeV. The difference in the CMS and ALICE R_{pPb} results stems primarily from differences in the charged-hadron spectra measured in pp collisions at $\sqrt{s}$ = 7 TeV.

Future direct measurement of the spectra of jets and charged particles in pp collisions at a center-of-mass energy of 5.02 TeV is necessary to better constrain the fragmentation functions and also to reduce the dominant systematic uncertainties in the charged-particle nuclear modification factor.

Spectra of high mass bosons in pPb collisions. — We have measured the Z boson production cross section in the muon decay channel in pPb collisions. The results are presented in the center-of-mass frame with positive rapidity values corresponding to the proton fragmentation region. The Z boson candidates are selected as an opposite-charge muon pair in the 60–120 GeV/c^2 mass range where both muons have p_T > 20 GeV/c and are within the $|\eta_{lab}|$ < 2.4 muon detector coverage. The measured inclusive Z boson production cross section in pPb collisions for the range $-2.5 < y_{CM} < 1.5$ is $\sigma_{pPb}(Z \rightarrow \mu\mu)$ = 94.1 ± 2.1 (stat.) ± 2.4 (syst.) ± 3.3 (lumi.) nb using the calibrated integrated luminosity. For the same restricted rapidity range, the POWHEG simulation predicts 94.0 ± 4.7 nb after multiplying by the number of nucleons in the Pb nucleus (A = 208), which corresponds to the hypothesis of binary collision scaling in pPb.
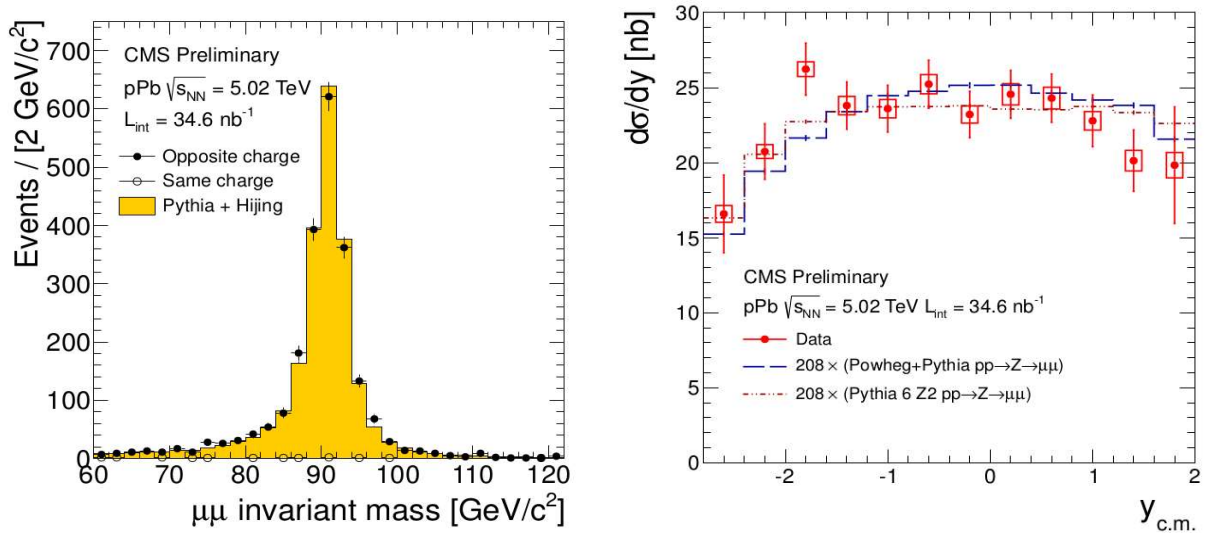

Figure 3. Left: *Invariant mass of selected muon pairs from pPb data compared to a simulation that was normalized to the number of events in data in the signal mass regions.* **Right:** *Differential cross section of Z bosons in pPb collisions as a function of rapidity compared to predictions from* POWHEG+PYTHIA *generator with CT10NLO PDF set, from* PYTHIA *generator with Z2 underlying event tune. All theory predictions are scaled by A = 208.*

The differential cross section as a function of Z boson rapidity is consistent with the theory predictions. The forward-backward ratio, defined as $d\sigma(+y)/d\sigma(-y)$, is expected to be more sensitive to nuclear effects, because normalization uncertainties cancel both in theory and in experiment. Due to the large statistical uncertainties, this measurement is unable to distinguish between different nPDF sets but it can constrain their uncertainties by adding new data points to the global fits in a previously unexplored region of the Q^2–x phase space. The differential cross section as a function of Z boson transverse momentum has been measured and apart from very low transverse momenta it is in good agreement with the predictions from PYTHIA. The results of the presented measurement provide new data points in a previously unexplored region of phase space for constraining nuclear PDF fits.

Thus, Z boson production is unmodified by the hot and dense QCD medium produced in heavy ion collisions, and its yield scales with the number of binary nucleon-nucleon collisions. The nuclear modification factor does not exhibit large deviations from unity showing that nuclear effects are small with respect to the uncertainties of the pPb measurements. The results were compared to NLO theory predictions with and without nuclear modification, that show hints of nuclear effects but more luminosity is needed to distinguish between different nPDF sets. These measurements set constraints for the global fits of nPDFs in a previously unexplored region of phase space.

Quark and gluon jets. — We have studied the proton-to-pion ratio in jets produced in simulated proton-proton collisions at $\sqrt{s}$ = 7 TeV using the PYTHIA 6.4 Monte Carlo (MC) event generator. We compared the p/π ratio in the selected quark-like and gluon-like jets to a reference sample of tagged quark- and gluon-jets. The contamination in the selected jets significantly influences the observed ratios. Thus, despite the different fragmentation of jets originating from quarks or gluons, we see no difference in the proton-to-pion ratio inside these jets, within the used MC model. To see whether this statement holds, we suggest proceeding with similar study using experimental data.

Grants

Publications

Articles

1. Münzer R et al. incl. <u>Fodor Z</u>, <u>Kecskemeti J</u>, <u>Seres Z</u> (67 authors): SiΛvio: A trigger for Λ-hyperons. **NUCL INSTRUM METH A**, 745: pp. 38-49. (2014)

See also: R-I.3,

CMS collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2014, here we list only a short selection of appearances in journals with the highest impact factor.

1. Chatrchyan S et al. incl. <u>Bencze Gy</u>, <u>Hajdu Cs</u>, <u>Hidas P</u>, <u>Horvath D</u>, <u>Sikler F</u>, <u>Veszpremi V</u>, <u>Vesztergombi Gy</u>, <u>Zsigmond AJ</u> [2200 authors]: Evidence for the direct decay of the 125 GeV Higgs boson to fermions. ***NATURE PHYSICS*** 10: pp. 557-560. (2014)

2. Bodwin GT et al. incl. <u>Bencze Gy</u>, <u>Hajdu Cs</u>, <u>Hidas P</u>, <u>Horvath D</u>, <u>Sikler F</u>, <u>Veszpremi V</u>, <u>Vesztergombi Gy</u>, <u>Zsigmond AJ</u> [2200 authors]: Fragmentation contributions to J/ψ production at the Tevatron and the LHC. **PHYS REV LETT**, 113:(2) Paper 022001. (2014)

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NA49 Collaboration

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See also: R-B. ALICE Collaboration, R-I. NA61/SHINE Collaboration

R-I. "Lendület" innovative particle detector development

"Momentum" research team

Dezső Varga, György Bencze, Gyula Bencédi[#], Ervin Dénes, Gergő Hamar[#], Gábor Kiss[#], Tivadar Kiss, András László, Krisztina Márton[#], László Oláh[#], Éva Oláh[#], Tamás Tölyhi

The activities of the group can be divided into two categories. The first concerns the rapid evolution of the laboratory infrastructure necessary for long-term future commitments. The second concerns initiating or continuing specific research subjects, developments on the high resolution single photon UV scanning, results from the Low Momentum Particle Detector (LMPD) for the NA61 Experiment, cosmic muon detection, activities for the ALICE Experiment, and education activities. These are reported below.

Refurbishment of the laboratory environment started last year and has been completed to match the necessary scientific requirements. This involved a substantial commitment on the side of the participants, including training in low-dust environments and precision gas systems. The main lab room (Building 2, room 111) includes equipment for the most sensitive test activities: gas distribution, precision high voltages, and various data acquisition systems (DAQ). The "Construction Lab" (Building 2) includes the clean compartment of 8 m^2 area, with a flat table assured for ISO5 (grade 100) quality. These developments are critical for the long-term competitiveness of the group. The laboratory became part of the National Research Infrastructure Survey and Roadmap (NEKIFUT).

Among the research objectives, the Leopard project (high-resolution scanning of thick gas electron multiplier (TGEM) structures with single UV photons) continued to be successful and has seen considerable improvements within the framework of the RD51 Collaboration. Now the classical GEMs, with a hole diameter of 50 μm, became visible, and therefore became an integral part of the AIDA2020 project; Task 12.4.4, with Wigner RCP as project leader. Figure 1 below shows high-resolution images of these, including a hole-by-hole gain map showing increased gain at the GEM edge (upper part of right panel).
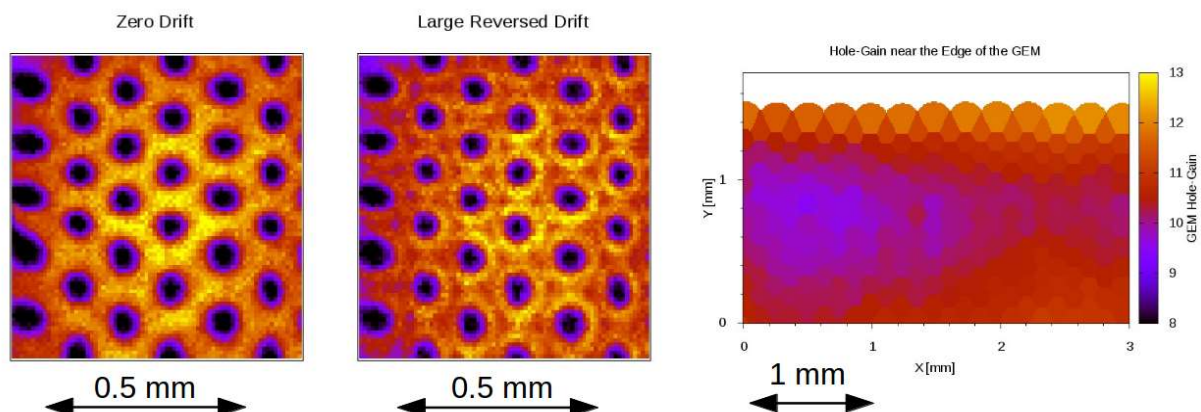

Figure 1. *Leopard images of a classical GEM layer. With improved resolution of 15 micron, the fine structures (left and middle) as well as single hole gains (right) are quantified.*

[#] Ph.D. student

Members of our research group are key participants at the **CERN NA61 (Shine) Experiment**. The Low Momentum Particle Detector, built in 2011-2012, has been fully calibrated during the year and its data has been analyzed. The purpose of the LMPD is to detect slow particles that are characteristic of the collision centrality in hadron-nucleus interactions. Figure 2 shows an image of the detector; single tracks emerging from the target are clearly detected (left panel).
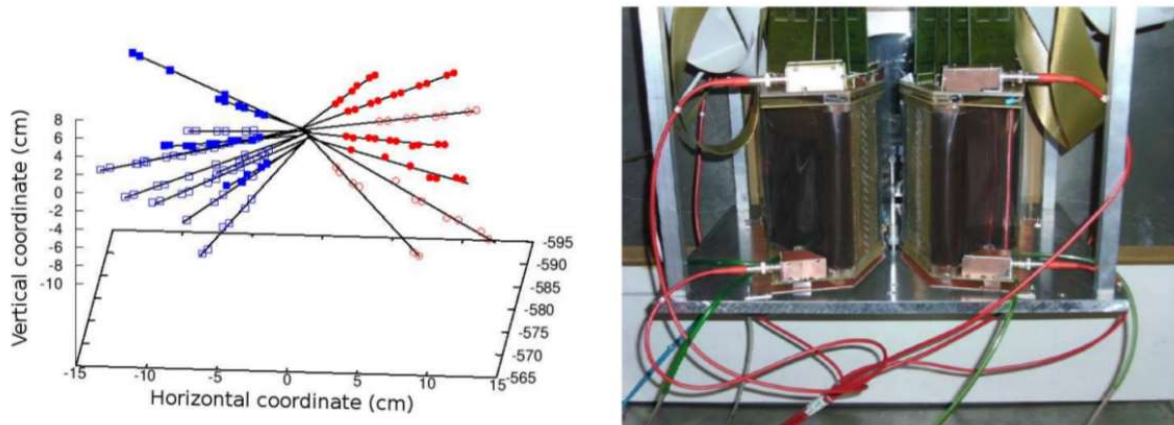

Figure 2. *The Low Momentum Particle Detector of the NA61 Experiment at CERN, constructed in 2011-2012. The tracks are clearly identified (left) emerging from the target which sits in the middle of the two halves of the detector (right)*

After the full calibration performed at CERN, and refined data analysis, published results show excellent tracking performance and demonstrated particle identification. The image of the target is shown in the left panel of Figure 3, whereas the capability to separate the particle charge (mostly protons and He isotopes) is shown in the right panel.
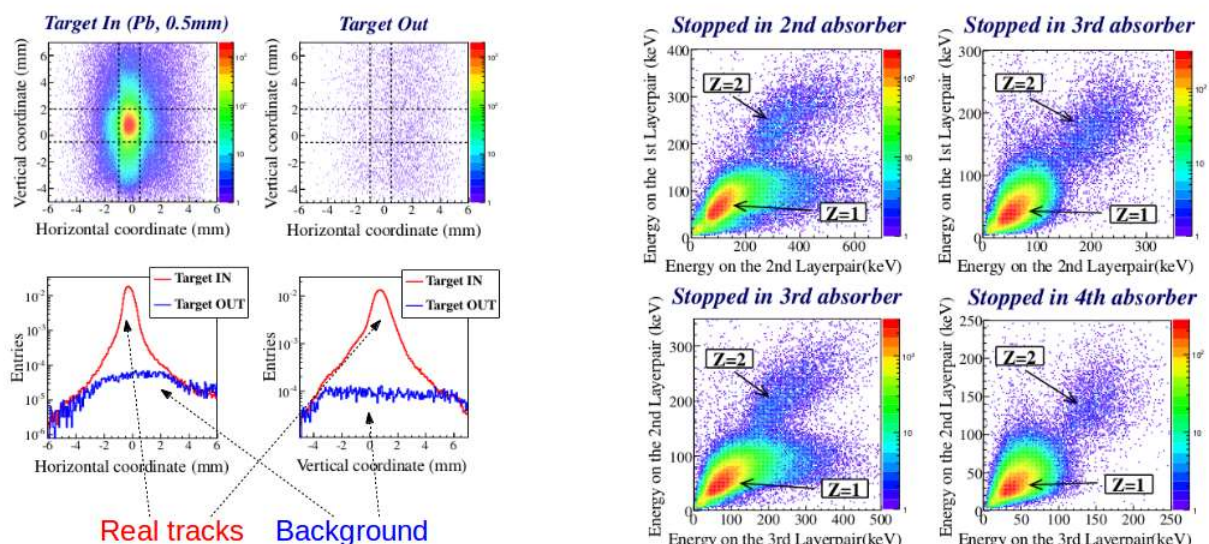

Figure 3. *The LMPD tracking performance is well demonstrated by the low level of background contamination below 1% fraction, whereas with a real target installed the trajectories emerge from a small spot (left). The LMPD can identify particles by ionization: H and He nuclei are clearly separated (right)*

Research activities for **cosmic muon detectors** were aimed at two directions: one is the earlier established underground flux observation, the other is transmission tomography to map the 3D structures of material placed inside the detector system. An example of the latter is shown in Figure 4, where the test objects appear clearly measured by cosmic muon scattering strength. Such detectors may find applications in security systems, for which a collaboration between NKE (National Security and Public Service University) and Wigner RCP has been initiated.
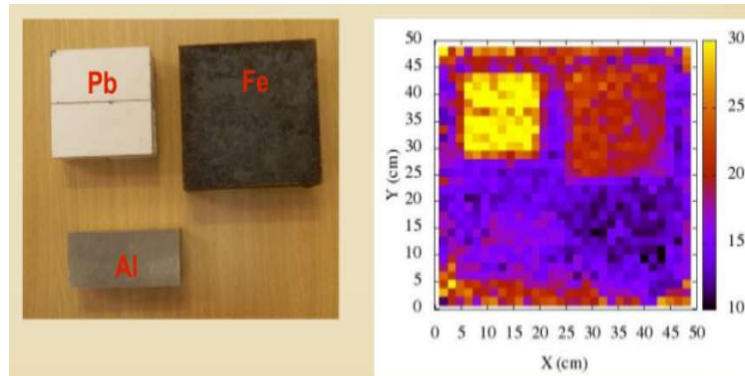

Figure 4. *Test objects (left) placed inside a cosmic muon detector can be imaged (right) by measuring muon scattering. High-Z materials such as lead provide a very strong signal, even if so thick that X-rays can not penetrate them.*

The collaboration with the **ALICE Experiment at CERN** has received a new boost from our group's entry to the Time Projection Chamber (TPC) Upgrade project. GEM detectors will replace the TPC readout chambers to enable continuous event readout, and consequently reach a 100-fold gain in speed.

Secondary school students, along with their teacher, Éva Oláh, were highly active. This activity received an "Útravaló" grant to support the education of students and common work. Approximately 10 students participated in the building and performance demonstration of the multi-wire proportional chamber (MWPC).

Grant
 "Momentum" Program of the HAS (D. Varga, 2013-2018)

International cooperation
CERN NA61 Collaboration (A. Laszlo and K. Marton), CERN RD51 Collaboration (Gy. Bencze, G. Hamar and D. Varga), CERN ALICE Collaboration (G. Hamar, Gy. Bencedi and D. Varga)

Long term visitor
Kristian Engeseth, Bergen University (D. Varga, 3 weeks)

Publications

Articles

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

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

R-J. Standard model and new physics

Wigner research group

Viktor Veszprémi, Dániel Barna[A], Márton Bartók[#], Lajos Diósi, Csaba Hajdu, András Házi[#], Pál Hidas, Dezső Horváth, Gabriella Pásztor[A], József Tóth, Tamás Vámi[#], György Vesztergombi

Physics analyses. — Our group has been participating in the studies of the newly-discovered Higgs boson and have shown that its properties indeed correspond to the predictions of the Standard Model. We presented this result both at international conferences and institutional seminars, and also in two books.

We have performed searches for supersymmetric particles in 8 TeV proton-proton collision data which was collected in 2012. In these searches, we were looking for possible signatures of gluino-pair production and decays to top squarks where b-jets, a lepton, multiple light flavor jets, and missing transverse momentum were present. We also measured the reconstruction and identification efficiencies of electrons and muons by performing an auxiliary measurement of events where leptonically decaying Z bosons and multiple jets are produced. No excess was observed in these searches and the results were interpreted as exclusion limits on the mass parameter space of simplified models of on- (real) and off-shell (virtual) top squarks production via gluino pairs.

Theoretical work. — Theoretical activity in quantum and gravity foundations, as well as in open quantum system dynamics has been continued. The yet hypothetical gravity-related spontaneous wave-function collapse has been derived for the first time in acoustic modes of bulk matter. Proposals of various related experimental tests have been outlined including a specific Cavendish experiment to test a possible quantum-delay of Newton gravitational force.

Thorough investigations of the Gaussian class of non-Markovian open quantum systems have led to a general mathematical structure showing strong resemblance with the well-known and widely-used special Markovian case; that is to say, with the famous Lindblad structure and master equations.

Work on instrumentation. — Our team continued to contribute strongly to the operation, calibration, and data-reconstruction of the CMS Tracker detectors: the inner silicon pixel, and outer silicon strip detectors. We have provided a coordinator for the CMS Tracker Detector Performance group, and one for its CMS Pixel calibration and local reconstruction subgroup.

The two most important performance parameters of the pixel detector are hit detection efficiency and position measurement resolution. They determine the efficiency and accuracy of charged particle track reconstruction. Charged particle tracks are used in the determination of the secondary (decay) vertices of heavy flavor jets, which are produced in

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[A] Associate fellow
[#] Ph.D. student

the supersymmetric events of our interest. We have found an efficiency loss at the per cent level in data acquired by the pixel detector which was not reflected by the simulation. We have improved the simulation of the CMS pixel detector and presented the results in a conference. We also measured the radiation damage experienced by the pixel detector. Radiation damage has an impact on the resolution of the hit position measurement. We found disagreement between the detector performance and its simulation in the official CMS software. We have implemented a new method which transforms the charge distribution of clusters in the pixel according to the expected radiation damage at given operational configuration (bias voltage, temperature, etc.) One of the most important aspects of detector readiness is the maintenance of the calibration databases which is entirely the responsibility of our group. We improved the resolution measurement also by introducing a new calibration object to correct for the apparent shift of cluster positions due to the presence of magnetic field as function of the irradiation in the silicon bulk.

Detector construction. — Radiation-induced damage of sensors and readout electronics degrades the resolution of position measurements in the CMS Pixel detector to the extent that the detector is rendered unusable. Therefore it will need to be replaced. This will happen in two steps in the next couple of decades called phase I and II upgrades. Our group has played a leading role in studying radiation effects and now we are also key contributors to the design of the new-generation pixel detector. We have designed and built the first prototypes for the control and readout electronics of the CMS Phase I Pixel upgrade detector.

The Liquid Argon Calorimeter is a basic component of the ATLAS detector. Its capabilities of detecting electrons, photons, jets and missing energy are crucial ingredients of discovering theoretically predicted new physics phenomena, like Supersymmetry, and of analyzing features of the Standard Model, including detailed experimental study of the Higgs boson. Because of the significant increase of the LHC luminosity in the coming years, the LAr Phase I Upgrade Project was defined and accepted to maintain and improve the performance of this detector. Being involved in the LAr group of CPPM, which is responsible for the upgraded back-end electronics of the level1 electromagnetic calorimeter's trigger system, we joined this effort with the aim of defining software algorithms to perform fast (trigger) electron selection. During data-acquisition, it is used in real-time identification of multi-lepton final states which are the result of associated production of charginos and neutralinos, while rejecting background as much as possible. This year, the first steps to reproduce the results of the TDR and check the existing software tools have been done and presented at several internal ATLAS working meetings.

Maintaining the CMS grid computing infrastructure. — The CMS computing grid is used in the reconstruction of both simulated and collision data which are analyzed in our searches for new physics. Stable operation of the T2_HU_Budapest grid site continued in 2014 giving us the third position in the site availability ranking of CMS T2 sites. Hardware developments included an upgrade of the external network connection to 10 Gbits/s, and the addition of 192 WN CPU cores and 40 TB disk storage.

Grant

Publications

Articles

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Book chapter

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See also: R-P.1

ATLAS collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2014, here we list only a short selection of appearances in journals with the highest impact factor.

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PHYS, (9) Paper 103. 54 p. (2014)

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See also: R-H. CMS Collaboration, R-H. NA49 Collaboration, R-I. NA61/SHINE Collaboration

R-K. Femtosecond spectroscopy and X-ray spectroscopy

"Momentum" research team

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Novel experimental and theoretical insights into the mechanism of light-induced spin-state switching. — Switchable transition-metal-based molecular systems have great potential in future information technology as very high density devices with rapid transitions. Light-switching in such complex compounds to a proper metastable state is possible at low temperatures only (typically below 30–50 K). Unveiling the details of the relaxation processes that follow the light excitation could lead to a complete understanding of the involved mechanisms, which may promote the design of more efficient systems. Here we report experimental and theoretical results that bring us closer to these aims.

Time-resolved X-ray spectroscopy reveals intermediates of molecular photoswitching with lifetimes on the order of femtoseconds. — A prototype light-switchable compound that has become a benchmark system for ultrafast studies, $[Fe(bipy)_3]^{2+}$ (bipy: 2,2'-bipyridine), can be excited from its singlet ground state to a quintet state. Changing the spin momentum by two ($\Delta S=2$) on the $3d^6$ iron in this molecule cannot take place in a single step, yet the characteristic time of this spin-state transition is rather short, about 300 fs. To understand the detailed mechanism of the spin-state switching it is crucial to reveal the elementary processes of this 300 fs identifying the transient states in the sequence that follows the $^1A_1 \rightarrow {}^1MLCT$ (Metal-to-Ligand Charge Transfer) excitation, on the way to the $^5T_2$ state. As known from spectroscopy and theory, several metal- or ligand-centered triplet states can be found between the ^1MLCT and the quintet states. According to the more than 20-year-old description of Andreas Hauser, the de-excitation takes place in consecutive steps of inter-system crossings and internal conversions via these states. Others doubted whether these can all take place on a sub-picosecond time scale, and suggested that strong coupling between the ^3MLCT and the quintet, whose potential crosses the $^{1,3}MLCT$ band close to its minimum, might explain the rapid transition better. A very recent theoretical work, however, claimed that the steps via the triplets could indeed be fast, and suggested the sequence $^1A_1 \rightarrow {}^1MLCT\ (\rightarrow {}^3MLCT) \rightarrow {}^3T_2 \rightarrow {}^3T_1 \rightarrow {}^5T_2$. Optical studies could not resolve the possible intermediate triplet states. Therefore, we carried out ultrafast optical-pump–X-ray-probe experiments at the Linac Coherent Light Source (LCLS) of the Stanford Linear Accelerator Center. In previous works we have shown that hard X-ray emission spectroscopy (XES) is particularly sensitive to the spin state of transition metal ions, and demonstrated that this can be exploited even in ultrafast experiments. Applying this technique at the Kβ line in LCLS could indeed resolve the temporal evolution of transient states with 100 fs time resolution. The experimental set-up and the main results are shown in Figure 1. The time evolution of the transient XES spectra is shown in Fig. 1b, which is constructed for each measured time delay as the difference of the measured XES signal from the ground state

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spectrum. Fitting appropriate reference XES difference curves to this surface allowed us to identify the MLCT and metal-centered triplet intermediates, and to characterize the time dependence of their populations. A cartoon of the identified states and transitions is seen in Fig. 1c, while the derived kinetics with the characteristic times are shown in Fig. 1d. Our result provides experimental evidence for the involvement of at least one of the ^3T triplet states in the de-excitation cascade, and thus excludes the direct transition from the MLCT band to the quintet, in very good agreement with the latest theoretical expectations. However, the achieved 100 fs experimental resolution have not allowed us to unravel all details of the de-excitation, as this would require improving the time resolution by an order of magnitude. Nevertheless, this work constitutes a milestone in both the ultrafast application of X-ray spectroscopy and the understanding of photoswitchable molecules.
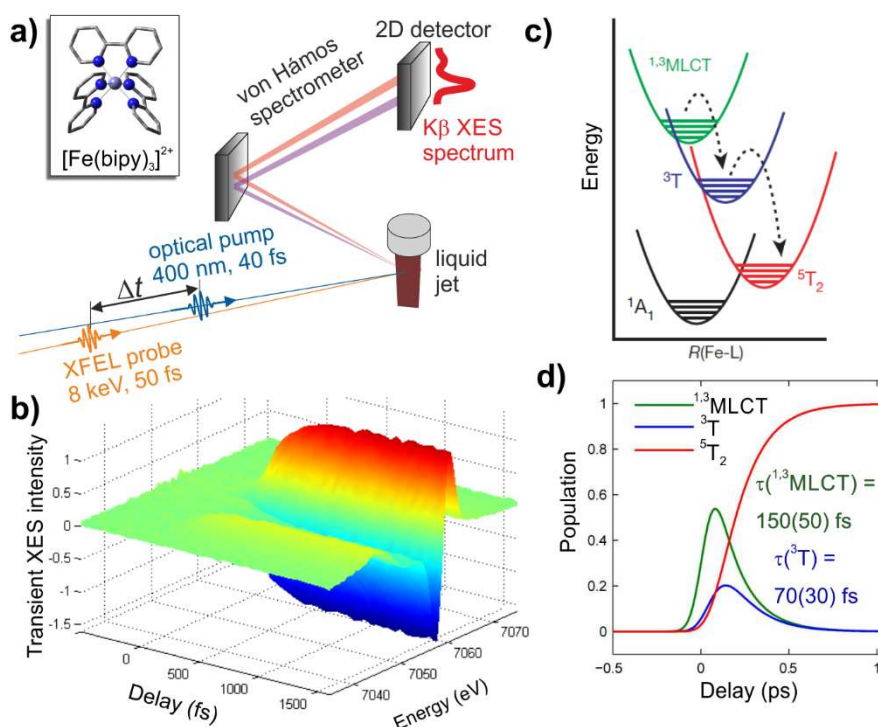

Figure 1. *The molecular structure of [Fe(bipy)$_3$]$^{2+}$ and the experimental setup used at the XPP beamline of LCLS (a). Time evolution of the transient XES signal (b). Schematics of the observed states and transitions (c), and kinetics determined from fitting the transient XES (d).*

Quantum-chemical modelling of electronic states relevant to transitions in light-excited molecules. — First-principle theoretical modelling of the properties of complexes, including the determination of the potential energy curves of the electronic states involved in the mechanism of the molecular switching is vital to the interpretation of the experimental data, and shall lead to a better understanding of the de-excitation mechanisms of these systems. Moreover, it can pave the way to effective optimization of the molecular properties via ligand engineering leading to systems with high potential towards applications.

Relevant molecular electronic states and their potential energy surfaces have been studied in detail using density functional theory (DFT), time-dependent DFT (TD-DFT), and multiconfigurational second order perturbation theory (CASPT2) methods. Figure 2 displays

our DFT and TD-DFT results of the $[Fe(bipy)_3]^{2+}$ molecule (the same that have been discussed above with respect to experimental results), obtained with B3LYP* functional and TZVP basis set. The figure represents a fairly realistic picture of the potential energy curve structure of the different states that were schematically represented in Fig. 1c. The arrows signify the expected $^1A_1 \rightarrow {}^1MLCT \rightarrow {}^3MLCT \rightarrow {}^3T_2 \rightarrow {}^3T_1 \rightarrow {}^5T_2 \rightarrow {}^1A_1$ set of transitions of the full photocycle. It is evident that this energy structure is fully compatible with the experimental findings, and shows that such calculated potential energy surfaces can be predicted with fair confidence.

The pattern of the potential energy curves for all Fe(II) switchable compounds is qualitatively similar to the one for $[Fe(bipy)_3]^{2+}$. The main difference between these molecular compounds is characterized by the energy difference between the lowest singlet ($^1A_1$) and quintet ($^5T_2$) electronic states, which determines whether the complex can be trapped in the excited high spin state for long enough times, a property highly important for molecular switching applications. In molecules with a large gap, usually referred to as complexes with high ligand field splitting, relaxation to the singlet ground state occurs at a reasonably high rate at room temperature, often characterized by a time scale of about a nanosecond. Actually, the energy gap between the quintet and singlet states are usually smaller than that in $[Fe(bipy)_3]^{2+}$, resulting in even slower relaxation to the ground state for most Fe(II) compounds. Therefore, it was astonishingly found in 2013 that in the case of the iron(II) complex with the tridentate ligand 2,6-bis(imidazol-2-ylidene)pyridine transient absorption measurements revealed the excited-state deactivation back to the ground state occurs within 10 ps. (The structure of the complex can be seen in the top of Fig 2b; the ligand is denoted as "CNC" after the atoms that bond to the iron.) This particular behavior hints that the energy of the states are rather unusual. It has been suggested that in this system the lowest excited state of the Fe(II) ion is a triplet and not a quintet, so the quintet state does not participate in the relaxation processes. Spin-orbit interaction between the singlet and triplet electronic states can cause a sufficiently strong coupling, which can be correlated with short lifetime. This expectation has been confirmed by our DFT and TD-DFT calculations. As can be seen in Fig. 2, when compared to the case of $[Fe(bipy)_3]^{2+}$, the potential energy curve of the quintet state in $[Fe(CNC)_2]^{2+}$ is shifted toward larger values of the Fe–ligand bond lengths, and the energy minimum of the lowest quintet state exceeds that of the lowest triplet. Moreover, the intersection points of the quintet curve and the MLCT band as well as the metal-centered triplet curves are located far more out than what would be optimal for a transition to the quintet. The destabilization of the quintet state, and the strongly modified potential energy surface with radically shifted intersection points provide a clear indication of why no significant quintet population is observed. A possible deactivation pathway is represented by arrows.
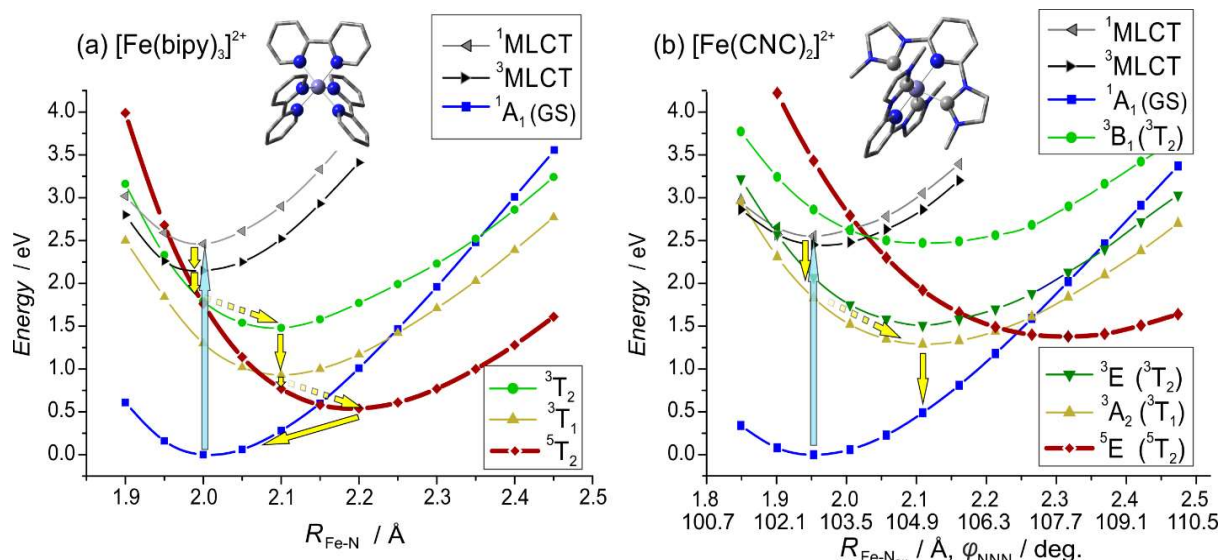
Figure 2. *Selected DFT and TD-DFT potential energy curves for [Fe(bipy)₃]²⁺ (a) and [Fe(CNC)₂]²⁺ (b) along configuration coordinates which connect their singlet and quintet minima. For the latter complex the symmetry is reduced to D₂d, but in parenthesis the octahedral parent terms are also given. The arrows indicate potential transitions for each photocycle.*

Interestingly, such complex behavior can result in a longer-lived ³MLCT state, which plays a major role in the mechanism of light-harvesting systems. The photosensitivity of ruthenium-based complex molecules combined with their long-lived ³MLCT states make them highly favorable for such systems. However, the low abundance of ruthenium would necessarily make Ru-based devices production uneconomical. Using the earth-abundant, inexpensive, and environmentally benign iron instead of ruthenium as photosensitizers would be an important step to promote light-harvesting and photocatalytic applications on a large scale.

Grants

International cooperation

Main cooperation: 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)

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See also: R-M.5

R-S. Space Physics

Wigner research group

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Space Weather

The Sun, the planets and other solar system objects are coupled together by charged particles and fields, which fill interplanetary space. The details of this complex plasma interaction are the subject of space weather studies. It includes questions about how particles and fields of solar origin interact with solar system objects. The final goal of these studies is to understand how our global environment influences life on Earth. In this year we investigated several aspects of space weather, including the distribution of interplanetary magnetic flux, supra-thermal electrons and ions.
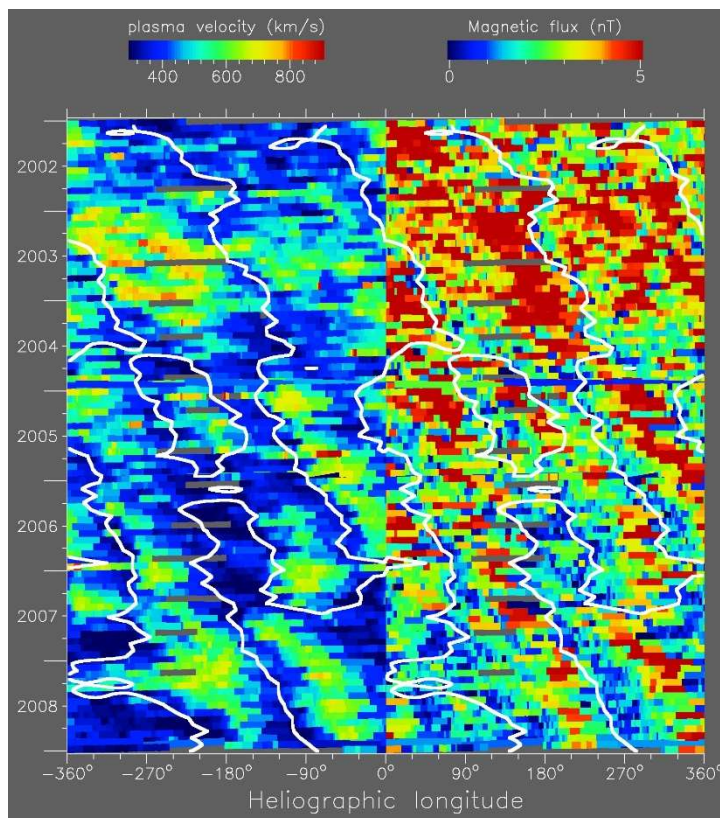
Magnetic flux in the Heliosphere. — Traditionally the open magnetic flux of the Sun is determined from the radial component of the magnetic field measured in interplanetary space. We have demonstrated that the determination of the magnetic flux can be improved significantly if care is taken to remove the effect of fluctuations of the field. Using the new method we were able to show that the magnetic flux is uniformly distributed by heliographic latitude. However the improved method unexpectedly revealed significant longitudinal variations.

Figure 1. Plasma velocity (left) and magnetic flux (right) in 2002 - 2009.

Plasma parameters measured near to the Earth were mapped back to the surface of the Sun. The data were organized according to the Carrington longitude of the source (horizontal axis). Long lived recurrent structures are clearly visible in solar wind speed, magnetic flux and magnetic sector (white line). The structures slightly drift right in the Carrington frame.

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The study supports the idea that the high magnetic fluxes are associated with slow-fast solar wind interfaces. Possible explanation of the high magnetic flux is the non-radial expansion of the solar wind.

Ion heating near the ion composition boundary at Venus. — The measurements of the ASPERA-4 electron spectrometer on board Venus Express confirmed the existence of a boundary layer above the ionopause of Venus. The upper end of the interaction layer where planetary ions disappear is called the ion composition boundary (ICB). Due to the interaction of the two plasma populations near the ICB – the shocked solar wind and planetary ions – instabilities are excited. Significant collisionless momentum and energy exchange takes place due to wave-particle interaction, creating a highly turbulent layer. In earlier works we proposed that modified two-stream instabilities (MTSI) are excited there. We investigated the properties of the modified two-stream instability, and the ion heating and ion acceleration mechanism in the framework of a numerical hybrid model which retains electron inertia. We have shown that MTSI is an effective heating mechanism, which is able to account for the recently observed charged particle heating in this region.

Jovian electrons. — We studied co-rotating interplanetary regions (CIRs) which are quasi-stationary structures in the interplanetary medium and act as magnetic traps for energetic electrons emitted from the magnetosphere of Jupiter. When such a trap passes by Earth, enhanced electron fluxes are observed. A particularly long series was observed during the last solar minimum in 2007-2009 with an average period of about 26 days. By performing numerical simulations a combined effect of the CIR and magnetic connection was obtained and fitted to the observations at SOHO and STEREO.
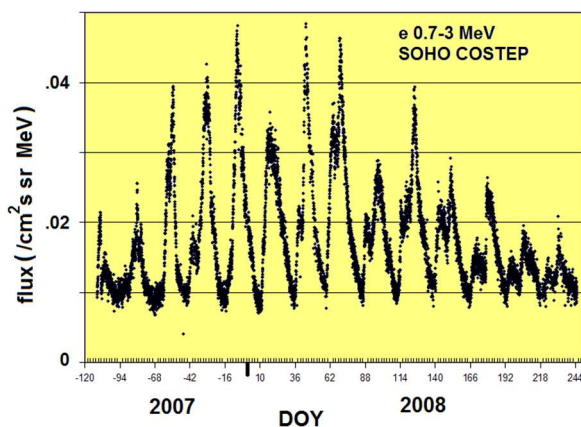

Figure 2. *2007-9: during an extremely long quiet period a series of Jovian electron peaks were observed.*
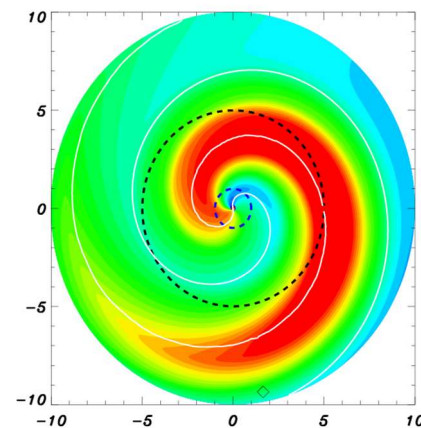
Figure 3. *Results of simulation of electrons fluxes due to the appearance of electron traps in 2008*

Supra-thermal ions. — Energy spectra and relative abundances of low-energy (0.04-1 MeV/n) ^{3}He, ^{4}He, C, O, Fe ions were investigated using data from the ACE mission in supra-thermal particle fluxes between 1998 and 2014. The unique prolonged solar activity minimum in 2007-9 allowed the observation of supra-thermal ion fluxes from near-equatorial coronal holes. We found that the values of the C/O and Fe/O ratio from coronal holes at solar minimum and maximum correlate with the bulk solar wind values of C/O and

Fe/O. This suggests that the bulk solar wind is the source of further accelerated ions forming the high energy tail.

Dust – Plasma interaction. — We modeled the possible effects (transient density enhancements of the Martian orbiting dust torus) caused by the meteor showers due to comet Siding Spring's close encounter with Mars in October 2014. Its dust tail can 'sand-blast' both Phobos and Deimos, dramatically increasing their dust production for a few hours. We determined the temporal and spatial evolution of the dust clouds raised during highly enhanced production rates that last only hours-to-days.

We also made model calculations supporting the development of the Nanodust Analyzer (NDA) instrument.

Planets and Magnetospheres

The magnetosphere of Earth. — The three-dimensional structure of mirror type (linearly polarized) magnetic fluctuations was investigated based on magnetic field and plasma data measured by the four Cluster spacecraft between the terrestrial bow shock and magnetopause and also in the interplanetary field. Some of the observed individual magnetic depressions showed axial symmetry, while some others formed sheet-like structures. We worked out a scenario, which is able to explain these observations, in which mirror type oscillations first form as planar waves and later decay to axially symmetric structures around the magnetic field lines.

An international team in which our scientists participated investigated the position and shape of the magnetopause of Earth and found out the role of magnetosheath magnetic field line stress and pressure in the evolution of these characteristic features of the magnetosphere.

Plasma structures in the magnetosphere of Saturn. — Gaining an understanding of the structure of the magnetosphere of Saturn is one of the key scientific goals of the Cassini mission, but despite a decade of successful measurements this structure is still poorly understood. Using the velocity moments derived from the ion measurements of the CAPS plasma spectrometer on board Cassini, we were able to uncover an important aspect of this structure. We found that the dense plasma near the magnetic equator rotates around the planet at high speed, while the dilute plasma of higher latitudes rotates significantly slower. The latitudinal gradient observed in the azimuthal speed is suggested to be a direct consequence of the sub-corotation of the plasma in the outer magnetosphere, with highest speeds occurring on field lines at lowest latitudes mapping to the rapidly rotating inner regions of the plasma sheet, and the speed falling as one approaches the lobe, where the field lines are connected to strongly sub-corotating plasma. The azimuthal velocities show oscillatory behavior with a period near the planetary rotation period, which can also be explained by the strong dependence on magnetic latitude, taking into account the flapping motion of the dense plasma sheet.

Most of the parameters that describe the magnetized plasma filling up the vast magnetosphere of Saturn exhibit periodic behavior. The fundamental period reflected in many magnetospheric phenomena is the rotational period of the planet, but the relationship is not at all trivial. In most cases reasonable periodic behavior can be found only

for relatively short time intervals, and often even in these intervals abrupt phase-shifts occur and higher frequencies appear.
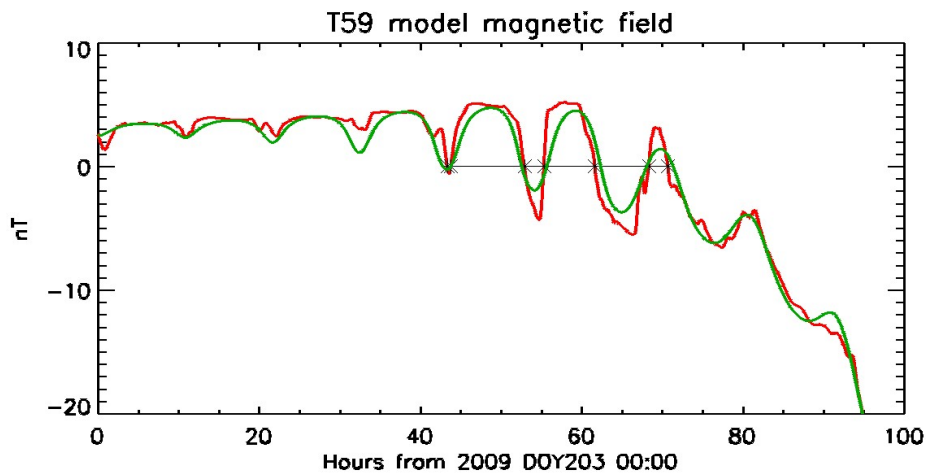

Figure 4. *The radial component of the magnetic field near the T59 Titan encounter. Red: measured, green: modeled.*

We worked out a new method to analyze these quasi-periodic variations of the plasma properties. In essence, we assume that the motion of the plasma sheet is periodic and that the observed quasi-periodic variations are due to the interplay of this periodic motion and the effects governing the spatial dependence of the plasma parameters, especially their dependence on the distance (d) from the central plasma sheet. We found that relatively simple F(d) functions are able to reproduce the observed complex temporal dependence of plasma properties.

Cometary physics. — We modeled the possible escape of charged nano-sized dust particles from the positively charged (sunlit) surface of comet P67 and provided a method for their observation by the ion and electron sensor (IES) instrument on-board Rosetta. We show that when the comet activity is low between 3.25 and 2.7 AU, the cometary surface and a part of the dust particles become charged due to the charging currents of the solar wind and photo-ionization as a result of solar radiation. Due to the nucleus' surface potential nano-size dust becomes immediately accelerated when it collects Q=+1e positive charge by photoelectron emission. The energy of this charged nanodust is higher than 4 eV and it could be detected not far from the sub-solar region by the IES.

We actively participate in the operation and data analysis of the Rosetta Plasma Consortium (RPC) experiment on board the Rosetta comet-chaser spacecraft. The first measurements performed around comet 67P reveal the birth of an induced cometary magnetosphere. A multitude of exciting new discoveries were made including the "song of the comet" (low-frequency periodic fluctuations detected by the magnetometer); low-energy pick-up ions; electron bursts; solar-wind deflection – to name a few of the completely unexpected new results of the RPC. The unique environment and interactions amount to new physics never seen before.

Grants

PECS Arrangement No. 4000105014/11, "Participation in the Venus Express mission" (K. Szegő, 2012-2014)

PECS Arrangement No. 4200098080, "Participation in the development of the Rosetta Plasma Consortium experiment onboard the orbiter" (K. Szegő, 2013-2014)

PECS Arrangement No. 4200098091, Participation in the SERENA / PICAM instrument development on MPO of the BepiColombo mission (K. Szegő, 2013-2014)

PECS Arrangement No. 4200098078, Participation in the development of the Command and Data Management Subsystem (CDMS) for the Rosetta Lander (K. Szegő, 2013-2014)

Hungarian space research development URKUT_10-1-2011-0006 "Participation in the NASA STEREO space mission" (K. Kecskeméty, 2013-2014)

Hungarian space research development URKUT_10-1-2011-0011 "Participation in the NASA Cassini space mission" (Z. Németh, 2013-2014)

International cooperation

International team of the Cassini Plasma Spectrometer (CAPS), (Károly Szegő, Zoltán Németh)

International team of the Cassini Magnetometer (MAG), (Géza Erdős)

International team of the Rosetta Plasma Consortium (RPC), (Károly Szegő, Zoltán Németh)

International team of the Cluster mission, (Mariella Tátrallyay)

Max Planck Institute for Solar System Research in Katlenburg-Lindau, Germany, Magnetospheric Imaging Instrument, (Zsófia Bebesi)

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S-A. Strongly correlated systems

"Momentum" research team

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In this year, we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG) and *Tree Tensor Network State* algorithm (TTNS). We have accomplished the following partial tasks in accordance to our project plan:

Tensor factorization and mathematical aspects. — We presented the Coupled-Cluster (CC) method and the DMRG method in a unified way, from the perspective of recent developments in tensor product approximation. In a recent 110 pages invited review article we have given a pedagogical introduction to the theoretical background of this novel field and demonstrated the underlying benefits through numerical applications on a text book example. Among the various optimization tasks we have discussed those which are connected to a controlled manipulation of the entanglement which is in fact the key ingredient of the methods considered in the paper.

Tensor factorization and algorithmic developments. — The improvement of our TTNS code formed the basis for our work in which we have shown that accuracy and convergence can significantly increase when stepping from the two-neighbour *Matrix Product State* (MPS) arrangement to the three-neighbour tree structure. It was also illustrated that this superior performance can be attributed to the more flexible tree network, which can reflect better the correlation or entanglement relations of the active orbitals. Additionally, we introduced a novel algorithm to optimize the tree tensor network topology based on quantum information theory and entanglement to fully exploit the flexibility of the TTNS ansatz. It has been stated recently several times in the literature that a higher-order DMRG/MPS is required to study systems with numerous strongly correlated orbitals. Our work shows a significant improvement towards an efficient TTNS implementation with orbital dependent tensor orders and system-specific tensor topology, which could match the expectations of the community and would be applicable to state-of-the-art multi-reference problems.

Relativistic quantum chemistry. — We presented the first implementation of the relativistic quantum chemical two- and four-component density matrix renormalization group algorithm that includes a variational description of scalar-relativistic effects and spin-orbit coupling. Numerical results based on the four-component Dirac-Coulomb Hamiltonian were presented for thallium hydride, which is the standard reference molecule for correlated relativistic benchmarks.

Algorithmic developments exploiting the power of novel kilo-processor architectures. — In the numerical analysis of strongly correlated quantum lattice models, one of the leading algorithms developed to balance the size of the effective Hilbert space and the accuracy of

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the simulation is the DMRG algorithm, in which the run-time is dominated by the iterative diagonalization of the Hamilton operator. Since the most time-consuming step of the diagonalization can be expressed as a list of dense matrix operations, the DMRG is an appealing candidate to fully utilize the computing power residing in novel kilo-processor architectures. In our pilot project a smart hybrid CPU-GPU implementation was presented, which exploited the power of both CPU (Central Processing Unit) and GPU (Graphical Processing Unit) and tolerates problems exceeding the GPU memory size. Furthermore, a new NVIDIA CUDA kernel has been designed for asymmetric matrix-vector multiplication to accelerate the rest of the diagonalization. Besides the evaluation of the GPU implementation, the practical limits of a field-programmable gate array (FPGA) implementation were also discussed.

Entanglement in uranium-based complexes. — The accurate description of the complexation of the CUO molecule by Ne and Ar noble gas matrices represents a challenging task for present-day quantum chemistry. Especially, the accurate prediction of the spin ground state of different CUO-noble-gas complexes remains elusive. In our work, the interaction of the CUO unit with the surrounding noble gas matrices has been investigated in terms of complexation energies and dissected into its molecular orbital quantum entanglement patterns. Our analysis elucidated the anticipated singlet-triplet ground-state reversal of the CUO molecule diluted in different noble gas matrices and demonstrated that the strongest uranium-noble gas interaction is found for CUOAr4 in its triplet configuration.

Entanglement and chemical bonding. — The chemical bond is an important local concept to understand chemical compounds and processes. Unfortunately, like most local concepts, the chemical bond and the bond order do not correspond to any physical observable and thus cannot be determined as an expectation value of a quantum chemical operator. We have recently demonstrated that one- and two-orbital-based entanglement measures can be utilized to interpret electronic wave functions in terms of orbital correlation. Orbital entanglement emerged to be a powerful tool to provide a qualitative understanding of bond-forming and bond-breaking processes, and allowed for an estimation of bond orders of simple diatomic molecules beyond the classical bonding models. In our work we demonstrated that the orbital entanglement analysis can be extended to polyatomic molecules to understand chemical bonding.

Metal-Insulator-like Transition (MIT) and entanglement. — We have studied the Metal-Insulator-like Transition (MIT) in lithium and beryllium ring-shaped clusters through ab-initio Density Matrix Renormalization Group (DMRG) method. Performing accurate calculations for different interatomic distances and using Quantum Information Theory (QIT), we investigated the changes occurring in the wave function between a metallic-like state and an insulating state built from free atoms. We also discussed entanglement and relevant excitations among the molecular orbitals in the Li and Be rings and showed that the transition bond length can be detected using orbital entropy functions. Also, the effect of different orbital bases on the effectiveness of the DMRG procedure has been analyzed by comparing the convergence behavior.

Nickel-ethene bond-formation. — We presented a conceptually new approach to dissect bond-formation processes in metal-driven catalysis by using concepts from quantum

information theory. Our method used the entanglement and correlation among molecular orbitals to analyze changes in electronic structure that accompany chemical processes. As a proof-of-principle example, the evolution of nickel-ethene bond-formation was dissected which allowed us to monitor the interplay of back-bonding and π-donation along the reaction coordinate. Furthermore, the reaction pathway of nickel-ethene complexation was analyzed by using quantum chemistry methods, revealing the presence of a transition state. Our study supported the crucial role of metal-to-ligand back-donation in the bond-forming process of nickel-ethene.

Entanglement and correlations in quantum many-body systems. — We defined a generalized, entanglement-based correlation function related to the mutual information of two localized, typically single-site, subsystems of a larger many-body system. The two-site mutual information is defined in terms of the von Neumann entropy of the single-site and two-site density matrices, which, in turn, can be written in terms of expectation values of transition operators between localized states. It can be used to map out entanglement patterns between the subsystems (that is, sites) of the system. By defining generalized correlation functions as two-point correlation functions of transition operators, we found that the long-distance decay of the mutual information follows the square of that of the most slowly decaying generalized correlation function. We showed how the generalized correlation functions are related to conventional correlation functions for spin and fermion lattice models. We explored the behavior of the mutual information, the generalized correlation functions, and their relation for the general spin-1/2 Heisenberg model and for SU(n) Hubbard models with n=2,3,4, and 5, and demonstrated the principles on known phases of the spin and SU(2) Hubbard models and obtained results characterizing the dimerized, trimerized, and quadrimerized phases in the SU(3), SU(4), and SU(5) Hubbard models, respectively. In addition, we extended the picture of the two-site mutual information and the corresponding generalized correlation functions to the n-site case.

Periodic Anderson model. — We investigated the effect of the Coulomb interaction, U_{cf}, between conduction and f-electrons in the periodic Anderson model using the Density Matrix Renormalization Group algorithm. We calculated the excitation spectrum of the half-filled symmetric model with an emphasis on the spin and charge excitations. In the one-dimensional version of the model, it was found that the spin gap was smaller than the charge gap below a certain value of U_{cf} and the reversed inequality was valid for stronger U_{cf}. This behavior was also verified by the behavior of the spin and density correlation functions. We also performed a quantum information analysis of the model and determined the entanglement map of f- and conduction electrons. It was revealed that for a certain U_{cf} the ground state is dominated by the configuration in which the conduction and f electrons are strongly entangled, and the ground state is almost a product state. For larger U_{cf}, the sites are occupied alternately dominantly by two f-electrons or by two conduction electrons.

Ultracold Atoms. — In the work "Phase Separation of Super Fluids in the Chain of Four-Component Ultracold Atoms" we have investigated the competition of various exotic superfluid states in a chain of spin-polarized ultracold fermionic atoms with hyper spin F=3/2 and s-wave contact interactions. We showed that the ground state is an exotic inhomogeneous mixture in which two distinct superfluid phases – spin-carrying pairs and singlet quartets – form alternating domains in an extended region of the parameter space.

Graphene nanoribbons. — The possibility that non-magnetic materials such as carbon could exhibit a novel type of s-p electron magnetism has attracted much attention over the years, not least because such magnetic order is predicted to be stable at high temperatures. We found that the magnetic order on graphene edges of controlled zigzag orientation can be stable even at room temperature, raising hopes of graphene-based spintronic devices operating under ambient conditions.

Grants

International cooperation
ETH Zürich, (Zürich, Switzerland), Development of the relativistic DMRG algorithm (S. Knecht, M. Reiher)

Philipps Universität Marburg, (Marburg, Germany), Optical properties of polydiacetylenes (F. Gebhard); Entanglement scaling in momentum space DMRG (G. Ehlers, R.M. Noack)

Freie Universität, (Berlin, Germany), Basis optimization using matrix product state (MPS) based approach (C. Krumnow, R. Schneider, J. Eisert); Ab initio description of metal Insulator transitions (E. Fertitta, B. Paulus)

Universität Wien, (Vienna, Austria), Development of tree tensor network state (TTNS) algorithm (V. Murg, F. Verstraete)

Technische Universität Berlin, (Berlin, Germany), Tensor factorizations in high dimensional problems (M. Pfeffer, R. Schneider)

McMaster University, (McMaster, Canada), Bond braking and formation through entanglement (K. Boguslawski, P. Tecmer, P. Ayers)

Ustav Fyzikalni Chemie J. Heyrovskeho AV CR, (Prague, Czech Republic), Development of the quantum chemistry version of the DMRG method (L. Veis, J. Pittner)

Long-term visitor
Libor Veis, Ustav Fyzikalni Chemie J. Heyrovskeho AV CR, Prague, Czech Republic (Oct. 2014-March 2015; host: Ö. Legeza)

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S-D. Semiconductor nanostructures

"Momentum" research team

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

Development of new type biomarkers. — Biologists urgently need biomarker systems which trace, for example, 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 "Lendület" Semiconductor Nanostructures Research Group is, however, seeking for solutions that can be applied in vivo. Diamond-based structures consisting of carbon atoms are good candidates as well as silicon carbide nanoparticles with favorable zeta-potential. We have shown by time-dependent density-functional theory calculations that nickel-vacancy point defects embedded into diamond nanoparticles (DNPs) with different sizes can act as multi-color biomarkers where the same type of defect can produce fluorescence at various wave lengths due to quantum confinement in DNPs. Another important result has been achieved for the very important nitrogen-vacancy defect in diamond. As the quantum-optics protocols of the nitrogen-vacancy (NV) centre rely on its negative charge state in diamond, the control of the charge state of the NV centre is a prerequisite to apply them in sensor applications where NV centres should be placed as close as possible to the surface of diamond for efficient sensing of the targeted nano-objects. Advanced technologies have made possible to implant NV centres not deeper than 1 nm below the surface in a controlled fashion, and luminescent ultra-small DNPs of about 5 nm in size could be also fabricated where NV centres are naturally located very close to the surface of a DNP (Fig. 1). In this work, we showed by accurate quantum mechanical simulations in collaboration with Prof. Frauenheim group at Bremen University that typical diamond surfaces possess image states with sub-bandgap energies which compromise the photo-stability of the NV centres placed within a few nm of the surface. This occurs due to the mixture of the NV-related gap states and the surface image states which is a novel and distinct process from the well-established band bending effect. We find that certain types of hydrogen, oxygen and fluorine coverage of diamond surface may lead to blinking or bleaching due to the presence of acceptor surface states. We identified a combination of surface terminators that is perfect for NV-centre-based nanoscale sensing.
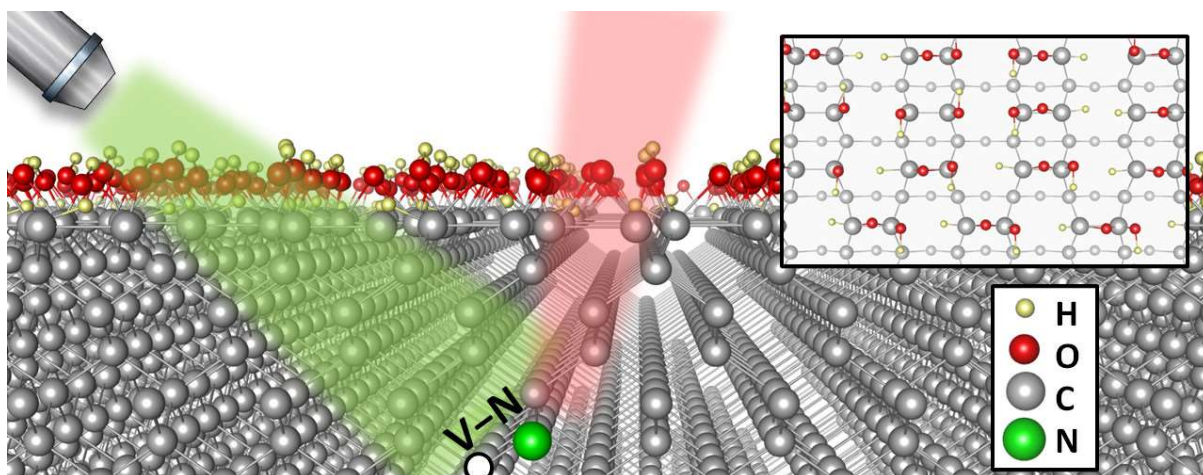

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Figure 1. *Fluorescent nitrogen-vacancy colour centre beneath the "ideal" diamond surface for sensing*
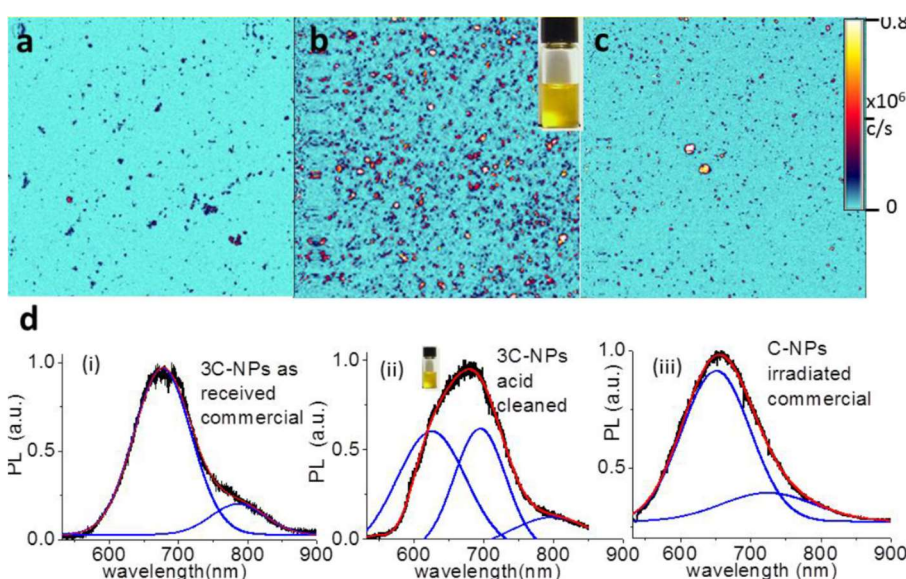

Figure 2. *Single-photon emitters in SiC nanoparticles. Sample **b** was produced in Wigner ADMIL.*

Our group members at Wigner ADMIL laboratory have succeeded in manufacturing carbon antisite–vacancy colour centres in silicon carbide nanoparticles. In collaboration with Australian researchers, we showed that these colour centres behave as single-photon emitters (Fig. 2), and, therefore, may be used in the future in nanometrology and quantum informatics. The biocompatibility of SiC makes these defects ideal candidates for biosensing at the molecular level. According to our single advanced density functional theory calculations, the photoluminescence can be associated with the double-positive-charge state of the carbon antisite-vacancy pair in 3C-SiC, in contrast with the previous assignment (Si-vacancy). SiC nanocrystals (SiC NCs) are very complex systems. While the core of the crystal is crystalline SiC, the surface contains different organic and silico-organic groups. These groups are responsible for the extreme stability of SiC NCs in aqueous media even at high salt concentration, and they highly influence the optical and chemical properties of the NCs. For employing SiC as a biomarker, chemical and physical properties of the nanocrystals have to be well known and controllable. SiC NCs made from highly porous SiC source are mostly carboxyl terminated. We have shown by means of combined experimental and theoretical study (Fig. 3) that heating of NCs carboxyl groups transforms them to anhydride groups which have high reactivity, allowing clean chemistry for labeling biomolecules.
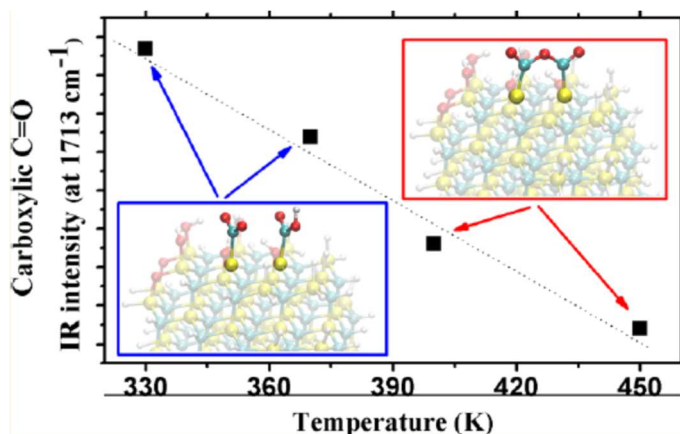
Figure 3. The infrared absorption band of carboxyl group at 1713 cm^{-1} reduces at elevated temperatures on SiC surface (blue frame) because of its transformation to anhydride group (red frame)

Quantum bits. — Further 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. In collaboration with Awschalom group (now at Chicago University), we have shown that divacancy spins are more sensitive to the perturbation of the external electric fields. Our *ab-initio* simulations revealed that not the piezo effect but the inherent polarizability of the SiC lattice is responsible for this phenomenon. We have developed a code to calculate the electron spin-electron spin dipole-dipole interaction to study this issue (Fig. 4). A very important step has been achieved in realizing quantum bits in SiC: in collaboration with German and Swedish researchers, we have shown that single Si-vacancy spins can be coherently manipulated by light at room temperature with a coherence time exceeding 80 microseconds.
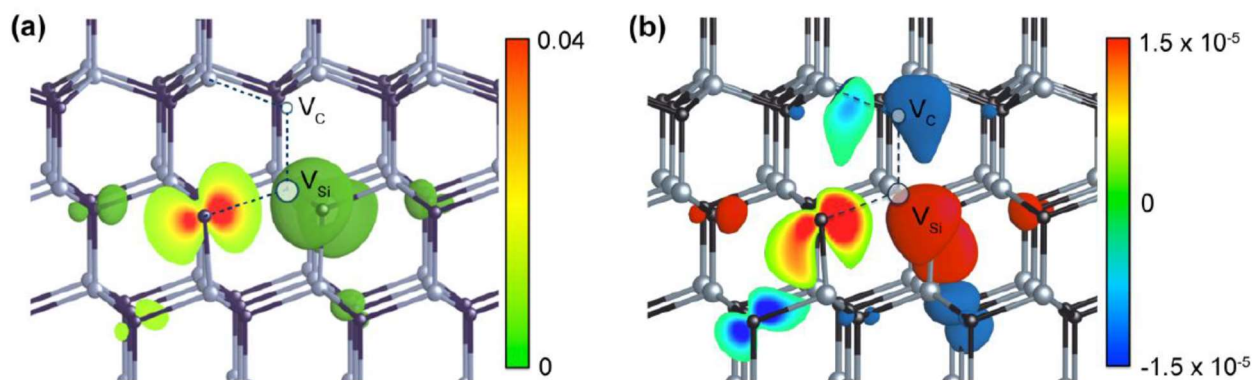

Figure 4. Calculated spin density on a divacancy defect in 4H-SiC (a) Ground state at so-called hh configuration, and (b) its change upon external electric field of 0.1 eV/Å pointing upward parallel to the defect symmetry axis.

Development of solar cells. — Efficiency of present, relatively cheap state-of-the-art photo-voltaics is theoretically limited to about 32%, even after future enhancements. The widespread polysilicon solar cells seen on the roofs of buildings have an even lower efficiency, down to about the half of the above limit. This means that at least 68 percent of light energy is wasted to heating the solar cells. Solution to the solar-cell inefficiency problem can be based on impact ionization by directing more energy in the electronic sector. One high-energy photon absorbed by the solar cell creates here not only one but two or three charge carriers. This results in high current, thus improves power efficiency by a half or similar magnitude. Note that in this very intensive field of research, percentage

points of efficiency improvement are regarded as a breakthrough. Intensive research has been carried out for quite long time to find materials where impact ionization is efficient in comparison with the poor results of bulk silicon. In collaboration with Manousakis group at Florida State University, we proposed that strongly correlated materials are strong candidates for realizing efficient photovoltaic cells because of the enhanced carrier multiplication rates. The idea is sketched on Fig. 5. We have shown by first-principles calculations that the carrier multiplication rate is two orders of magnitude higher in VO_2 than in Si and much higher than the rate of hot electron/hole decay due to phonons. As VO_2 is proto-typical of strongly correlated materials, we think that the family of strongly correlated materials exhibit similar properties. This may lead to a "single-photon-in" – "two-electrons-out" operation of solar cells in strongly correlated materials that can significantly increase the efficiency of this type of solar cells compared to the case of conventional semiconductors.
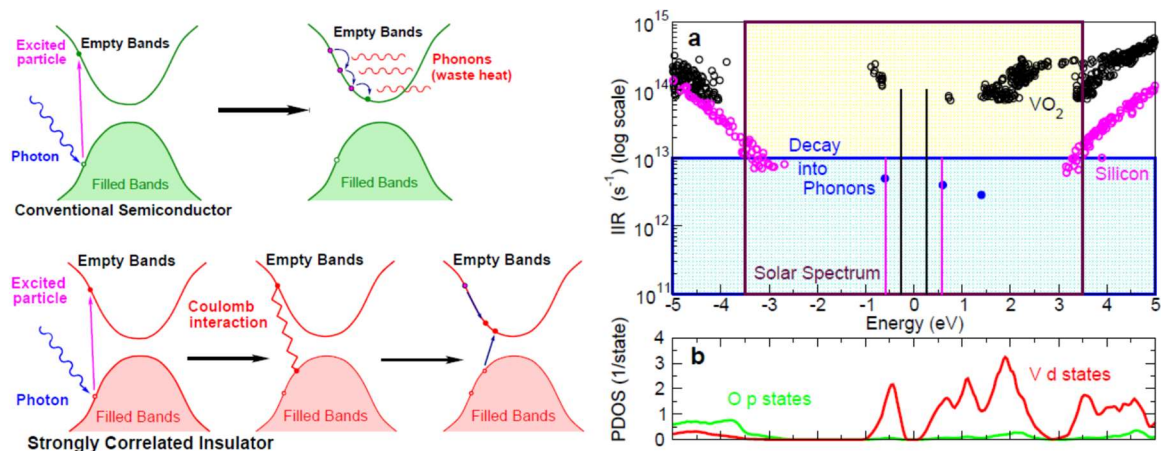

Figure 5. *Left panel: The standard process in conventional semiconductors is shown in the top, while the expected process in strongly correlated insulators is shown in the bottom row. Right panel: Carrier multiplication rates for VO₂ and Si, and the corresponding projected density of states (PDOS) of VO₂ orbitals; the d-orbitals are "correlated" ones responsible for the increased impact ionization rates*

Alternative absorber materials are also much sought-after in photo-voltaics. Tin monosulfide (SnS) is a quasi-2D material which is a metastable crystalline form of Sn and S. From solar-cell application point of view, the very attractive property of SnS is the strong absorption starting at about 1.3 eV. However, a real SnS material is very defective, and often exhibits unintentional p-type doping. In collaboration with Kaxiras group at Harvard University, we found that for the intrinsic defect, an Sn-vacancy acceptor defect is responsible for the intrinsic p-type conductivity of SnS. For the extrinsic defects, we find support for the experimental suggestion that P, under S-rich conditions, prefers to substitutionally occupy the Sn site rather than the S site, and this leads to n-type behavior. Additionally, we support the notion of previous experimental implications that Sb acts as a donor in Sn. We also show that Cl prefers to substitute for S atoms where it acts as a donor.

Grants

OTKA K101819: Design, fabrication and analysis of luminescent silicon carbide nanocrystals for in vivo biomarker applications (A. Gali, 2012-2016)

OTKA 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 (A. Gali, 2013-2017)

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

"Momentum" Program of the H.A.S. (A. Gali, 2010-2015)

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)

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See also: S-F.7, S-F.14

S-H. Partially ordered systems

Wigner research group

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Granular materials. — The formation and evolution of shear zones in granular materials have been investigated by X-ray tomography and optical methods.

Shear localization and the formation of wide shear zones is a puzzling phenomenon connected to yielding of granular materials. The evolution of wide shear zones was investigated experimentally and numerically for quasi-static dry granular flows in split-bottom shear cells. Reynolds dilatancy, positional order and orientational order effects compete in the shear zone. We studied granular packing consisting of beads, irregular grains, such as sand, and elongated particles and compared their behavior. X-ray tomography was used to determine the particle positions and orientations in a cylindrical split-bottom shear cell. Packing densities and the arrangements of individual particles in the shear zone were evaluated (see Fig. 1a).
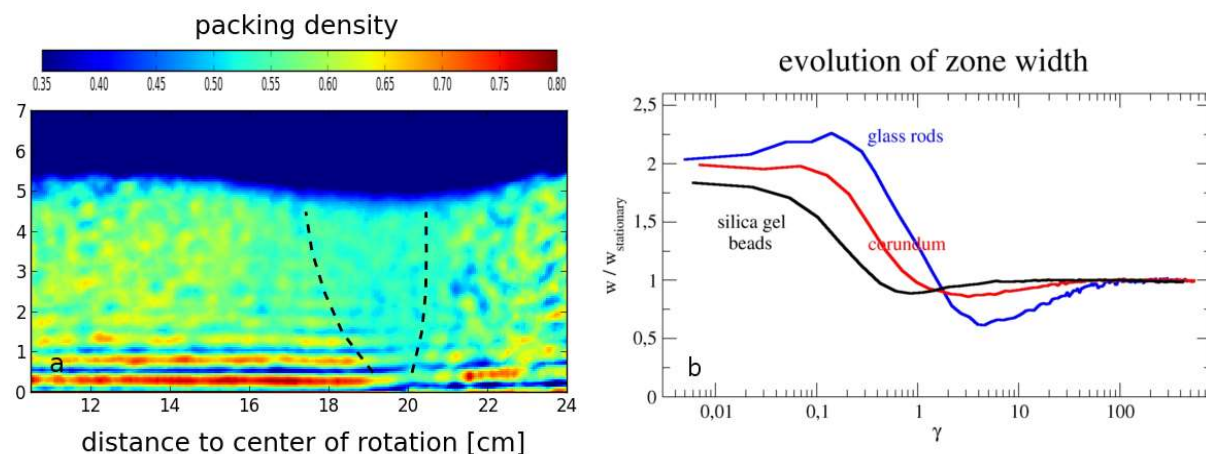

Figure 1. (a) *Packing density of a granular material obtained by X-ray tomography in a cylindrical split-bottom shear cell,* (b) *evolution of the width of the shear zone as a function of the local deformation.*

Shearing an initially random sample, the zone width was found to significantly decrease in the first stage of the process (see Fig. 1b). The characteristic shear strain associated with this decrease is about unity meaning that narrowing of the zone is realized relatively quickly; that is, the neighboring layers only need to move about one particle diameter. This typical shear strain is systematically increasing with shape anisotropy; that is, when the grain shape changes from spherical to irregular (for example, sand) and becomes elongated (pegs). The strongly decreasing tendency of the zone width is followed by a slight increase which is more pronounced for rodlike particles than for grains with smaller shape anisotropy (beads or irregular particles). The evolution of the zone width is connected to shear-induced

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packing density change and for nonspherical particles it also involves grain reorientation effects. Even though aligned cylinders in principle may achieve higher packing densities, this alignment compensates for the effect of dilatancy only partially. The final zone width is significantly smaller for irregular grains than for spherical beads.

Liquid crystal composite materials. — The influence of the shape anisotropy of magnetic particles on the isotropic–nematic phase transition has been studied in magnetic-nanoparticle-doped nematic liquid crystals (ferronematics). Liquid crystals (LC) have been doped with spherical or rod-like magnetic particles of different size and volume concentrations. The phase transition from isotropic to nematic phase has been observed by polarising microscope as well as by capacitance measurements. The influence of the concentration and the shape anisotropy of the magnetic particles on the isotropic–nematic phase transition in LC has been demonstrated. The results are in a good agreement with recent theoretical predictions.

The magneto-optical and dielectric properties of ferronematics have been investigated experimentally. The studies have focused on the effect of a very small orienting bias magnetic field B_{bias}, and of the nematic director pre-tilt at the boundary surfaces in these systems which are sensitive to low magnetic fields. Based on the results, we assert that B_{bias} is not necessarily required for a detectable response to low magnetic fields, and that the initial pre-tilt as well as the aggregation of the nanoparticles play an important role.

Photo-sensitive mesogenic materials and surfaces. — A new azobenzene-group-containing monomer and several respective functional side-chain polymers grafted on a methylhydrosiloxane backbone (with two different degrees of polymerization; with and without the addition of a photoreactive benzophenone derivative) are designed, synthesized, and characterized. The resulting materials clearly show self-assembly behavior and possess a nematic liquid-crystal phase over a broad temperature range, which extends down to below 0 °C. The optical properties of these new photochromic liquid-crystalline materials are determined from the absorbance spectra of oriented samples and by photo-induced birefringence studies. The results indicate a considerable dichroism of the side-chain liquid-crystalline polymers (SCLCPs), and hence demonstrate their potential applicability for optical data storage (Fig. 2).
Liquid-crystal layers sandwiched between a reference plate and a photosensitive substrate have been investigated. We focused on the reverse geometry, where the cell was illuminated by a laser beam from the reference side. In planar cells, both static and dynamic instabilities occurred, depending on the angle between the laser polarization and the director orientation on the reference plate. In cells where the molecules were aligned along the normal of the reference plate, a dynamic pattern was observed at all angles of polarization. A simple model based on a photo-induced surface torque accounts for the findings and predicts that, at certain thicknesses, the dynamic instability is forbidden. Experiments on wedge-like cells confirmed this prediction. Light-scattering studies revealed some basic properties of the instabilities.

Pattern formation in liquid crystals - Two types of electric-field-induced pattern formation (electroconvection, EC and flexodomains, FD) were investigated in various liquid crystals in international collaborations.
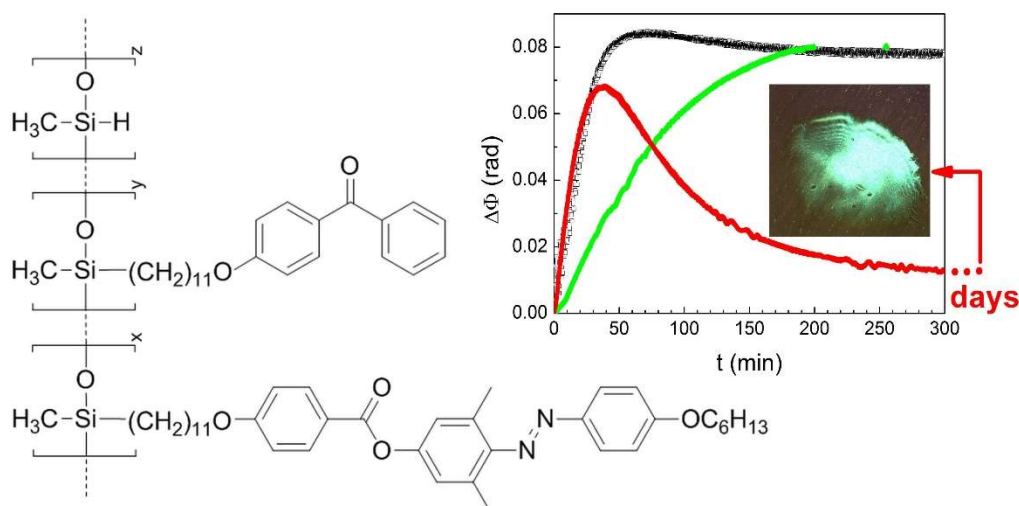
Figure 2. *Chemical composition of the side-chain liquid crystalline polymers and the temporal evolution of the photo-induced phase shift (birefringence) in the nematic monomer (black symbols), and in the polymer in the glass state (green symbols), as well as in its nematic phase (red symbols), demonstrating of the applicability of these materials for optical data storage.*

The effect of superimposed ac and dc electric fields on the formation of EC and FD patterns in nematic liquid crystals was studied experimentally and theoretically. For selected ac frequencies, the extended standard model of the electro-hydrodynamic instabilities was used to characterize the onset of pattern formation in the two-dimensional parameter space of the magnitudes of the ac and dc electric field components. Numerical as well as approximate analytical calculations demonstrated that, depending on the type of patterns and on the ac frequency, the combined action of ac and dc fields may either enhance or suppress the formation of patterns.

Experimental tests of the theoretical predictions showed that an enhancement of pattern formation was found only at very low frequencies in the conductive regime of EC. In all other cases, the superposition of ac and dc voltages inhibited the pattern-forming mechanism; therefore, the pattern-free region extended to much higher voltages than the individual ac or dc thresholds (Figs. 3A and 3B). In addition, a dc-bias-induced reduction of the electrical conductivity and a shift of the crossover frequency from the conductive to dielectric EC regimes were also detected. The dc voltage dependent conductivity allowed to give a qualitative explanation for the deviation from the theoretical predictions in the conductive EC regime. However, the discrepancies found in the dielectric EC regime still represent a challenging problem and indicate the need for an extension of the theoretical description.

The formation of flexoelectric (FD) patterns was studied under the influence of external electric and magnetic fields in a nematic liquid crystal. The critical voltage and wave vector of flexodomains were measured in different geometries and were also calculated from the continuum theory. The experimental and simulated results showed an excellent agreement. We demonstrated that upon altering the orientation of the magnetic field with respect to the director, the critical voltage and wavenumber behave substantially differently. In the geometry of the twist Fréedericksz transition, a non-monotonic dependence on the magnetic field was found (Fig. 3 (C)).
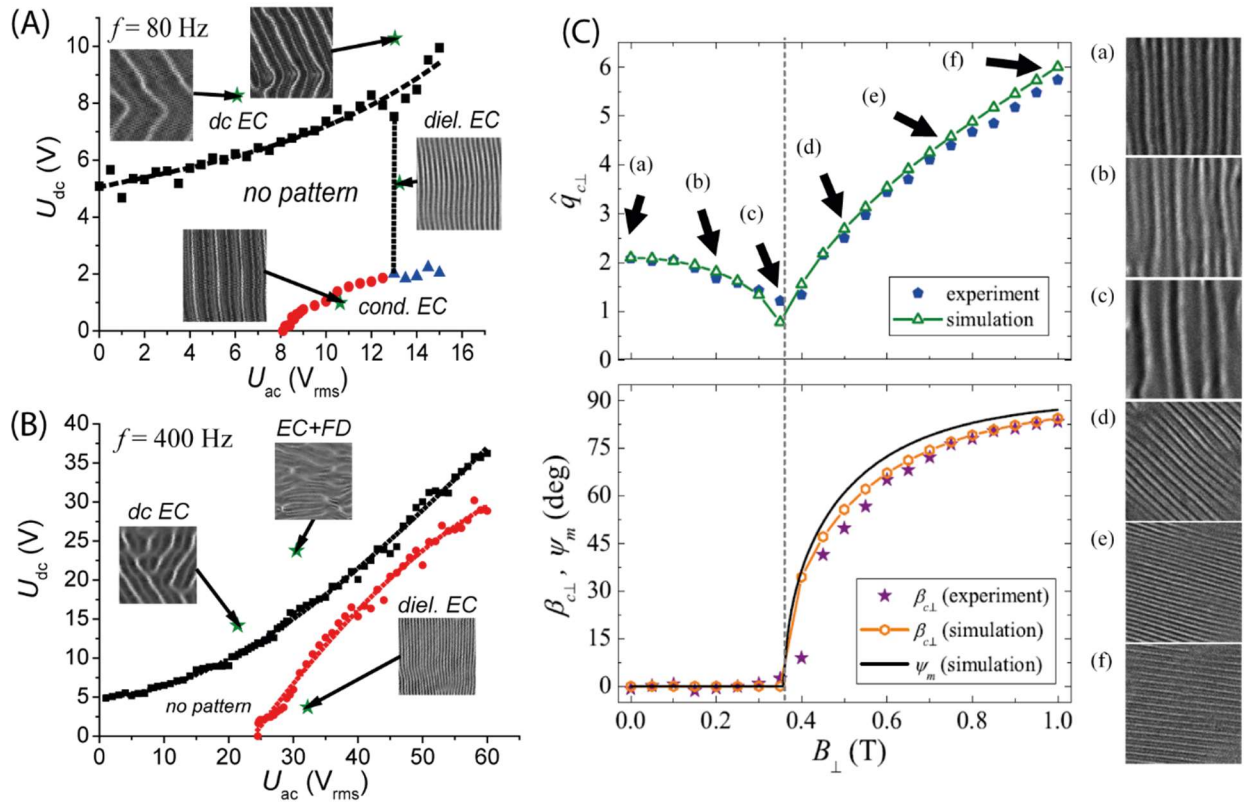
Figure 3. *Morphological phase diagram of a Phase5 sample at f = 80 Hz (A) and f = 400 Hz (B). The lines indicate the stability limit curves, while stars label those U_{ac} - U_{dc} combinations where the images (covering an area of 52 μm × 52 μm) were taken. The initial director lies along the horizontal direction. (C) The magnetic inductance dependence of the dimensionless critical wavenumber $\hat{q}_{c\perp}$, stripe angle $\beta_{c\perp}$ of flexodomains, and maximal director twist angle ψ_m in the perpendicular geometry. The solid and connected open symbols were obtained by experiments and numerical simulations, respectively. The corresponding images (a)-(f) cover an area of 106 μm x 106 μm. The initial director lies along the vertical direction.*

In an ether-bridged bent-core nematic liquid crystal material (BCN), two kinds of non-standard EC patterns appearing in different frequency ranges were detected and their characteristics were compared. One was a longitudinal pattern in the high-frequency range of several hundred Hz with stripes running parallel to the orientation of the BCN and with a periodicity of approximately the cell thickness; the other one was in the form of oblique stripes, which result in a zigzag pattern, and appear in the low-frequency range of several tens of Hz. In addition, within an intermediate-frequency range, transformations from oblique to longitudinal and then to normal stripes occurred at increased ac voltages. When the temperature increased and approached the clearing temperature, the contrast of longitudinal and oblique stripes enhanced and the frequency range of existence became wider, while the onset voltages increased only moderately instead of diverging, thus suggesting an isotropic mechanism of pattern formation.

Properties of bent-core and rod-like liquid crystal mixtures - Binary mixtures of bent-shaped and rod-like liquid crystalline compounds have been prepared and analyzed. Phase transition temperatures were measured by differential scanning calorimetry, phases were identified by polarizing optical microscopy and X-ray diffraction. A model was proposed for

the packing of molecules of different size and shape. In a similar binary system of strongly polar liquid crystals, the dielectric and viscoelastic properties were explored. The splay and bend elastic moduli were found to exhibit an unusual temperature dependence which was proposed to be due to the polar interactions.

Synthesis of mesogenic compounds. — Three series of bent-core mesogens having pyridine as the central unit have been synthesized and characterized. A series of 2,6-diaminopyridine derivatives capable of forming inter- and intramolecular hydrogen bonds exhibit very high melting points. A decrease in the polarity of the central part of the bent-core obtained by replacing the amide with ester linkages results in derivatives with lower melting points and formation of B2- and B7-like mesophases. The introduction of the olefinic groups, which connect the pyridine ring with the inner aromatic rings, helps to further lower the polarity of the central part in the five-ring system and leads to the formation of B1 and B7 phases. The phases have been determined by optical microscopy observations and differential scanning calorimetry (DSC) and confirmed by X-ray studies. The bending angles and the polarity of the investigated five-ring systems have been calculated by the density-functional-theory (DFT) method (Fig. 4).
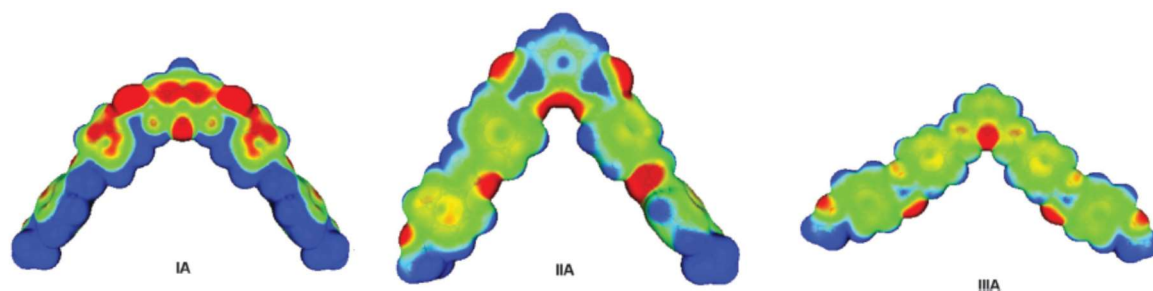

Figure 4. *Electrostatic potential surface of the most stable conformers of the cores of systems (blue to red colour – positive to negative part of the molecule).*

Grants

International cooperation
Centre for Nano and Soft Matter Sciences, INSA (Bangalore, India), Dynamics of soft condensed matter (N. Éber, 2013-2015)

Institute of Experimental Physics, SAS (Košice, Slovakia), Nanoparticles in anisotropic soft matter (T. Tóth-Katona, 2013-2015)

Institute of Physics, ASCR (Prague, Czech Republic), Synthesis, mixing, polymerization, crosslinking and physical characterization of photosensitive mesogenic monomers (T. Tóth-Katona, 2013-2015)

Guangdong University of Technology (Guanzhou, China), Nonlinear structures in mesogens (Á. Buka, 2013-2015)

Cadi Ayyad University (Marrakech, Morocco): Composite materials from natural resources (N. Éber, 2014-2016)

Long term visitor
Nemanja Trisovic, University of Belgrade, Serbia (K. Fodor-Csorba, 6 months)

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S-J. Gas Discharge Physics

Wigner research group

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Our research activities are related to the different physical and chemical aspects of low temperature, non-equilibrium plasmas at low (10-1000 Pa) and atmospheric pressures. First of all, we are interested in the operation of different types of gas discharges and the fundamental processes occurring in these systems, which make them applicable in various fields, such as chemical analysis, material synthesis, environmental protection, biomedicine and nanotechnology. On the other hand, we also make use of the plasma environment of the low-pressure gas discharges to study atomic processes as well as collective phenomena occurring in many-particle systems by using the dusty (strongly-coupled) plasma as a model system. A common aspect in the investigations conducted on these topics is the bottom-up approach we follow. This means that we seek for the understanding and description of the observed macroscopic phenomena at the most fundamental level, often down to the classical atomic scale and elementary interactions. In most of the studies we combine experiments with advanced numerical or analytical calculations to provide the most complete and detailed physical picture. Along the elucidation of the fundamental properties of gas discharges and the characterization of strongly coupled plasmas, we also contribute to the development and optimization of future emerging plasma technologies, such as biomedicine and nanotechnology. In the following we briefly introduce some of our recent achievements grouped around our four main research directions.

Gas discharge physics. – Gas discharges are non-equilibrium systems of unbounded electrons and ions in low-pressure gas backgrounds. The electric field, induced in the discharge volume by an external electric circuit drives, through the acceleration of charged particles, the elementary collisions in the plasma. Discharge properties strongly depend on the composition of the gas and the characteristics of the driving voltage. Our mission is to provide fundamental understanding of the microscopic mechanisms in gas discharges, which are relevant to applications, paving the way to the improvement of current technologies and development of new applications. During the last year we investigated the breakdown of low-pressure air under radiofrequency and direct-current electric fields experimentally and by a numerical kinetic model. The computations provided insight into the changes of electron kinetics across the different regimes, controlled by gas phase/surface processes, as a function of the frequency of excitation. Furthermore, we used particle-in-cell simulations to uncover the details of the heating dynamics of electrons in radiofrequency plasmas. Ambipolar electric fields were identified as an important source of electron heating besides the well-known mechanisms associated with the expansion of the space charge sheath at the electrodes. By improving the modeling techniques, the approximations used can be reduced and a more detailed analysis of the systems can be

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[#] Ph.D student
[A] Associate fellow

obtained. Recently, a novel approach to treat many-body Coulomb effects in low-ionization degree gas discharge plasmas has been developed which combines the molecular dynamics description of many-body interactions between electrons and Monte Carlo type description of collision processes between electrons and the background gas. This approach eliminates the need for a binary collision approximation of Coulomb collisions that has been present in all previous Monte Carlo transport simulations as well as in solutions of the Boltzmann equation.

Strongly coupled plasmas. – In contrast to gas discharges, strongly coupled plasmas are systems of charged particles, where the long-ranged electrostatic interaction between charges dominates the dynamics over the thermal motion of the particles. Such plasmas are realized in dense astrophysical objects, cold ion traps, charged colloidal suspensions, and, our system of interest, dusty plasmas. Dusty plasmas are gas discharges with micron-sized solid grains immersed into it. In this case, the grains charge up in the discharge plasma and become trapped in the electric field present in the discharge. As the dynamics of the dust grains and the gas discharge have very different characteristic time scales, the ensemble of charged dust grains can be treated independently of the discharge. The dust component can be well approximated with the one-component plasma model featuring screened Coulomb (Yukawa) inter-particle interactions. The dust grains tend to form crystalline solid or liquid structures, resulting in a model system ideal to study classical phenomena in condensed matter on the particle level. Recently, we have developed a molecular dynamics method to compute the linear and quadratic density-response functions of strongly-coupled Yukawa liquids. The agreement between the results obtained from this approach and from the Fluctuation-Dissipation Theorem (FDT) in the linear regime has verified our computational methods. Based on this, the agreement in the quadratic case has provided a support for the validity of the quadratic FDT that has not been tested so far for similar physical systems.
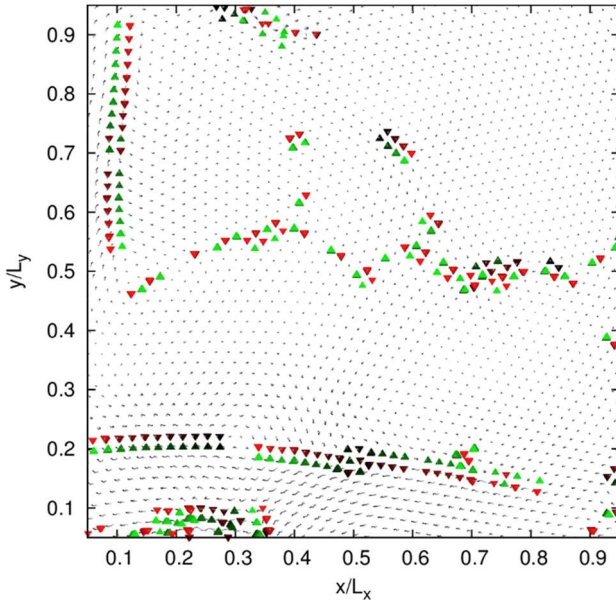
Figure 1. *Defect maps of subsequent system snapshots from the experiment. Colors lighten with elapsing time. ▼ particles with 7 neighbors; ▲ particles with 5 neighbors.*

Dusty plasmas. — They are special manifestations of strongly-coupled plasmas where micrometer-sized solid particles are immersed into a low-pressure gas discharge. These dust grains acquire high electric charge and form a strongly interacting ensemble, which behaves qualitatively similar to classical atomic matter (solids and liquids). Due to their characteristic time and distance scales, these systems can easily be observed on the individual particle level and thus give insight into the microscopic details of well-known macroscopic processes. This time, we have used our dusty-plasma experiment to identify the microphysics behind the slow plastic deformation (creep) that happens due to a constant homogeneous shearing force. We have observed the creation of pairs of oppositely

oriented dislocations (see Fig. 1), the rapid (supersonic) glide motion and annihilation of these dislocations at domain walls as being the dominant microphysical processes.

Discharge plasmas for biomedicine. — In the field of biomedicine, we aim to contribute to the understanding of the effect of discharge plasmas on the wound-healing process. In the last decade, it has been found that the direct treatment of wounds by discharge plasmas can accelerate the healing process. In order to understand this effect (that is, the interaction of plasma species with the skin cells) we treated keratinocyte cells with an atmospheric pressure plasma source called plasma needle (the plasma is generated at the tip of a needle as shown in Fig. 2.) and followed the cell proliferation. The wound has been modeled with a scratch made on the cell culture. The cells attached to the bottom of the plate are covered with phosphate buffered saline solution (PBS) during treatment (as shown in Fig. 2.a.) in order not to dry out. We managed to find treatment conditions, related to the discharge input power, treatment time and volume of PBS that covers the cells, where a positive effect on the cell proliferation can be achieved. A maximum in the scratch closing is observed both in function of input power (around 20 W) and treatment time (around 10 s). In order to clarify these relations further experiments will be conducted. The interaction of the plasma species with the cell medium and the cells is very complex. We are developing plasma and liquid diagnostics, which drive us closer to the understanding of plasma and liquid chemistry of the system.
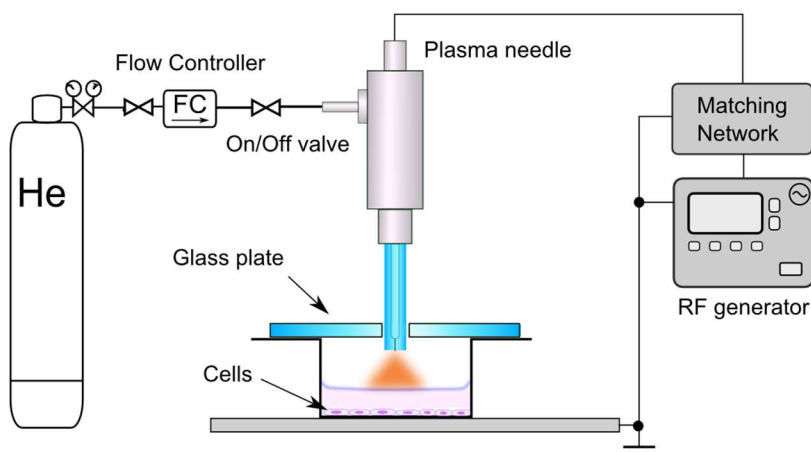

Figure 2.a. *Schematic presentation of the plasma source "plasma needle" used for cell treatment.*

Figure 2.b. *The structure of the visible glow of the plasma needle.*

Analytical plasmas: Electrolyte cathode atmospheric pressure glow discharge (ELCAD). — The most powerful multi-purpose material analysis techniques are based on the light emission spectra, unique to excited chemical elements and molecules. The ELCAD technique is useful to analyze liquid samples, as the cathode of the atmospheric glow discharge is the liquid itself. As result of sputtering and evaporation of the liquid, the chemicals penetrate into the discharge plasma, where the excitation due to electron collisions drives the emission of light. High-resolution spectral analysis results in the detection and identification of trace elements down to the ppm level even in industrial environment, including waste water monitoring. During the last year an electrolyte cathode atmospheric glow discharge atomic emission spectrometry (ELCAD-AES) method was developed for the detection of the industrially relevant In, Rh and Te in water samples. The method uses analytical lines in the

UV-VIS spectrum, free from spectral overlap interferences, and sensitive enough for quantifying the analytes at mg L^{-1} or lower levels. The studies conducted have shown that the detection of Te and Rh is very difficult, the emission intensities of interference-free transitions are very low. The emission intensities are highly sample pH dependent; that is, analytical signals can only be detected at pHs lower than 2. However, the use of acidity lower than pH 1 causes lower plasma volume; that is, the contraction of plasma into the sample introduction capillary creating discharge instabilities resulting in frequent self-extinction. The detection limits for In, Rh, and Te were found to be 0.01, 0.5, and 2.4 mg L^{-1}, respectively, while the precision expressed as relative standard deviation (RSD) not higher than 4.6, 6.4, and 7.4 %, respectively. Samples with high salt content (for example, well water) caused positive matrix effects (1.4 - 3.2-fold signal enhancements), but also approx. 1.5-times higher RSDs.

Grants

OTKA K-105476: High performance modelling and simulation of low-temperature and strongly coupled plasmas (Z. Donkó, 2013-2016)

OTKA NN 103150: Dusty plasma: a laboratory for classical many-particle physics (P. Hartmann, 2012-2015)

OTKA K 104531: High and low-frequency discharges for biomedical applications and nanostructuring (K. Kutasi, 2012-2016)

COST Action MP1101 Biomedical Applications of Atmospheric Pressure Plasma Technology (Management Committee Member: K. Kutasi 2012-2015)

COST Action TD1208 Electrical discharges with liquids for future applications (Management Committee Members: K. Kutasi, I. Korolov 2013-2016)

"Wigner research group" support

International cooperation

Boston College

Ruhr Universität Bochum

Baylor University Texas

Institute of Physics Belgrade (Belgrade, Serbia), Interaction of discharge plasmas with living cells (Zoran Lj. Petrovic, Nevena Puac)

Josef Stefan Institute Ljubljana (Ljubljana, Slovenia), Surface treatments in afterglow plasmas (Miran Mozetic)

Institut Jean Lamour École des Mines Nancy (Nancy, France), Gabriel Lippmann Centre Luxembourg (Luxembourg) Elementary processes in afterglow plasmas (Thierry Belmonte, David Duday)

Publications

Articles

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7. Iwashita S, Schungel E, Schulze J, <u>Hartmann P</u>, <u>Donko Z</u>, Uchida G, Koga K, Shiratani M, Czarnetzki U: Dust hour glass in a capacitive RF discharge. **IEEE T PLASMA SCI**, 42:(10) pp. 2672-2673. (2014)

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Other

20. <u>Donkó Z</u>, <u>Korolov I</u>, <u>Magyar P</u>: Franck-Hertz-kísérlet: 100 éve és ma (The Franck-Hertz experiment: 100 years ago and today, in Hungarian). **FIZIKAI SZEMLE**, 64:(4) pp. 125-131. (2014)

S-K. Liquid Structure

Wigner research group

László Pusztai, Pál Jóvári, László Kőszegi[A], György Mészáros[A], Ildikó Pethes, Szilvia Pothoczki, Erzsébet Sváb[A], László Temleitner, Orsolya Gereben[A]

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 2014.
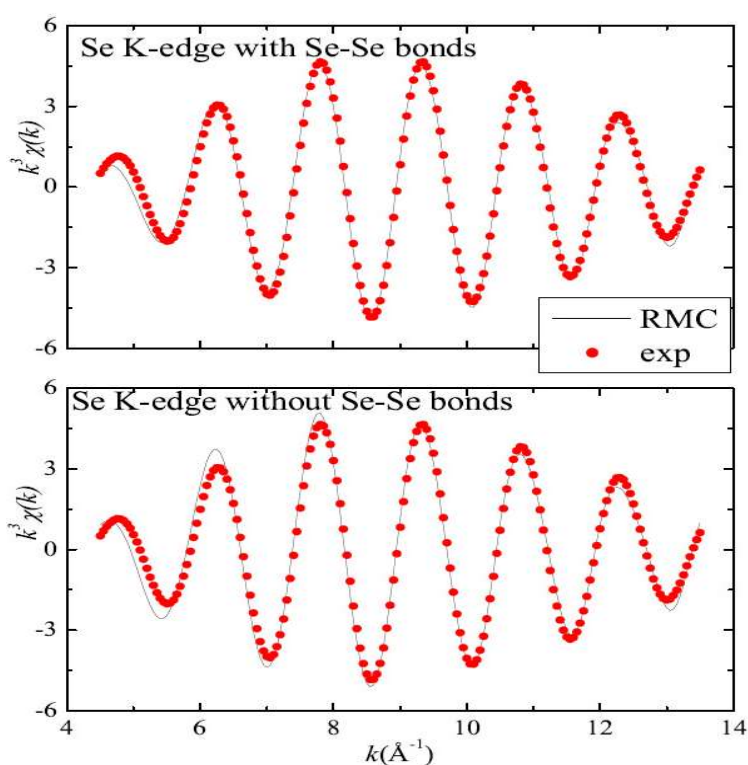

Figure 1. *Comparison of experimental and model Se K-edge EXAFS data of $Ge_{33}As_{20}Se_{47}$ obtained by fitting simultaneously X-ray diffraction and Ge-, As and Se K-edge EXAFS measurements. Upper panel: Se-Se bonds allowed, lower panel: Se-Se bonds forbidden.*

Covalent glasses. — The structure of *Te-rich* (75-80 at.% Te) and *Te-poor* (40 at.% Te) *Ge-As-Te glasses* has been investigated by diffraction and EXAFS (extended X-ray absorption fine structure) measurements. Large scale structural models have been created by fitting simultaneously diffraction and EXAFS data sets by the reverse Monte Carlo simulation technique. It is found that As-As bonds improve the fit quality in the case of Te-rich glasses while no Ge-Ge bonding is necessary in these compositions. Chemical ordering is expected in the Te-poor glasses: Te-Te homonuclear bonds are not observed while Ge binds preferentially to Te rather than to As. Ge-As and Ge-Te coordination numbers do not change significantly with increasing Ge content.

[A] Associate fellow

The structure of *Ge$_x$As$_{10}$Se$_{90-x}$ (x=10, 17.5, 22.5, 27.5, 30, 35) glasses* as well as some other compositions extensively used in infrared optics, for example, GASIR® (Ge$_{22}$As$_{20}$Se$_{58}$) and AMTIR-1 (Ge$_{33}$As$_{12}$Se$_{55}$) has also been studied by a similar combination of experimental techniques and reverse Monte Carlo simulation. Ge-As-Se glasses are characterized by the lack of preferential bonding and behave as random covalent networks: Ge-Ge, Ge-As or As-As bonds can be found in Se-rich compositions while Se-Se bonding remains in strongly Se-deficient glasses as well. This is illustrated by Figure 1 where we compare Se K-edge fits of Ge$_{33}$As$_{20}$Se$_{47}$ obtained with (upper panel) and without (lower panel) Se-Se bonds.

It is to be mentioned that amorphous Ge-Sb-Te alloys are characterized by strong chemical short-range order: Ge-Ge and Ge-Sb bonds are formed only in case of tellurium-deficient compositions. Chemical ordering is somewhat weaker in Ge-As-Te glasses as As-As bonds can already be observed in Te-rich compositions. Finally, Ge-As-Se glasses are random covalent networks with no observable chemical short range order. These results suggest that chemical ordering is stronger in IV-V-VI glasses consisting of heavier components.
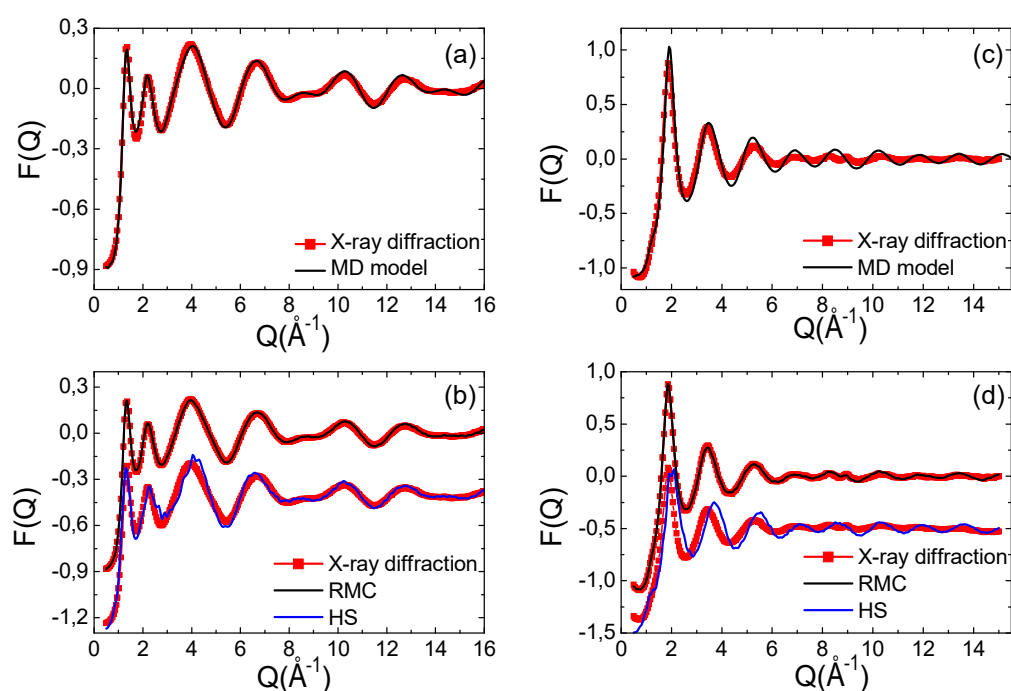

Figure 2. *(a) and (b) X-ray total scattering structure factors of liquid PCl$_3$. Clearly, the molecular dynamics (MD) simulation was able to reproduce the measured data nearly quantitatively, and even the hard-sphere-like (HS) reference system resembles the real material quite well. Reverse Monte Carlo (RMC) modeling, as expected, provides full agreement with experiment. (c) and (d) X-ray scattering structure factors of liquid PI$_3$. Here, contrary to the case of phosphorus trichloride, only RMC modeling achieves full consistency with X-ray diffraction data. The hard sphere reference system proves to be only a very crude approximation of the real liquid.*

Molecular liquids. — Synchrotron X-ray diffraction measurements have been conducted on *liquid phosphorus trichloride, tribromide and triiodide*. Molecular Dynamics simulations for these molecular liquids were performed with a dual purpose: (1) to establish whether

existing intermolecular potential functions can provide a picture that is consistent with diffraction data; (2) to generate reliable starting configurations for subsequent Reverse Monte Carlo modelling. Structural models that were fully consistent with experimental diffraction information within errors have been prepared by means of the Reverse Monte Carlo method, see Figure 2. Comparison with reference systems, generated by hard-sphere-like Monte Carlo simulations, was also carried out for demonstrating the extent that simple space filling effects determine the structure of the liquids (and thus, also estimating the information content of measured data). Total scattering structure factors, partial radial distribution functions and orientational correlations as a function of distances between the molecular centres have been calculated from the models. In general, antiparallel-like arrangements of the primary molecular axes are found to be the most favourable orientation of two neighbouring molecules. In liquid PBr_3 electrostatic interactions seem to play a more important role in determining intermolecular correlations than in the other two liquids; molecular arrangements in both PCl_3 and PI_3 are largely driven by steric effects.
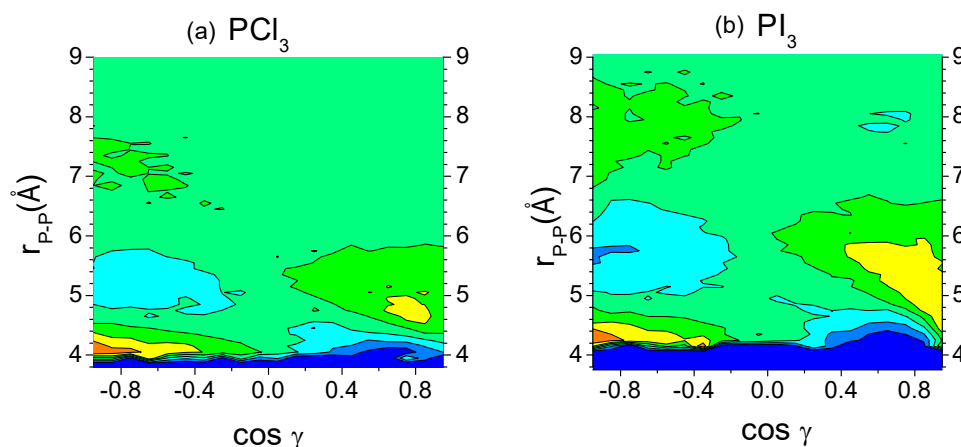

Figure 3. *Dipole-dipole (or molecular axis-molecular axis) correlation functions. (a) PCl$_3$_RMC model; (b) PI$_3$_RMC model.*

Dipole-dipole orientational correlation functions for liquid PCl_3 and PI_3 are shown in Figure 3 as calculated from the RMC particle configurations. The angle between two dipole vectors has been determined for every molecular pair and their distribution is depicted as the function of the P-P distances in the figure. Concerning the shortest centre-centre distances (within the first P-P coordination shell, up to about 8 Å), two clear regions emerge. The highest intensities at around 4 Å belong to the antiparallel orientation ($\cos \gamma = -1$). The other representative arrangement, the parallel orientation with $\cos \gamma = 1$, is less concentrated into a narrow distance range and appears with much lower intensity.

Liquid carbon tetrabromide, CBr_4, is one of the prototypical molecular liquids containing highly symmetric (in this case, tetrahedral) molecules. Surprisingly, the partial radial distribution functions (PRDF) of this material have so far been determined, using computer modelling, on the basis of only one measured diffraction data set (that has always happened to be the neutron-weighted total scattering structure factor). With the aim of improving this situation, we have performed synchrotron X-ray diffraction experiments on the liquid phase at about 400 K, using the BL04B2 high energy beamline of the SPring-8 synchrotron facility

(Hyogo, Japan). The new X-ray data, as well as previously measured neutron diffraction results, have been subjected to Reverse Monte Carlo modelling. RMC calculations using one (neutron OR X-ray), two (neutron AND X-ray) and zero (hard sphere reference, HS) experimental data sets were carried out. As it can be seen in Figure 4, particle configurations in full agreement with measured data could be produced in each case. All the three (C-C, C-Br and Br-Br) PRDF-s from each model could be calculated; the main finding is that PRDF-s based on the neutron diffraction data only are an equally valid representation of the liquid with those obtained on the basis of the two measurements, even though the two total structure factors appear to be rather different. A possible rationalization of this finding is that when dealing with molecules of such high symmetry, the positions of the 'ligands' (in the present case, of bromine atoms) determine the position of the central atoms (here, of carbon atoms).
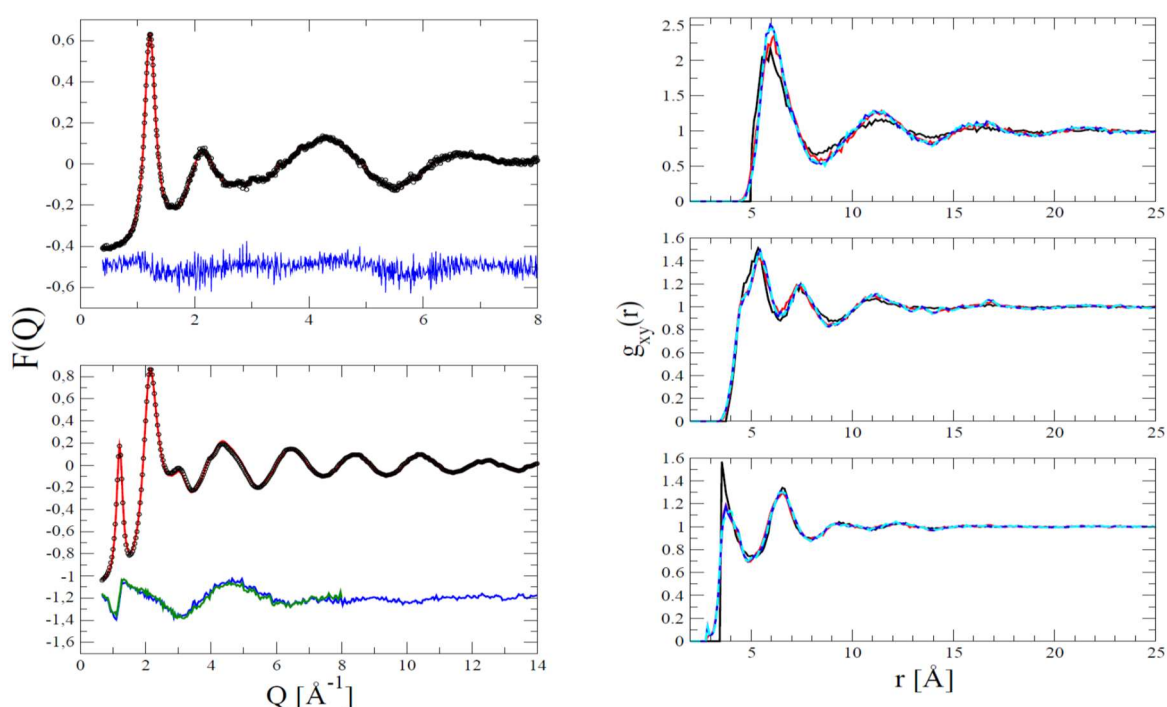
Figure 4. Left panel: Agreement of RMC models with experimental total structure factors of liquid CBr_4. Upper part: neutron diffraction; lower panel: x-ray diffraction (this work). Circles: experimental data; red solid lines: RMC model; blue lines: residuum. **Right panel**: Partial radial distribution functions calculated for the various models of liquid carbon tetrachloride. Black solid line: hard sphere reference; red line: neutron data only; blue line: neutron and X-ray data were both made use of. Upper part: C-C PRDF; middle part: intermolecular C-Br PRDF; bottom part: intermolecular Br-Br PRDF. Note that the addition of the X-ray data to the model has not altered these real space functions.

Grants

SNK-63/2013 (MTA-BAS Hungarian-Bulgarian bilateral) Investigation of the short- and long range order in multifunctional materials; (E. Sváb, 2014)

„Wigner research group" support

Publications

Articles

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11. Silva-Santisteban A, Henao A, Pothoczki S, Bermejo FJ, Tamarit JL, Guardia E, Cuello GJ, Pardo LC: Short range order of CCl4: RMC and MD methods. **J PHYS CONF SER**, 549:(1) Paper 012014. 4 p. (2014)

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

Ultrafast nanooptics Lendület research team

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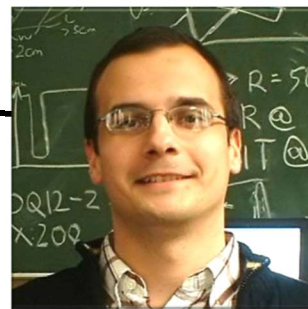
Strong-field interactions and nano-optics experiments. — We investigated the mechanism of the known and disputed phenomenon of THz generation from plasmonic nanostructures experimentally. We delivered an explanation for the observed phenomena by demonstrating that it is mainly optical rectification from the nanostructured surface that contributes to THz generation at low laser intensities, while for high intensities, radiation from photo-emitted and photo-accelerated electrons that takes over in determining the THz radiation.

We also preformed the genetic optimization of a so-called light field synthesizer device. It has been demonstrated recently that ultrashort optical waveforms can be synthesized from different colored channels in the visible domain. We investigated what happens when we generate high-order harmonics with such synthesized waveforms and optimized them for the generation of desired attosecond pulses. We found that attosecond pulses as short as 50 as can be generated with this method and that we can even generate double atto pulses with tunable separation between 300 as and 900 as.

Femtosecond photonics. — We performed a set of fiber optics experiments related to femtosecond pulse compression in various optical fibers. These yielded some fundamental new discoveries in the field of non-linear fiber optics on the conversion of the chirp of laser pulses upon pulse compression in large-mode-area (LMA) photonic crystal fibres. Additional published contributions to this research field include developing and demonstrating a new method for sensitive intracavity testing of large-aperture femtosecond mirrors and the numerical analysis of potential broadband all-dielectric grating structures for pulse compression in high-brightness lasers.

Surface plasmon studies. — Recently, we have reported on our new experimental results, showing anomalous intensity dependence of the laser–assisted surface tunneling microscope signals and time-of-flight spectra of photoelectrons liberated by multiplasmon absorption from a gold nanolayer. We have associated to these findings the picture of plasmon–induced electron pairing, which may be understood on the basis of our earlier non-perturbative study, where we have derived the laser–induced effective potential *between free electrons in vacuum*. As an example, in Figure 2 we show the spatial dependence of such an effective potential for the elastic channel of non-relativistic e–e scattering. We note that, in contrast to several earlier considerations on "photon-induced interband pairing", in our works the Volkov type description of two electrons embedded in

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[#] Ph.D student
[E] Professor Emeritus

the laser (plasmon) field has been the key element in the derivation of the effective e–e attraction, and interband effects did not need to be taken into account.
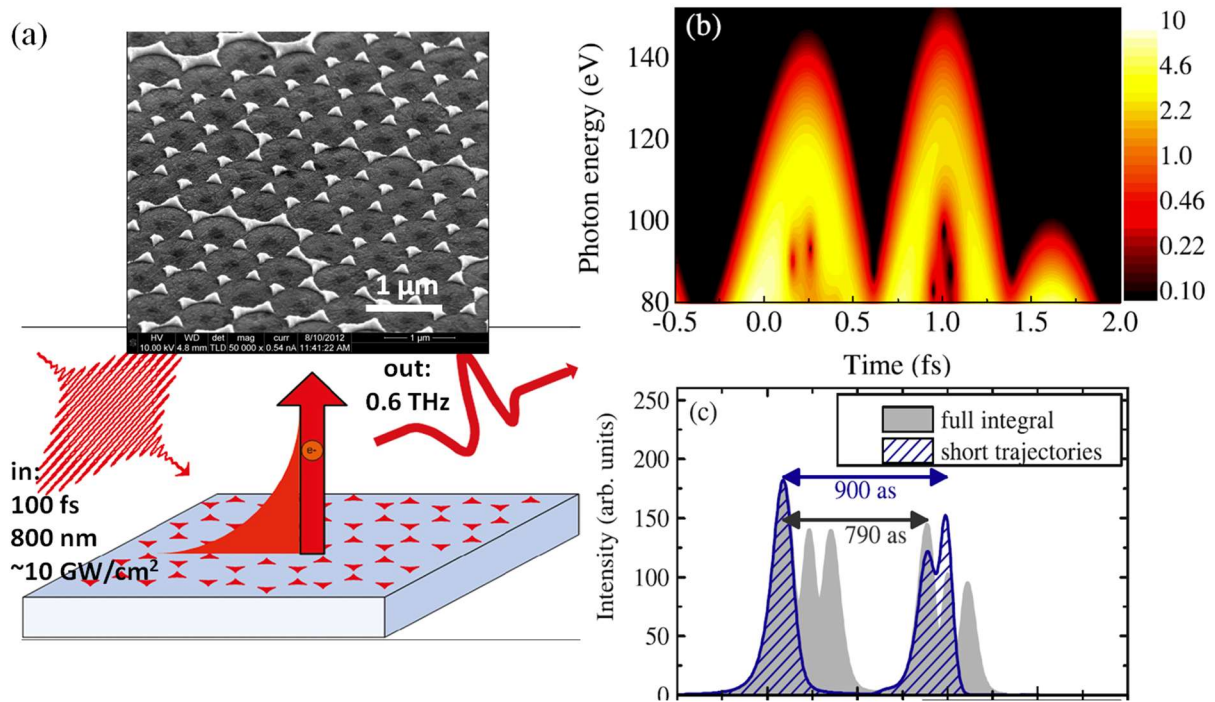
Figure 1. *(a) Generation of THz radiation with femtosecond laser pulses from plasmonic nanostructures showing a typical sample used for the experiments and the experimental geometry. (b) Time-frequency analysis of a double attosecond pulse (with 900 as separation) generated with ultrashort, synthesized optical waveforms out of a lightwave synthesizer. (c) Time structure of the generated double attosecond pulse by looking at the singe-atom response of the medium (grey area) and filtering the short trajectory components of the high-harmonic radiation (striped area).*
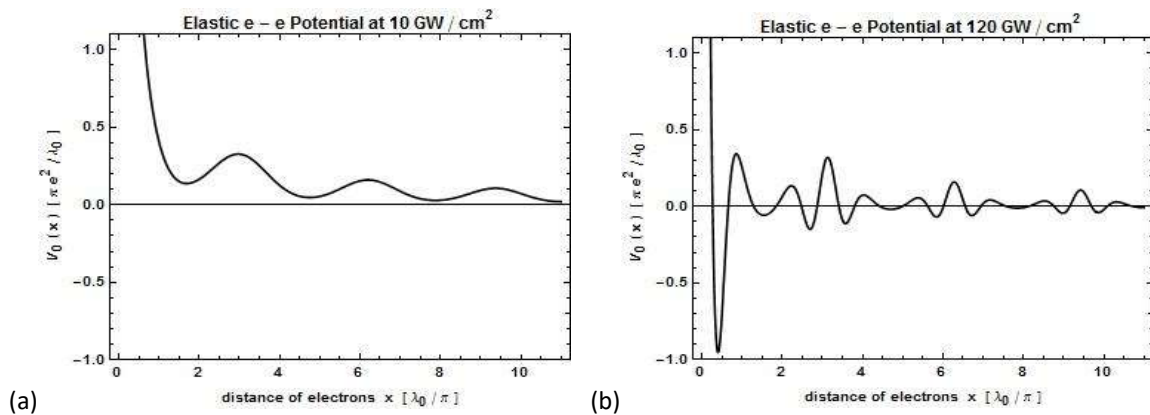
Figure 2. *Variation of the electron-electron effective potential along the propagation direction of the plasmon wave, in the case of the elastic scattering of an e–e pair for I = 10 GW/cm² (a) and for I = 10 GW/cm² (b) incoming laser intensity. As the incoming intensity (and the corresponding plasmon–enhanced local field amplitude) is increased, the original Coulomb repulsion between the two electrons is softened, and even regions of effective attraction appear. A similar behaviour is characteristic for the multiplasmon inelastic channels.*

Theoretical quantum optics. — Concerning theoretical quantum optics, we have shown that the eigenstates of the simple new exponential phase operator, defined by the polar decomposition of the quantized amplitude of a linear oscillator (which may represent a mode of the radiation field), are SU(1,1) coherent states. In terms of these coherent states, we have represented a variant of the quantum saw-tooth phase operator in the original Hilbert space. In Figure 3, we illustrate the dependence on the action-angle parameters of the quantum phase function found and a corresponding quantum sampling function. The method developed by us, which leads to the generalized spectral decomposition of the phase operator, may for example be useful in describing the quantum phase properties of extreme radiation fields (like attosecond light pulses), or, in general, may be applied in quantum signal analysis.

(a)

(b)
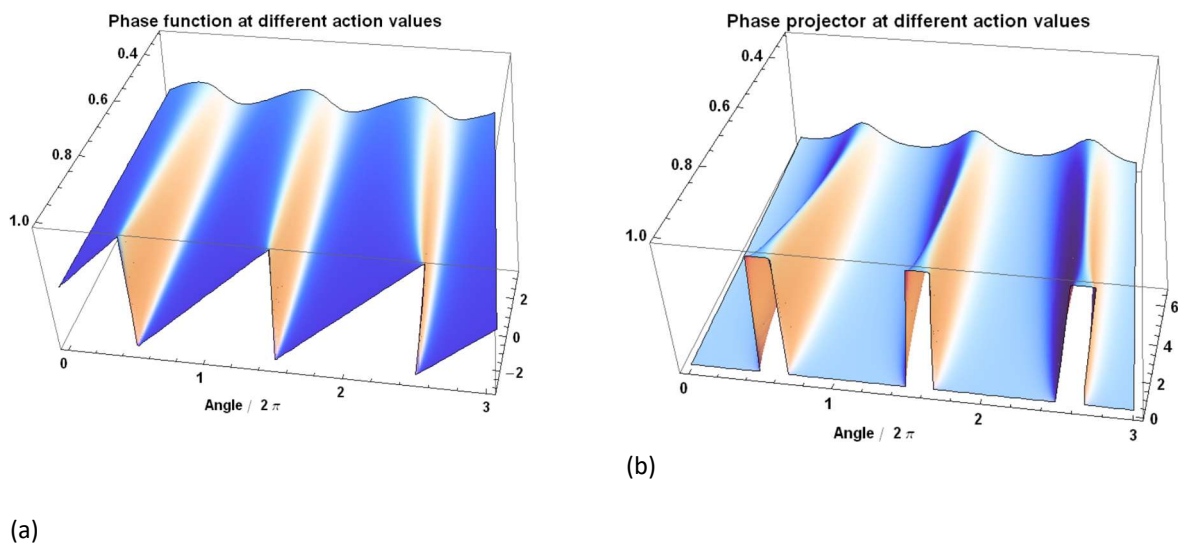
Figure 3. *Three-dimensional plot of the quantum phase function (a) for increasing action parameter values in the angle interval corresponding to three cycles of the harmonic oscillator. In this range, the expectation values of the photon number vary from 0.5 up to 1800. For large action values the quantum phase function approaches the well-known saw-tooth phase function of classical Fourier analysis. In figure (b), the three-dimensional plot of the quantum phase-sampling function is shown in the same parameter range. This figure illustrates that for larger and larger action values, these "projectors" sharply cut an angle interval of width equal to 1/6 of the oscillator's evolution cycle, thus they approach an ideal phase-sampling function.*

Grants

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

International cooperation

Max Planck Institute of Quantum Optics (Garching, Germany), Ultrafast strong-field nanoplasmonics (P. Dombi)

University of Alberta, Edmonton, Canada, Field-enhanced electron acceleration with few-cycle laser pulses (P. Dombi)

Institute of Photonic Sciences, Barcelona, Ultrafast electron acceleration experiments with mid-infrared lasers (P. Dombi, P. Rácz)

Karl-Franzens Universität, Graz, Austria, Investigation of femtosecond photoemission from nanostructures (P. Dombi)

School of Physics and Astronomy, University of Exeter, THz emission from nanostructures (P. Dombi)

Institute for Quantum Optics, University of Ulm (Ulm, Germany), Wigner functions (S. Varró) Surface plasmon research. (S. Varró and N. Kroó).

Institute for Applied Physics, Theoretical Quantum Physics, Technical University of Darmstadt (Darmstadt, Germany), Quantum optics. (S. Varró)

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See also: R-B.2, R-P.1, R-P.3, R-P.9, S-O.8

S-S. Quantum Optics and Quantum Information

"Momentum" research team

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Cavity Quantum Electrodynamics. — The fundamental description of the interaction of atomistic matter with the electromagnetic field in the Coulomb gauge is known to suffer from the presence of an awkward term containing the square of the vector potential. In most of the practical cases, for optically dilute atomic samples, this term can be neglected and the observable effects are ultimately accounted for in terms of a simplified model, such as the Jaynes--Cummings one. In typical quantum optical systems, such a phenomenological approach with properly adjusted parameters usually gives a satisfactory quantitative accuracy. However, there are situations where even the qualitative behaviour of the system is questionable because of the confusion around this term. A prominent example is the Dicke model where the very existence of the predicted super-radiant phase transition depends on the validity of the adopted effective model. Another important field in this respect is the so-called ultra-strong coupling regime realized by novel artificial systems where the Coulomb gauge entailing the A-square term is not well suited to the consistent description of light-matter interaction and the self-interaction within the polarizable medium.

We showed that cavity quantum electrodynamics (that is, when the field itself as well as the light-matter interaction are significantly influenced by the presence of boundaries) can be established at a fundamental level on a Hamiltonian which eliminates the problem of the A-square term. We present a canonical transformation which makes manifest that this term is compensated by the instantaneous dipole-dipole interaction term, and the remaining terms are of a simple linear form. From our approach it follows, for example, that there is no principle that would prevent the super-radiant phase transition in the case of an ensemble of atomic dipoles in a cavity. The canonical transformation is analogous to the Power--Zienau--Woolley (PZW) transformation in free space, however, in our approach we allow for arbitrary geometry, thereby treating a general cavity QED system.

Ultracold gases, Bose-Einstein condensates. — Ultracold atoms coupled to the radiation field of an optical resonator realise a long-range interacting many-body system which proved to be suitable for the quantum simulation of the super-radiant quantum phase transition. A few relevant modes describe with surprising accuracy the self-organization criticality in the frame of the Dicke model. The corresponding quasi-particles of the bosonic superfluid have limited lifetime which has a substantial influence on the nature of criticality. Dissipation and the accompanying quantum fluctuations substantially modify the correlation functions and the critical exponents. We found recently that the presence of criticality, in

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turn, can lead to a drastic modulation of the quasiparticle damping rate when sweeping the control parameter.

We developed a general theory for calculating the damping rate of elementary density-wave excitations in a Bose-Einstein condensate strongly coupled to a single radiation mode of an optical cavity. We found a huge resonant enhancement in the Beliaev damping of the density-wave mode which constitutes the polariton-like soft mode of the self-organization phase transition. The resonant enhancement takes place, both in the normal and ordered phases, outside the critical region. In the polariton mode, only a very small photonic component dresses the density wave mode, but this leads to a large frequency variation (that is, mode softening) due to the presence of the critical point. The available four-particle collisional processes involving the polariton mode, the condensate and two other phonon excitation of the condensate are significantly influenced by the polariton frequency.

We showed that the large damping rate of the polariton mode is accompanied by a significant frequency shift. Going beyond the Born-Markov approximation and determining the poles of the retarded Green's function of the polariton, we reveal a strong coupling between the polariton and a collective mode in the phonon bath formed by the other density-wave modes.
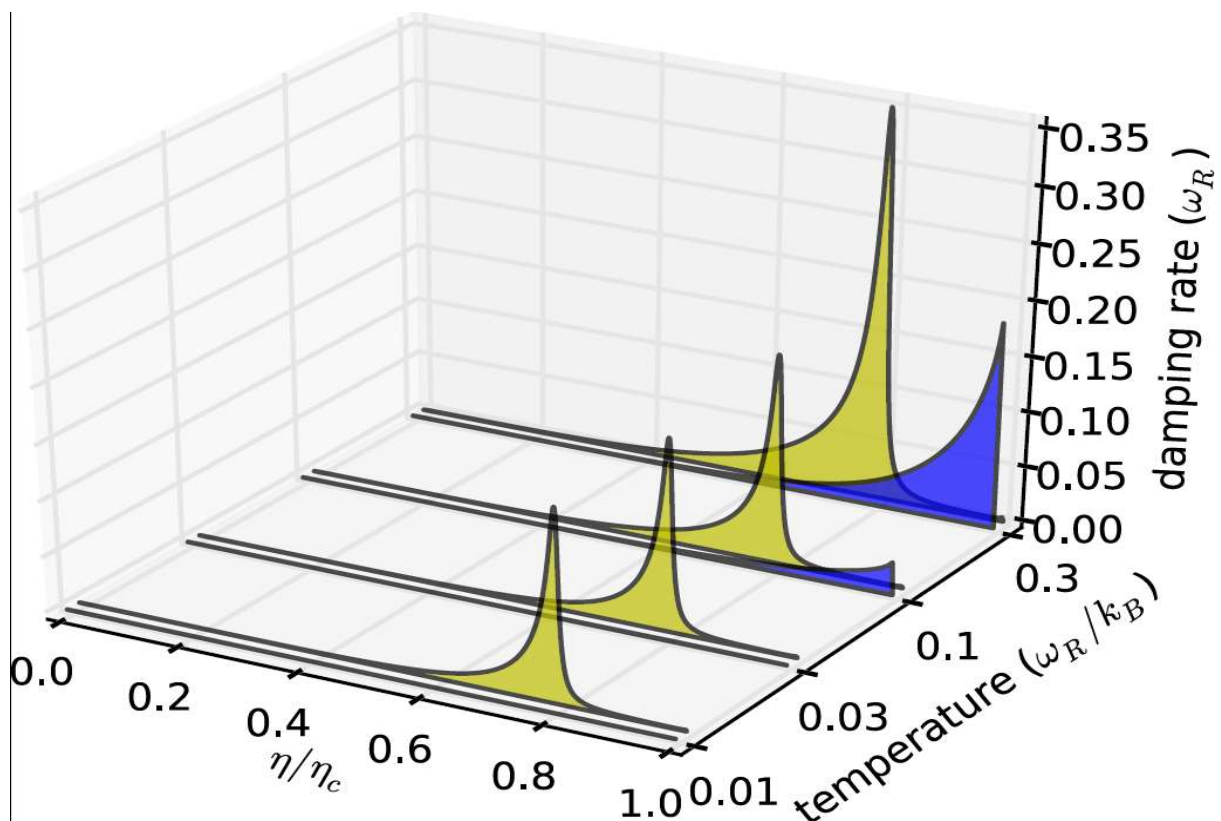
Figure 1. *Photonic tuning of damping. The Beliaev (yellow) and Landau (blue) damping rates are plotted for various temperatures as a function of the normalized pumping strength of the external laser illuminating the atoms from a direction perpendicular to the cavity axis. The Beliaev damping, being dominant at low temperatures, undergoes a resonant enhancement of many orders of magnitude. The Landau damping rate increases towards the critical point but is suppressed for temperatures well below the recoil temperature.*

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Hybrid quantum systems. — We showed how the vibrational modes of a nanowire may be coherently manipulated with a Bose-Einstein condensate of ultracold atoms. We considered the magneto-mechanical coupling between paramagnetic atoms and a suspended nanowire carrying dc current. Atomic spin flips produce a back-action on the wire vibrations, which can lead to mechanical mode amplification. In contrast to systems considered before, the condensate has a finite energy bandwidth in the range of the chemical potential and we explored the consequences of this on the parametric drive. Applying the resolvent method, we determined the threshold coupling for parametric amplification and we also found a significant frequency shift of the vibration due to magneto-mechanical dressing.

Figure 2. *Bose–Einstein condensate (BEC) trapped near a current-carrying nanowire. Mechanical vibrations of the nanowire modulate the magnetic field felt by the BEC thus inducing transitions form the m_F = −1 to t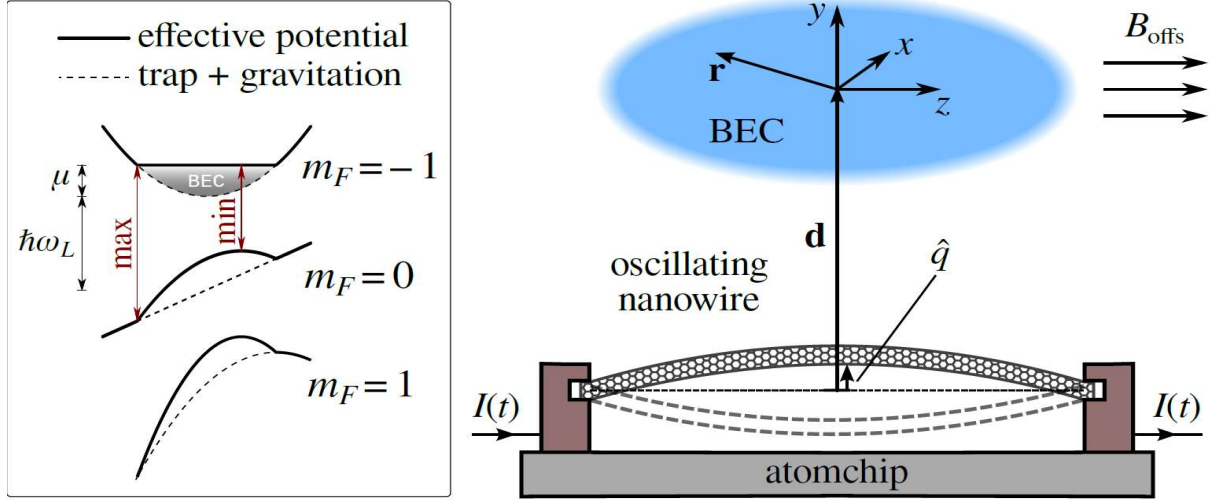he m_F = 0 Zeeman sublevel. The inset shows trapping, gravitational, and scattering potentials for the three Zeeman sublevels.*

Quantum information processing, quantum walks, and chaotic dynamics of entangled qubits. — Randomly breaking connections in a graph alter its transport properties, a model used to describe percolation. In the case of quantum walks, dynamic percolation graphs represent a special type of imperfections, where the connections appear and disappear randomly in each step during the time evolution. We presented an analytical method to solve the evolution on finite percolation graphs in the long-time limit. We completely solved the case of the one-dimensional percolation graphs and found non-trivial asymptotic effects: (quasi-)periodic oscillations, and exponentially localized edge states can emerge. On two-dimensional systems, we demonstrated new effects like localization in the asymptotic limit, and a special directional symmetry breaking.

Topological phases. — One of the main tasks of condensed matter theory today is the classification and realization of topological states of matter. For non-interacting electrons in closed systems with discrete symmetries (time-reversal, chiral, particle-hole), the theoretical part of this task is already completed, and summarized in the celebrated "periodic table of topological insulators". Current research focuses on a broader classification, by relaxing any of the constraints on "matter" placed above (that is, allowing for interactions) treating bosons as well as fermions, including less fundamental (for example, crystalline) symmetries, or treating open systems by allowing for periodic driving. We study topological phases of a type of periodically driven quantum systems: the discrete-

time quantum walks. These belong to the extremely driven limit; that is, their effective (Floquet) lattice Hamiltonian is a very poor approximation of the instantaneous Hamiltonian.
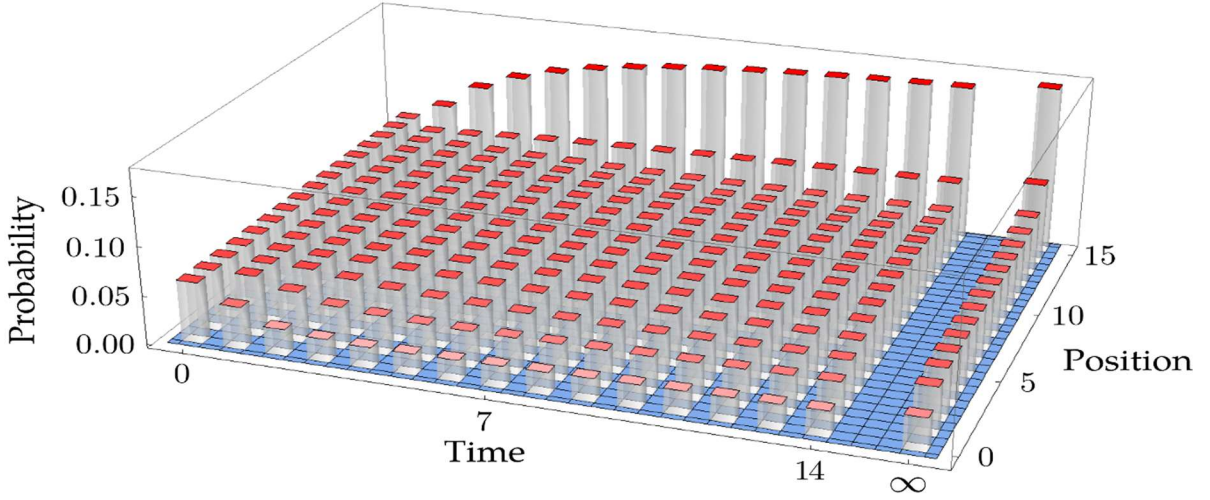

Figure 3. *Evolution of the position distribution corresponding to a quantum walk on a dynamical percolation chain graph with 16 vertices. The walk is started from a pure quantum state corresponding to a flat position distribution. Albeit the dynamical percolation is an isotropic effect, it results in a non-uniform behaviour. The infinity symbol marks the analytically calculated asymptotic distribution of the system.*

Using a generalization of the scattering theory of topological phases, we gave a complete classification of topological phases of one-dimensional quantum walks with discrete symmetries. We found the same classification as in the "periodic table of topological insulators", with the exception that every topological phase has two invariants, not just one, corresponding to edge states with quasi-energy 0 and π (in dimensionless units). We express the bulk topological invariants in terms of matrix invariants of the reflection matrix. This does not only constitute a practical theoretical tool to study (for example, the effects of disorder) but is also a quantity that could be directly measured in an optical experiment.

We gave the bulk-boundary correspondence for chiral symmetric one-dimensional periodically-driven lattice Hamiltonians, of which discrete-time quantum walks are a special case. We gave a sufficient condition for chiral symmetry: a period of the driving should consist of two parts, with a simple relation between the unitary operators representing the first and the second part. We obtained the pair of bulk topological invariants as winding numbers of blocks of the time evolution operator over the first part of the period. This led to simple drive protocols to tune the invariants, which we numerically verified on the periodically driven Su-Schrieffer-Heeger model of polyacetylene (as shown in Figure 4). Our theory gives the first consistent interpretation of the high number of Floquet-Majorana fermions seen by numerical simulations of periodically-driven quantum wires.
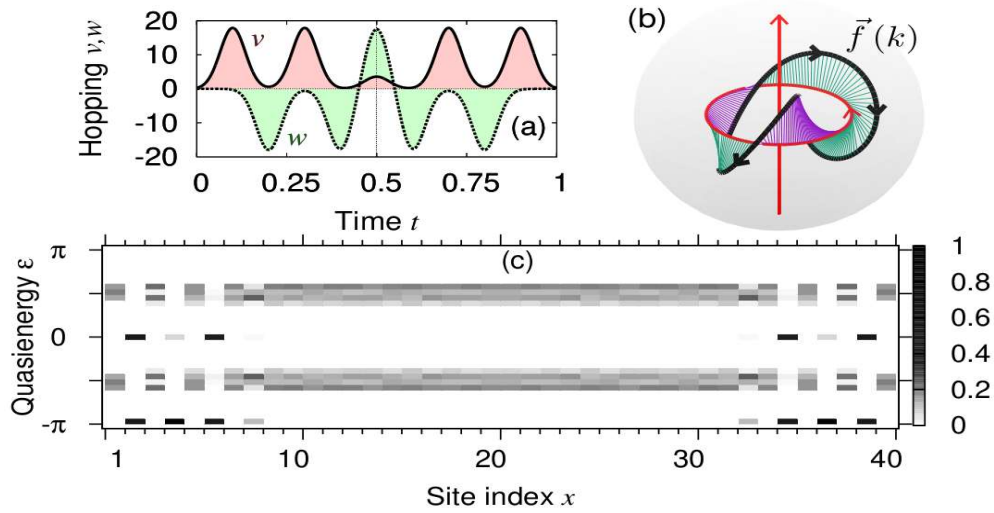
Figure 4. *Bulk topological invariants and end states in a periodically-driven quantum wire, described by the Su-Schrieffer-Heeger model with chiral symmetry. (a): A simple drive protocol for the intracell (v) and intercell (w) hopping amplitudes to ensure chiral symmetry and tune the topological invariants; (b): the topological invariants have a direct geometric interpretation: they are windings of the vector representing the time-evolution operator during a part of the period; (c): the end states predicted by the bulk invariants show up in the local density of states of the wire.*

Vibrational dynamics of simple molecules – It was shown that vibrational displacements satisfying the Eckart-Sayvetz conditions can be constructed by projection of unconstrained displacements. This result has a number of interesting direct and indirect ramifications: (i) The normal coordinates corresponding to an electronic state or an isotopologue of a molecule are transformed to those of another state or isotopologue by a linear and, in general, non-orthogonal transformation. (ii) Novel interpretation of axis switching. (iii) One may enhance the separation of rotational-large-amplitude internal motions and the vibrational motions beyond that offered by the standard use of the Eckart-Sayvetz conditions. (iv) The rotational-vibrational Hamiltonian given in terms of curvilinear internal coordinates may be derived with elementary mathematical tools while taking into account the Eckart conditions with or without enhancement.

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MÖB-DAAD: 40018 Properties of continuous-time quantum walks and their applications for modelling transport of electrons (T. Kiss, 2013-2014)

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domestic quantum-electronics research. Budapest, 28.11.2014, Eds.: Ádám P, Almási G, University of Pécs, Hungary, 2014. Paper E6. 2 p

See also: S-Q.7, S-Q.8, S-Q.11, S-Q.15.

INSTITUTE FOR
PARTICLE AND NUCLEAR PHYSICS

R-A. Field theory

Kornél Szlachányi, Gabriella Böhm, László Fehér, Gyula Fodor, Péter Forgács, Tamás Herpay, Árpád Lukács, Balázs Mikóczi, Júlia Nyíri, László Szabados, Péter Vecsernyés

Relativity and quantum cosmology. — The simplest explanation of the observed deviation of red-shift versus luminosity of distant supernovae explosions (Perlmutter, Schmidt; Nobel prize, 2011) from the expected one is the strict positivity of the cosmological constant in Einstein's field equations; that is, that the spacetime is asymptotically de Sitter. In cooperation with Prof. Paul Tod (Math. Institute and St. John's College, Oxford University) the structure of general, asymptotically de Sitter space-times was clarified. We found a well defined notion of energy-momentum and mass of the matter+gravity system, associated with a closed 2-surface of the future conformal infinity, such that the energy-momentum is future pointing and timelike, and is vanishing precisely when the spacetime is exactly the de Sitter spacetime.

We computed the full analytic time-dependent signal (that is, gravitational waveform) of eccentric compact binaries (black holes and/or neutron stars) based on the gravitational radiation formula up to first post-Newtonian order. Using generic perturbations of celestial mechanics the Hansen expansion was generalized to the first post-Newtonian order. The final result was an analytic ready-to-use first post-Newtonian eccentric waveform in the Fourier domain.

Periodically oscillating localized scalar field configurations were investigated when there is a negative cosmological constant. In this case the configurations are asymptotically anti de Sitter, which is important because of the AdS/CFT correspondence and the recently discovered instability of anti de Sitter spacetime. These objects were studied by a spectral numerical code, by high order perturbation methods, and we studied their stability by direct numerical evolution.

Causal and phase structures of quantum field theories. — Bell's local causality was formulated within the framework of local classical theories with or without primitive causality and local quantum theories with primitive causality. Sufficient conditions were found for a local physical theory to be locally causal.

The translation invariant phases of the XYZ quantum chain was classified. The field algebras of various Hubbard chains were constructed arising from localized and transportable morphism of their observable algebras.

Quantum symmetries. — Multiplier Hopf algebras of Van Daele (1994) provide a beautiful generalization of Hopf algebras having many features that were unavailable in ordinary Hopf algebras due to `infinities'. Various facts about Hopf algebras can be extended to the multiplier setting; in particular, the categories of representations (which here could mean either modules or comodules) of a multiplier Hopf algebra are monoidal. In the case of Hopf algebras, however, this fact has a deep explanation in terms of the induced Hopf monads, while in the multiplier setting such an analysis had been lacking so far.

This question was approached by formulating the definition of multiplier bialgebra and multiplier Hopf algebra in arbitrary braided monoidal categories, and developed the theory of these structures. This includes an analysis of the monoidal structure on the categories of representations and a conceptual explanation of its origin.

The 1-object case of skew monoidal categories was studied, which should be called skew monoidal monoids (SMM). A self-dual bialgebroid was constructed as the symmetry underlying both the module and comodule category of the SMM which is a submonoid of its base; that is to say, of the SMM itself. This symmetry is present even if the skew monoidal structure is not closed.

Grants
OTKA K 108384, A categorical study of quantum symmetries and their applications (Gabriella Böhm, 2013-2017)

Marie Curie IEF fellowship, Observatoire de Paris (Meudon) (Gyula Fodor, 2014 - 2016)

International cooperation
Observatoire de Paris (Gyula Fodor)

University of Glasgow, United Kingdom (Gabriella Böhm)

University of Granada, Spain (Gabriella Böhm)

Macquarie University, Sydney, Australia (Gabriella Böhm)

Nanjing Agricultural University, PR China (Gabriella Böhm)

Long term visitors
Ana Rovi, University of Glasgow (Gabriella Böhm, 2 weeks)

Ulrich Krähmer, University of Glasgow (Gabriella Böhm, 2 weeks)

Stephen Lack, Macquarie University, Sydney (Gabriella Böhm, 3 weeks)

Kenneth Paul Tod, Oxford University (László Szabados, 1 week)

Andrzej Rostworowski, Jagellonian University, Krakow (Gyula Fodor, 2 days)

Publications

Articles

1. Anisovich V V, Matveev M A, Nikonov V A, <u>Nyiri J</u>: Central production of lepton–antilepton pairs and heavy quark composite states in hadron diffractive collisions at ultrahigh energies. **INT J MOD PHYS A,** 29: Paper 1450176. 10 p. (2014)

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7. Fehér L, Kluck TJ: New compact forms of the trigonometric Ruijsenaars-Schneider system. **NUCL PHYS B,** 882:(1) pp. 97-127. (2014)

8. Feher L, Gorbe TF: Duality between the trigonometric BC(n) Sutherland system and a completed rational Ruijsenaars-Schneider-van Diejen system. **J MATH PHYS,** 55: Paper 102704. 31 p. (2014)

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12. Czinner VG: Thick Dirac-Nambu-Goto Branes on Black Hole Backgrounds. In: A García-Parrado, FC Mena, F Moura, E Vaz (eds.): Progress in Mathematical Relativity, Gravitation and Cosmology: Proceedings of the Spanish Relativity Meeting ERE2012, University of Minho, Guimarães, Portugal, September 3-7, 2012, Berlin: Springer Verlag, (Springer Proceedings in Mathematics & Statistics; 60.) 2014. pp. 223-226

See also: R-B.18

R-D. Femtoscopy

Tamás Csörgő, László Jenkovszky[A], Frigyes Nemes[#], András Ster, Márton Vargyas[#], Róbert Vértesi
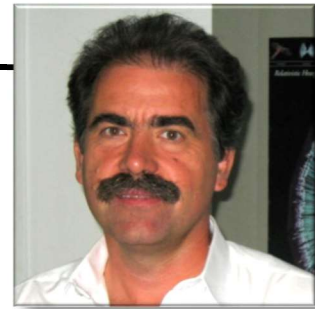
Exploring a new domain of QCD with elastic proton-proton scattering in the TOTEM experiment at CERN LHC and theoretical reconstruction of the internal structure of protons from TOTEM data. — Starting from 2014, T. Csörgő was elected to the Editorial Board of TOTEM, with responsibility in the final readings of all TOTEM papers and the duty of the submission of TOTEM papers to arXiv.org. The year 2014 also brought the first TOTEM-CMS joint paper, on the determination of pseudorapidity-density of charged particles in an unprecendentedly large pseudo-rapidity interval. Our most significant result was published in the TOTEM paper on the LHC optics determination from proton tracks measured by the Roman Pots of TOTEM, a paper prepared by the Hungarian PhD student F. Nemes (together with H. Niewodiamski), that forms also the experimental backbone of the PhD Thesis of F. Nemes (co-supervised by T. Csörgő and M. Csanád). This article appeared in the New Journal of Physics G and due to its originality and innovative content, it was selected by the Editors of the Institute of Physics (IoP, the publisher) for the Special Select Collection. This collection included only two articles on particle physics on this list of special topics from this journal. To interpret these TOTEM data, we devised a generalized Bialas-Bzdak model, and our first results indicate the appearance of geometrical scaling and related new scaling laws. The same data were also interpreted within the Glauber-Velasco model, and the results were presented by Professor R. J. Glauber in a video conference talk at the 10th Workshop on Particle Correlations and Femtoscopy (WPCF 2014) conference. The same results were also presented by T. Csörgő at other important international conferences: at the International Workshop on Collectivity (Orthodox Academy of Crete, Kolymbari, Greece) and also at the 2014 Low-X Meeting (Yukawa Institute for Theoretical Physics, Kyoto, Japan).

Search for the QCD Critical Point in the BNL RHIC experiment PHENIX and theoretical studies of exact solutions of fireball hydrodynamics. —During 2014, the main femtoscopy result from PHENIX was obtained by our collaborator's group, that of Professor Roy Lacey and his team at Stony Brook, that observed a non-monotonous behaviour in the excitation function of HBT radii in Au+Au collisions at RHIC. This provides an indication for the presence of a QCD Critical Point. These results were presented by Professor Lacey at the WPCF 2014 conference. This result gave a new momentum to the activity of our PHENIX group, in collaboration with the ELTE PHENIX group, because our on-going PHENIX data analysis is related exactly to this topic. In addition, we have reached an important

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[A] Associate fellow
[#] Ph.D student

theoretical milestone in 2014, by publishing two papers on exact solutions of rotating fireball hydrodynamics in the journal Physical Review C.

The 10th Workshop on Particle Correlations and Femtoscopy, WPCF 2014 was the most important annual world conference of the year in the area of femtoscopy. WPCF 2014 was organized in a Wigner – ELTE – KRF collaboration in Gyöngyös, Hungary, and chaired by T. Csörgő. We have successfully organized (with T. Csörgő as honorary chair) the 2014 edition of our annual Zimányi Winter School on Heavy Ion Collisions, despite catastrophic weather conditions and an unscheduled close-downs of Wigner RCP: we had six emergency relocations of the Zimanyi School in five days. Amidst exceptional weather conditions, M. Csanád, chair of Zimányi 2014, demonstrated his exceptional organization skills and, with the help of P. Lévai and other co-organizers including T. Csörgő, brought the meeting to a successful conclusion.

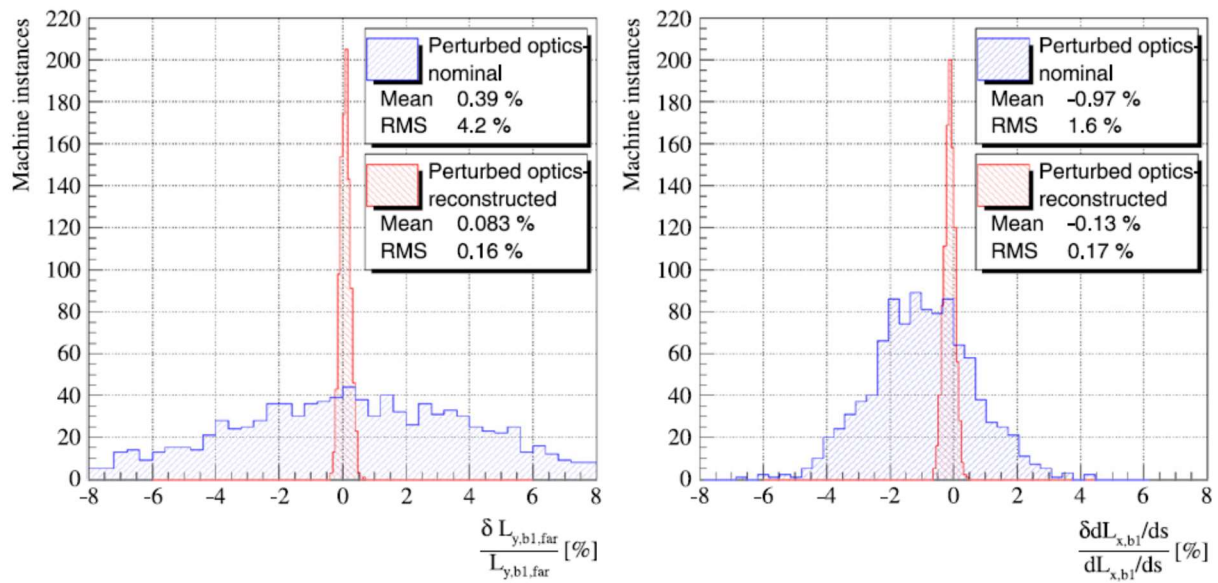**Figure 1.** *Optical functions of CERN LHC at IP5 (TOTEM), for a $\beta^* = 3.5$ m LHC optics, before (**Left**) and after (**Right**) the determination of the optical functions from proton tracks measured by the Roman Pots of the TOTEM experiment. The precise recalibration from TOTEM data made it possible for TOTEM to determine the total cross-section of proton-proton collisions at 7 and 8 TeV LHC collisions.*

Figure 2. *Secondary school students play with Quark Matter Outreach Card Games at the Berze Hits Particle Card Game Competition, organized in Gyöngyös, Hungary in a Wigner-ELTE-KRF Collaboration.*

Grants

International cooperation

Harvard University (Cambridge, MA, US)- Wigner RCP: Theoretical analysis of TOTEM data (T. Csörgő, R.J. Glauber, F. Nemes)

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

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: J. Sziklai, R. Vértesi)

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: F. Nemes, J. Sziklai).

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)

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Articles

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Others

7. <u>Csörgő T</u>, Novák T: World class workshop on femtoscopy in Gyöngyös, Hungary. **J CENT EUR GREEN INNOV**, 2:(4) pp. 189-194. (2014)

8. <u>Csörgő T</u>, Novák T: Femtoszkópiai világkonferencia Gyöngyösön (World class workshop on femtoscopy in Gyöngyös, Hungary, in Hungarian). **J CENT EUR GREEN INNOV**, 2:(4) pp. 183-187. (2014)

Phenix collaboration

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2. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Sziklai J</u>, <u>Vértesi R</u> [425 authors]: Cold-nuclear-matter effects on heavy-quark production at forward and backward rapidity in d+Au collisions at $\sqrt{s_{NN}}$=200 GeV. **PHYS REV LETT**, 112: Paper 252301. 8 p. (2014)

3. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Sziklai J</u>, <u>Vértesi R</u> [380 authors]: Inclusive double-helicity asymmetries in neutral-pion and eta-meson production in p $\to$+p $\to$ collisions at $\sqrt{s}$ =200 GeV. **PHYS REV D**, 90:(1) Paper 012007. 19 p. (2014)

4. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Ster A</u>, <u>Sziklai J</u>, <u>Vértesi R</u> [451 authors]: Measurement of transverse-single-spin asymmetries for midrapidity and forward-rapidity production of hadrons in polarized p+p collisions at $\sqrt{s}$=200 and 62.4 GeV. **PHYS REV D**, 90:(1) Paper 012006. 16 p. (2014)

5. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Sziklai J</u>, <u>Vértesi R</u> [386 authors]: Azimuthal-angle dependence of charged-pion-interferometry measurements with respect to second- and third-order event planes in Au plus Au collisions at $\sqrt{s_{NN}}$=200 GeV. **PHYS REV LETT**, 112:(22) Paper 222301. 6 p. (2014)

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at √s$_{NN}$=200 GeV. **PHYS REV C**, 90:(3) Paper 034903. 13 p. (2014)

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10. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Ster A</u>, <u>Sziklai J</u>, <u>Vargyas M</u>, <u>Vértesi R</u>, <u>Zimanyi J</u> [589 authors]: Measurement of K^0_S and K^{*0} in p + p, d + Au, and Cu + Cu collisions at √s$_{NN}$=200 GeV. **PHYS REV C**, 90:(5) Paper 054905. 18 p. (2014)

11. Adare A, et al. incl. <u>Csörgő T</u>, <u>Novák T</u>, <u>Ster A</u>, <u>Sziklai J</u>, <u>Vértesi R</u> [390 authors]: Nuclear matter effects on J/ψ production in asymmetric Cu+Au collisions at √s$_{NN}$ =200 GeV. **PHYS REV C**, 90:(6) Paper 064908. 10 p. (2014)

12. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Sziklai J</u>, <u>Vargyas M</u>, <u>Vértesi R</u> [523 authors]: Comparison of the space-time extent of the emission source in d+Au and Au+Au collisions at √s$_{NN}$=200 GeV. **NUCL PHYS A**, 931: pp. 1082-1087. (2014)

13. Adare A, et al. incl. <u>Csörgő T</u>, <u>Nagy MI</u>, <u>Ster A</u>, <u>Sziklai J</u>, <u>Vargyas M</u>, <u>Vértesi R</u> [673 authors]: PHENIX Collaboration. **NUCL PHYS A**, 931: pp. 1230-1236. (2014)

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TOTEM Collaboration

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2. Chatrchyan S, Khachatryan V, Sirunyan A M, Tumasyan A, et. al incl. <u>Bencze G</u>, <u>Hajdu C</u>, <u>Hidas P</u>, <u>Horvath D</u>, <u>Sikler F</u>, <u>Veszpremi V</u>, <u>Vesztergombi G</u>, <u>Zsigmond AJ</u>, <u>Csörgő T</u>, <u>Sziklai J</u>[2287 authors]: Measurement of pseudorapidity distributions of charged particles in proton-proton collisions at TeV by the CMS and TOTEM experiments. **EUR PHYS J C**, 74: Paper 3053. 26 p. (2014)

R-E. Theoretical neuroscience and complex systems

Fülöp Bazsó, Dorottya Cserpán[#], Péter Érdi, László Négyessy, Zoltán Somogyvári, László Zalányi
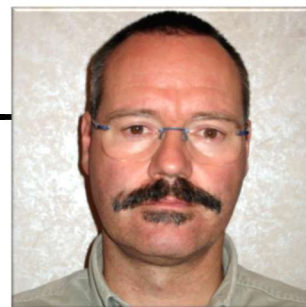
Regular structure and time series classification. — Inspired by the famous Szemerédi's Regularity Lemma, we propose a new algorithm for time series classification. Time series are represented in terms of a bipartite graph, and probabilistic model space is proposed to fit the actual data. Model selection uses Rissanen's minimal description length principle. Sets of nodes and the patterns of relations between them represent the structure of large objects, while the more detailed structure is random-like. The algorithm scales well with data size and the structure itself becomes more apparent as data size increases. Our method is useful in the broader context of big data science.

Determination of cortical and synaptic layers and synaptic dynamics based on extracellular multi-electrode potential measurements. — We have shown that it is possible to determine cellular and synaptic layers in the hippocampus and in the neocortex, based on an extracellular multi-electrode potential measurement. The specific laminar distribution of the efferent hippocampal pathways enables identification of the anatomical layers in the dendritic area based on the coherence (Figure 1). This method reliably determined the different anatomical layers not only in the hippocampus, but also identified three separate layers, corresponding to the superficial, middle and deep layers in the neocortex. Temporal dynamics of the LFP and CSD in hippocampal layers showed a spatiotemporal distribution of synaptic events leading to action potentials in pyramidal cells and interneurons.
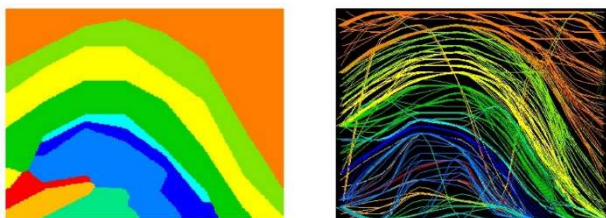
Figure 1. Laminar distribution of the efferent hippocampal pathways.

Modeling and studying cerebral cortical circuitries: from synapses to large scale. — We studied the connections between two, neighboring cortical areas that have similar functions but distinctive functional properties. We focused on the synaptic organization and the spatial characteristics of connectivity. Cortical interactions were also studied at large scale by way of network modeling. The model network representing the input-output combinations of the areas have short path lengths, low-level reciprocity and clustered organization (Figure 2). The results shed light on the importance of "marginal" areas.

[#] Ph.D student
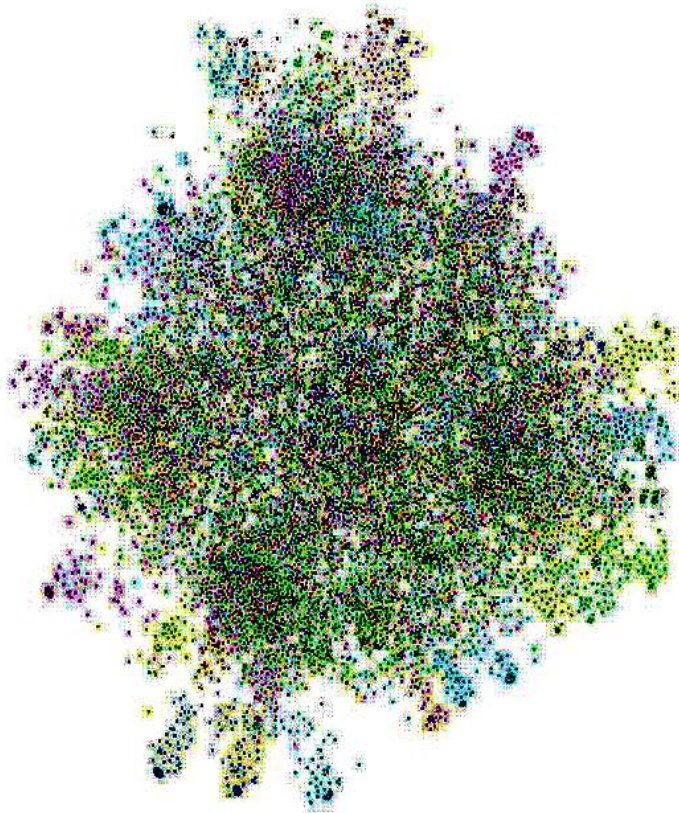
Figure 2. *Clustered organization of the network of input-output combinations of the cortical areas.*

International cooperation

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

Vanderbilt University, (Nashville, TN, USA), Imaging and mapping sensorimotor circuits in the primate (Anna Wang Roe).

New York University (New York, NY, USA), Microelectrode imaging, (György Buzsáki)

University of Texas, (Austin, TX, USA), Theory of budgetary politics (Bryan Jones)

University of Novi Sad, (Novi Sad, Serbia), Analysing and modeling neural signals (Tatjana Lončar-Turukalo)

Publications

Articles

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R-L. Functional nanostructures

László Bottyán, László Deák, István Dézsi[E], Miklós Dolgos[#], Márton Major, Dániel Géza Merkel, Béla Nagy[#], Dénes Lajos Nagy[E], Szilárd Sajti

The group conducts research on the structure and dynamics of inorganic and biomimetic nanostructures by nuclear solid-state methods: neutron, x-ray and synchrotron-based reflectometries. Development of the theory of these techniques is a particular strength of the group.

Stroboscopic detection of nuclear resonance scattering of synchrotron radiation. — In order to quantitatively evaluate the so-called "pseudo-reciprocity" that we recently demonstrated in a nuclear x-ray scattering experiment, the stroboscopic detection of nuclear resonance scattering (NRS) of synchrotron radiation was explored. The method is identical to interferometry and the developed theoretical treatment provides both the real and imaginary parts of the scattering amplitude of NRS.

Magnetic heterostructures

Off-specular neutron scattering and NRS of randomly patterned heterostructures: Magnetic domain structures were theoretically studied in order to extract the intra- and inter-layer (magnetic) domain-domain correlation functions using Poisson's point distributions.

Off-specular neutron scattering and NRS of laterally periodic heterostructures: A non-perturbative exact solution for anisotropic magnetic scattering in grazing incidence (GISANS and NR GISAXS methods) was found for spherical lateral inhomogeneities.

Superconductor/ferromagnet (SC/FM) proximity: Tiny changes in the magnetic structure of multilayers were detected by neutron reflectometry using spin asymmetry (SA) plots. According to modeling the inverse proximity effect in SC/FM bilayers shift the zero crossings of the SA, while changes in the FM layer magnetization does not. SA plots on MgO(100)/^{57}Fe(1 nm)/V(40 nm)/Pt(31 nm) reveal that the different cooling speeds alter vortex pinning so that changes in the magnetic structure may average out near the interface.

Mössbauer polarimetry: Using exponential escape function of the electrons from all resonance processes, a general expression of the electron yield in ^{57}Fe integral conversion electron Mössbauer spectroscopy was derived as a function of the incident angle of the γ-photons, the source polarization and the isotopic abundance of the source and the absorber, providing a firm basis to determine the alignment and direction of magnetization in the absorber.

[E] Professor Emeritus
[#] Ph.D student

<u>Nanoparticle heterostructures:</u> In a quest for high-strength, radiation-resistant alloys, the atomic and electronic structure of carbon-containing oxide-strengthened steels were studied and found to exhibit FCC structure. Multilayers composed of an electronic insulator an iron film and an insulator-covered iron nanoparticle composite layer were successfully synthetized and analyzed.

Laboratory automatization. — To increase productivity, reliability and long-term operational safety, all instruments of the ultra-vacuum deposition Thin Film Technology Laboratory (a registered national research infrastructure) have been hardware-upgraded and rendered under a common computer program control, such that most processes can be fully monitored and controlled remotely.

Grants and international cooperation
Taiwan_MTA_SNK-69_2013 MTA-Taiwan MOST (earlier NSRC) bilateral project: Studying exchange bias effects in ferromagnetic / antiferromagnetic thin films by polarized neutron reflectometry (L. Bottyán, 2013-2014)

TéT-10-1-2011-0671 Hungarian-Vietnamese Bilateral Intergovernmental S&T Cooperation: Porous materials and residual stress in metals studied by nuclear microscopies (L. Bottyán, 2012-2014)

Long-term visitor
Hartmut Spiering, Johannes Gutenberg-Universität Mainz, Institute of Inorganic and Analytical Chemistry, Germany, 1 to 22 November, 2014, (host: L. Deák)

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Article

1. Shabadi V, <u>Major M</u>, Komissinskiy P, Vafaee M, Radetinac A, Baghaie Yazdi M, Donner W, Alff L: Origin of superstructures in (double) perovskite thin films. **J APPL PHYS**, 116:(11) Paper 114901. (2014)

R-M. Ion beam physics

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

Migration of ion-implanted Ar and Zn in silica by backscattering spectrometry. — It is well known, that the refractive indices of lots of materials can be modified by ion implantation, which is important for waveguide fabrication. In this year the effect of Ar and Zn ion implantation on silica layers was investigated by Rutherford Backscattering Spectrometry (RBS) and Spectroscopic Ellipsometry (SE).

Silica layers produced by chemical vapour deposition technique on single crystal silicon wafers were implanted by Ar and Zn ions with a fluence of $1-2\times10^{16}$ Ar/cm^2 and 2.5×10^{16} Zn/cm^2, respectively. The composition and refractive indices of the implanted silica layers before and after annealing for 1h at 300 and 600 ^{o}C were determined by RBS and SE. It was found that the implanted Ar disappeared from the sample after annealing at 300 ^{o}C, while the Zn was found to be stable up to 500 ^{o}C. The migration of the implanted Ar was also studied by real-time RBS up to 500 ^{o}C (see Figure 1).
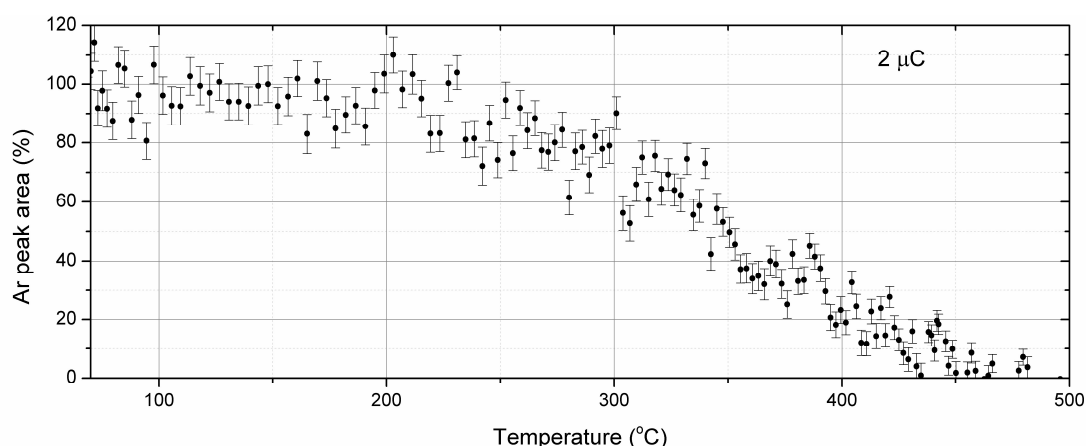
Figure 1. *In-situ annealing combined with RBS experiment performed on the Ar implanted sample with fluence of 1×10^{16} at/cm^2. The Ar starts to escape at 225 ^{o}C; there is another significant step at 350 ^{o}C.*

Although the refractive indices of the Ar implanted silica layers were increased compared to the as-grown samples, but after the annealing this increase in the refractive indices is vanished. In case of the Zn implanted silica layer both the distribution of the Zn and the change in the refractive indices was found to be stable. Zn implantation seems to be an ideal choice for producing waveguides.

[A] Associate fellow
[E] Professor Emeritus

CHARISMA. — Even in the last 3 months of the four years long CHARISMA (Cultural Heritage Advanced Research Infrastructures: Synergy for a multidisciplinary approach to conservation/restoration) EU FP7 Program research groups from Romania, England, Greece, Italy and Portugal got access to the external proton milli-beam PIXE setup at the Van de Graaff accelerator of Wigner to study. The intense joint research work carried on this important measuring facility of the FIXLAB of CHARISMA contributed to a great extent to the excellent performance of the Budapest Neutron Centre (BNC) consortium. This performance was highly acknowledged by the coordination body of CHARISMA.

In the joint research, non-destructive elemental analyses were performed on a variety of archaeological finds. Elemental concentrations and their ratios were determined in fifteen Prehistoric obsidian tools found in Transylvania, (Cluj-Kolozsvár, Oradea-Nagyvárad and Bánát areas). As provenance "fingerprints", the Ti to Mn and Rb to Zr ratios were used. The results confirm that the Transylvanian Neolithic samples have a Slovak Tokaj Mountains provenance. To verify that the concentrations and their ratios for Ti/Mn and Rb/Sr/Y/Zr can constitute a specific pattern for each geological area of obsidian provenance, mineralogical obsidian samples from Mexico, Brazil, Arizona (USA), China, Armenia, Lipari Island and Tokaj Mountains were also analyzed. The results confirmed the existence of unique characteristics that can be used to identify geological areas of provenance for obsidian tools.

Figure 2. *A mineralogical obsidian bombarded with external proton beam of 3 MeV energy for PIXE analysis. Due to ionoluminescence the analyzed spot is clearly seen in red on this particular sample.*

Grants

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Articles

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

Gagik Dzsotjan, József Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós Kedves, Béla Ráczkevi, Zsuzsanna Sörlei[A], Károly Varga-Umbrich[#]

Coherent control of atomic coherences in optically dense media. — We have proposed and analyzed different novel schemes of coherent adiabatic control using short frequency-chirped and transform-limited laser pulses including (i) schemes of robust creation of coherences between meta-stable (ground) atomic quantum states in optically thick media for enhancing different resonant nonlinear optical frequency mixing processes, (ii) schemes of extremely robust creation of coherences between the ground and excited atomic states in dilute gases and optically dense media. These coherences lead to the significant increase in the output, and efficient control of the frequency spectrum of high-order harmonics generated by the strong laser pulses in gases.
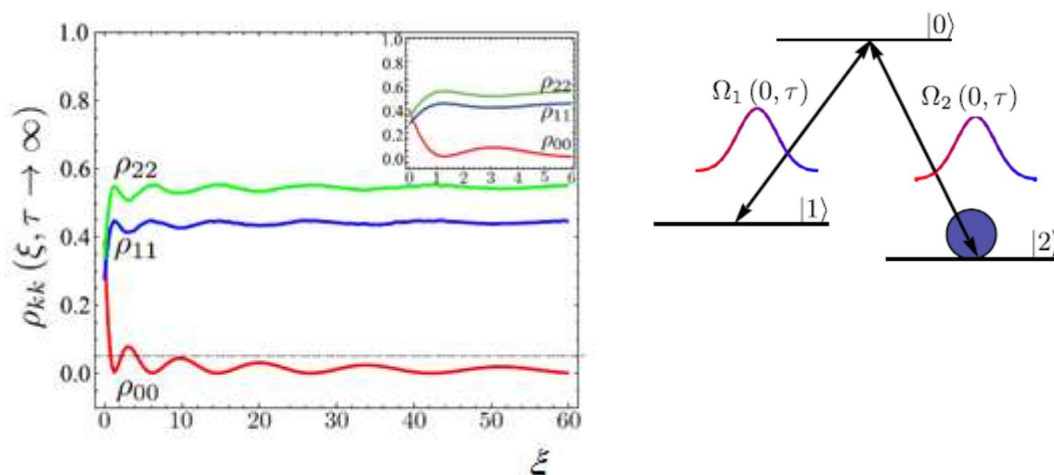
Figure 1. *(a)- Populations of the atomic states established at different propagation distances (absorption length) ξ in the case of a frequency chirped pulse pair; (b)- A schematic illustration of the interaction.*

Generation of harmonics in an atom driven by a strong ultra-short laser pulse. — We have analyzed interactions of ultra-short and intense laser pulses with atoms without application of the rotating wave approximation and obtained the spectrum of the radiation emitted by the atoms. These simulations allow us to understand the features of high-order harmonics generation, including the case, when it takes place in the field of intense frequency-chirped laser pulses.

[A] Associate fellow
[#] Ph.D. student
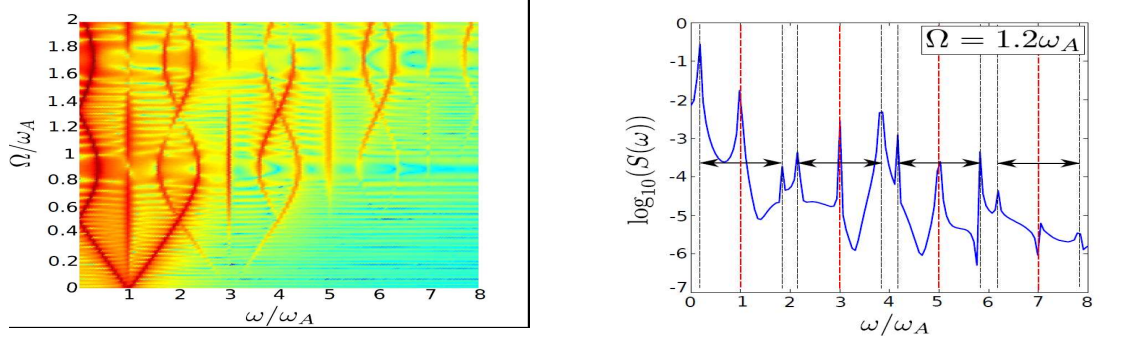
Figure 2. *Spectrum of generated harmonics*

Quantum memories based on photon-echo phenomenon - We have investigated the use of frequency-modulated control pulses and an ensemble of three-level atoms with a Λ-level scheme to serve as an optical quantum memory. If the full bandwidth of the chirped control pulses is large enough to encompass both optical transitions of the atoms, they can drive a cyclic permutation of the atomic states in the adiabatic regime. In this case, three consecutive control pulses can restore the original atomic states with the possibility of re-phasing the optical coherences to obtain an echo emission on the original transition. During an intermediate stage of the sequence, quantum information is stored in long-lived atomic spin coherences.
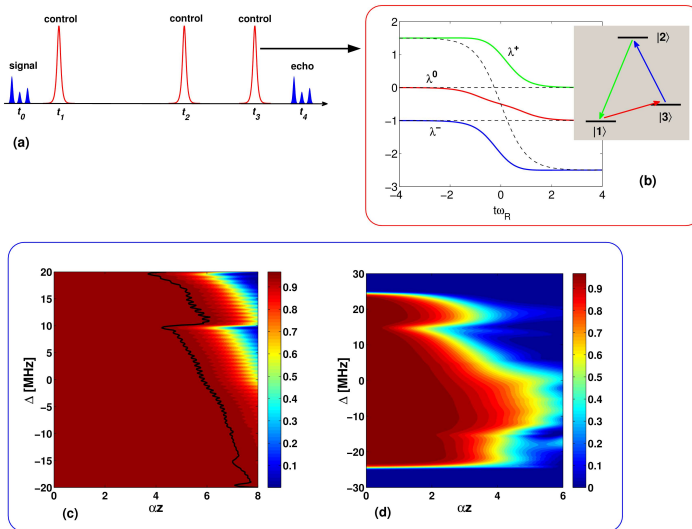
Figure 3. (a) *Time sequence of the signal, control and echo pulses.* **(b)** *The time evolution of the adiabatic eigenvalues of the atoms under the action of the control pulses and the permutation of the atomic states it induces (inset).* **(c)** *The probability with which the control pulses re-phase the atomic coherences in the ensemble as a function of optical depth and atomic resonance frequency. The case when ensemble spectral width is less than the control pulse bandwidth.* **(d)** *The same probability for the case when the ensemble spectral width is larger than the control pulse bandwidth.*

Generation of a highly homogeneous laser plasma: Theory. — We have demonstrated that ultra-short intense frequency-chirped laser pulses may be successfully applied for efficient excitation of Rubidium atoms that results in a substantial decrease of the ionization threshold. This is highly advantageous for generating a homogeneous laser plasma in extended geometries. This work is closely connected with the AWAKE (proton-driven wake-field particle acceleration in plasma) project at CERN and will contribute to transverse modulation of proton bunches into micro-bunches with a length comparable with that of the wavelength of the wake generated in the plasma. We have performed a numerical

analysis of the interaction of intense frequency-chirped laser pulses with Rubidium atoms in the framework of the AWAKE collaboration at CERN.

Experiment. — An experimental setup for the study of the ionization of Rubidium atoms by intense laser pulses of femtosecond duration from a Ti:Sapphire laser has been constructed and ionization of Rb atoms from a dispenser have been performed.
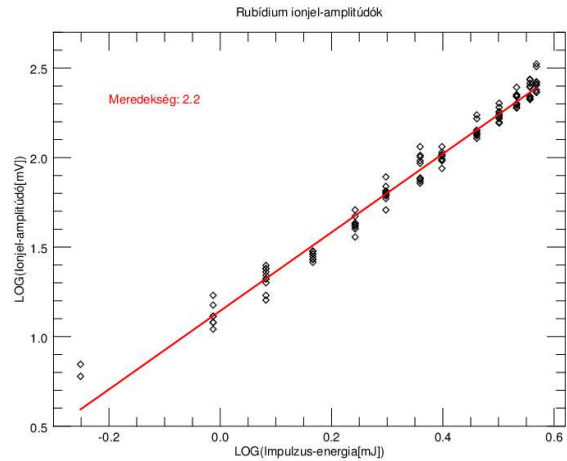
Figure 4. (a)- The experimental setup for generation of high homogeneity Rubidium plasma, (b)- Ionization efficiency of Rb atoms as a function of laser pulse energy in logarithmic scale.

Grants and international cooperation
TÁMOP-4.1.1.C-12- grant.

Infrastructure development grant of the Hungarian Academy of Sciences (G.P. Dzsotjan, 2013-2014)

Excellence Program Grant of the Hungarian Academy of Sciences (G.P. Dzsotjan, 2014-2015)

Dijon, France (G.P. Dzsotjan, 2013-2014)TéT_12_FR-1-2013-0019 French-Hungarian Bilateral with the University de Bourgogne, Dijon, France (G. Dzsotjan, 2013-2014)

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See also: R-P.1

R-O. ITER and fusion diagnostic development

Tamás Ilkei, Tétény Baross, Gábor Bodnár, Fruzsina Darányi, István Gábor Kiss, Botond Mészáros, Dániel Nagy, József Németh, Miklós Palánkai, Ádám Pataki, Gábor Veres

Tokamak Services for Diagnostics (TSD) F4E-FPA-328. — The ITER and fusion diagnostic development group plays a leading role in the TSD project, which concerns the supply of R&D and detailed designs for connectors, cable tails, looms, conduits and feedthroughs to feed and to transport electrical signals to and from various ITER diagnostic sensors in and out of the Vacuum Vessel. None of these components are foreseen to be replaceable, therefore a comprehensive assessment of the risks - failure of electrical contact at connectors, electrical interference, the effects of exposure to irradiation such as material transmutation, heating, and generation of spurious electrical signals - is required along with appropriate mitigation as part of the R&D/Design activities. In 2014 the group focused on the interface definition of various diagnostic sub-systems and services of a Tokamak through close collaboration with the ITER responsible parties. The group also conducted a comprehensive system-level analysis of ITER corresponding applicable documents to identify existing requirements, including (for example) load specifications, environmental constraints, operating conditions, safety and nuclear safety regulations, and interfaces with other ITER systems affecting the design of 'the item to be designed' and its integration in ITER. Furthermore, the activities of the group covers 3D modelling of space reservations for cable tails, looms and feedthroughs and execution of prototype tests, analysis and evaluation of test results including (for example) performance evaluation, mechanical, thermal, electrical, and vacuum compatibility. As a result of the successful collaboration in 2014, a further specific grant of two years duration is under negotiation.
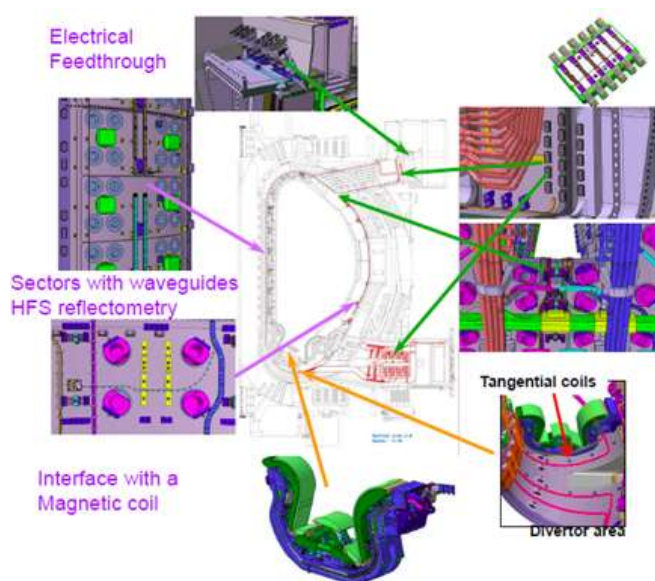
Figure 1. TSD components shown in the cross section of a Tokamak

Development and design of ITER bolometers. — In the 2014, a major four-year framework agreement was signed between a European consortium with Wigner's participation and the Joint Undertaking for the Development of Fusion Energy for the development and design of the ITER bolometry diagnostics including the development of the bolometer cameras themselves. The consortium is led by the Max-Planck-Institute for Plasma Physics and the second largest partner (with about 40 percent of the workload) is the Wigner RCP.

The first of Wigner RCP's tasks of the grant were the identification and analysis of the measurement and system requirements, and the evaluation of the available interface definitions. Of special importance among these were the measurement requirements that set the potential and the limits for physical measurements to conduct during the operational phase of ITER. A unique exercise was the analysis of the spatial resolution capability of the 480 lines-of-sight bolometer camera system.

Main plasma, 1 and 5 % noise
MTF = Modulation Transfer Function
ERF = Edge Response Function
LSF = Line Spread Function
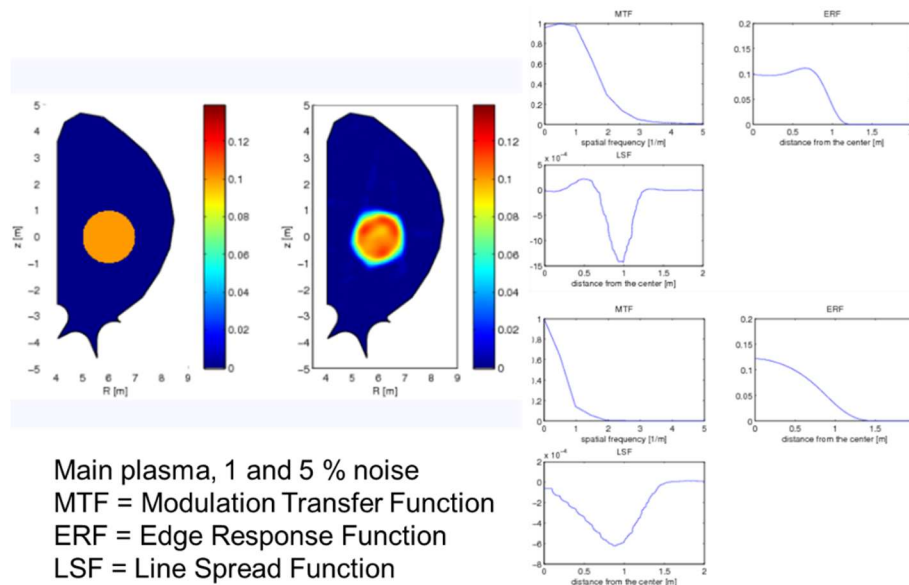
Figure 2. *The analysis of the spatial resolution capability of the ITER bolometer tomography system.*

For the calculations, we have followed the description in the ISO 15708-2:2002 standard and placed a cylinder of a given radius in the physical space where the definition of the spatial resolution is required; that is, in the main plasma (Figure 2. above). By using the LOSs and the etendues we have generated a simulated measurement. This simulated measurement is then modified with Gaussian noise of different amplitudes. After this, a tomographic back-calculation was performed. From the back-calculated image, several radial cuts were produced and averaged, resulting in an average radial cut of the cylinder. After derivation of the Edge Response Function (ERF) we obtained the Line-spread Function (LSF). The Fourier transform of the LSF yields the Modulation Transfer Function (MTF). We could then make the statement that the required spatial resolution is met, if the 1/(required resolution) modulation is transferred by the system with an efficiency of at least 20 percent.

Grants

F4E-FPA-384 (DG) Framework Partnership Agreement for the Development and Design of ITER bolometers (2014-2018)

F4E-FPA-328 (DG) Framework partnership Agreement for the Tokamak Services for diagnostics (2012-2016)

F4E-OMF-331 - Specific Contract of Engineering Framework Contract - LOT2: Preliminary Design of TBS Ancillary subsystems and integration in ITER (2012-2014)

International cooperation

Max Planck Institute for Plasma Physics (Garching, Germany), Development of ITER bolometers (lead party)

Fraunhofer ICT-IMM (Mainz, Germany), Development of ITER bolometers (cooperator)

Karlsruhe Institute for Technology (Karlsruhe, Germany) Test Blanket Module development (lead party)

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Conference proceedings
2. Bodnár G, Bató S, Zoletnik S, Refy DI, Brix M, Gomes R: Mechanical and thermal considerations for the JET Li-beam ion source upgrade. In: 28th Symposium on Fusion Technology (SOFT 2014), San Sebastián, Spain, 29.09.2014-03.10.2014, Paper P4.017. 12 p.
3. Bodnár G, Bató S, Zoletnik S, Refy DI, Brix M, Gomes R: Mechanical and Thermal Considerations for the JET Li-Beam Ion Source Upgrade. In: 28th Symposium on Fusion Technology (SOFT 2014), San Sebastián, Spain, 29.09.2014-03.10.2014, Paper P4.017. 12 p.

See also: R-Q.8, R-Q.9, R-R.7, R-R.9, R-R.10

R-P. Laser plasma

István B. Földes, Márk Aladi[#], Angéla Barna[#], Imre Ferenc Barna,
Róbert Bolla[#], Mihály Pocsai[#]

High harmonics signature of nanoplasmas in clusters. — High harmonics of ultrashort laser pulses in gases cover practically the full spectral range from the visible to kiloelectronvolt X-rays and in the same time they serve as attosecond pulse sources, too. High-harmonic generation from clusters seems to be a possible candidate for an efficient light source providing higher emission frequencies and higher conversion efficiency even if the upper limit of conversion is determined by ionization, too. Experiments were carried out with different gases with varying pressure which demonstrated this increase of conversion due to clusters (Fig. 1).

Figure 1. *Experimental arrangement.*
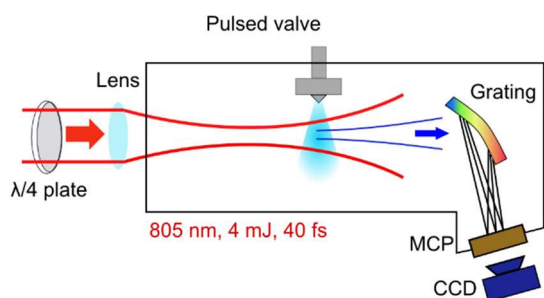
The experiments were carried out using the 40 fs Ti:sapphire laser which was focused into the gas jet. The position of the target could be varied as compared with the focal plane, thus varying the intensity and the conditions for phase matching in the same time. Single shot spectra were obtained using a toroidal vacuum UV (VUV) grating and microchannel plate (MCP) detector.

The steep increase of harmonics intensity with increasing pressure in Ar and Xe demonstrated the presence of clusters. Fig. 2a shows that the spectra are blue-shifted and the blue shift increases with increasing laser intensity. This is attributed to the increasing number of free electrons in the gas due to the higher ionization state caused by the increased intensity. The phase mismatch between the harmonics of order q and the laser beam contribution due to the free electrons can be described by the equation

$$\Delta k_{electron} \approx \frac{6\pi}{\lambda_\omega}\left(n_{q\omega} - n_\omega\right) = \frac{6\pi}{\lambda_\omega}\left(\sqrt{1 - \frac{\omega_p^2}{q^2\omega^2}} - \sqrt{1 - \frac{\omega_p^2}{\omega^2}}\right) \geq 0.$$

Here ω_p is the plasma frequency, ω is the frequency of the laser and λ_ω is its wavelength. This gives a positive contribution to the frequency shift. Conversely, if one assumes that nanoplasmas are present inside the clusters it gives a contribution of

$$\Delta k_{nanoplasma} = \frac{6\pi}{\lambda_\omega}\left(1 - \frac{2\pi n_e r^3 n_{cl}}{3n_{qcrit} - n_e}\right) - \frac{6\pi}{\lambda_\omega}\left(1 - \frac{2\pi n_e r^3 n_{cl}}{3n_{crit} - n_e}\right)$$ which is of opposite sign. In this

equation r is the radius of the clusters, n_{cl} is the density of the clusters, n_e is the electron-density in the cluster, n_{crit} and n_{qcrit} are the critical density for the laser and for the q-th harmonic, respectively. Thus the nanoplasmas give a frequency red shift, with opposite sign

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[#] Ph.D. student

to that of the free plasmas. This is demonstrated in Fig. 2b which shows that keeping the intensity constant a (relative) red shift can be observed with increasing pressure; that is, with increasing cluster size. As far as we know this is the first demonstration of the existence of nanoplasmas using high harmonics. At present polarization properties of high-harmonics generation are being investigated as illustrated in Fig. 1 which may give more insight into the effect of cluster nanoplasmas inside the clusters onto the generation of high-harmonics.
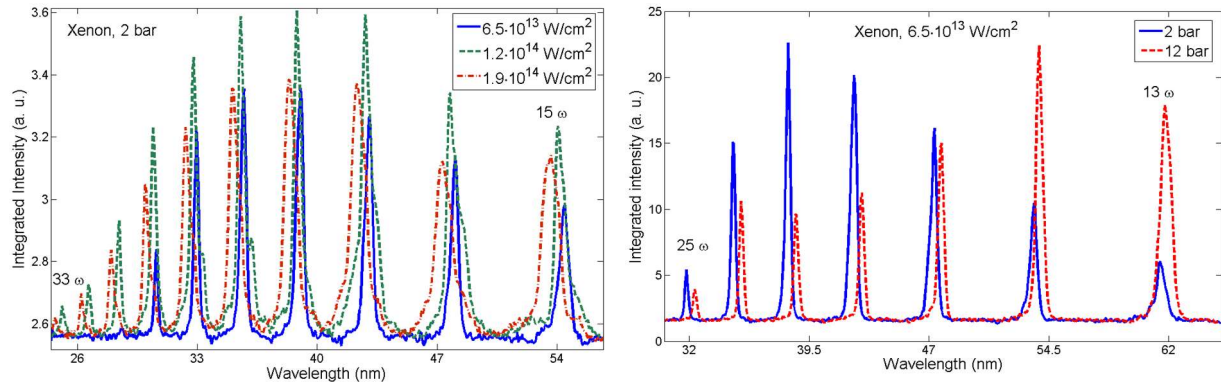
Figure 2. *High-harmonics spectra in xenon with constant pressure (a) and with constant laser intensity (b).*

Theoretical calculations were carried out considering nonlinear, power-law field-dependent electrical permittivity and magnetic permeability in order to investigate the time-dependent Maxwell equations with the self-similar Ansatz. The first-order hyperbolic partial differential equations conserve non-continuous initial conditions describing electromagnetic shock. Such phenomena may happen in complex materials induced by the planned powerful ultrashort laser pulses.

Grant
EUROFUSION, Enabling Research Towards Demonstration of Inertial Fusion for Energy (ToIFE), CfP-WP14-ER-01/CEA-12 (I. Földes, 2014-2017)

International cooperation
Max Planck Institute of Quantum Optics (Garching, Germany), within the frames of EURATOM

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R-Q. Beam emission spectroscopy

Dániel Dunai, Gábor Anda, Sándor Bató, Attila Bencze, Sándor Kálvin, Tibor Krizsanóczi, Máté Lampert[#], Gábor Petravich, Dániel Réfy[#], Balázs Tál[#], Sándor Zoletnik

Geodesic Acoustic mode measurements program. — In recent years the turbulence driven zonal flows in toroidal magnetized plasmas, in particular GAMs (Geodesic Acoustic Modes) are subject of intensive experimental studies. In 2014 Wigner RCP has been conducting, as principal investigator, an EUROFUSION Enabling Research project about the comparative experimental study of GAMs in various tokamaks where Beam Emission Spectroscopic (BES) measurements are available. This project includes more than 15 scientists from four European countries with an overall budget of about 100 kEUR. Measurements were done using both heating beam BES (e.g. KSTAR) and Lithium beam BES (e.g. COMPASS, ASDEX-U and JET). A fairly big amount of data have been collected which is now under extensive detailed analysis. Some preliminary conclusions can be drawn showing that some diagnostic improvement will be needed in future for conclusive results. For example the detected light level seems insufficient for GAM detection in ASDEX and maybe JET, while in COMPASS and KSTAR the situation looks promising, but an improvement of signal to noise ratio is needed.

KSTAR measurements. — The research group is responsible for the BES diagnostics operation and also partly for the data analysis on the Korean KSTAR tokamak, which is an advanced superconducting fusion device located in Daejeon. This collaboration started in 2010 and was carried out in recent years under the Joint Hungarian - Korean research laboratory cooperation. In 2014 several improvements have been implemented in preparation for the measurement campaign. The most important upgrade was that the number of measurement channels has been doubled, so the observation volume in the plasma has also been doubled. With this upgrade the entire Lithium beam is imaged, so more precise density reconstruction is available. The upgraded system measures the lithium or the heating beam emission with 500 kHz bandwidth and 3Ms sampling frequency. The previous years' lithium beam measurements featured relatively low light intensity with high background. To increase the signal to background ratio larger ion source was installed. The new insource with the optimized ion optics provides higher beam current, and thus higher measured intensity. Successful measurements were made with the system after the upgrade. The density reconstruction implementation and further fluctuation analysis is expected for 2015. The Lithium beam was injected in almost every shot, when it was possible, giving large amount data to be processed.

Great performance was achieved with Heating beam BES measurements, where the same hardware setup measures the hydrogen beam emission instead of the Lithium beam. These

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measurements can be characterized by low background and high signal to noise ratio. Study the edge and core plasma turbulence is available with this technique. A main physics goal was to explore the edge localized mode (ELM) precursor phenomenon and to compare the BES measurements with other fast diagnostics (Fig. 1).
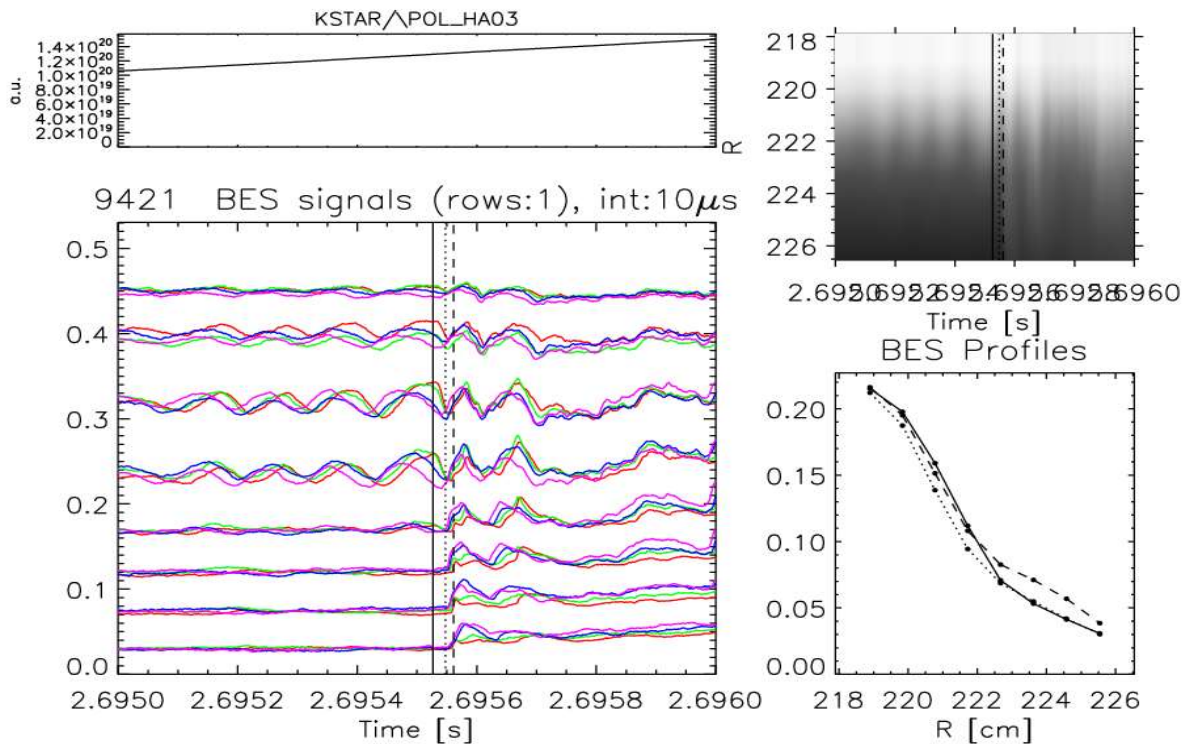
Figure 1. *KSTAR heating beam BES measurement results. The signals are recorded at different depth in the plasma, up is inside. Different colours show different poloidal channels at one radial location. Poloidal propagation of the ELM precursor structure is clearly observed*

JET program. — The BES research group also partly responsible for the operation as well as the upgrade of the Lithium beam emission spectroscopy diagnostic at JET tokamak device during this year. The upgrade of the ion source was the most important development in 2014. The emitter heating system has been replaced first, which included the installation of a new control system and new high voltage transformers. The implementation of an active cooling system became necessary due to the increased heating power. Certain optical elements were replaced in the fast camera system - which was installed back in 2011/12 - that increased the number of the measured channels. We managed to operate the emitter at peak performance for the end of the 2014 campaign after several technical difficulties at the commissioning of the system. The BES team provided at least one man full time continuously for the two shifts a day beam operation at JET during the physics campaign. The Li-BES diagnostic is a standard diagnostic at JET, which means that the entire community uses these results. Our scientific program is focused on the characterization of the turbulence and the zonal flows and their interaction, as well as doing fast (~10kHz) plasma profile reconstruction with the help of the fast camera. Making use of our capabilities, we try to investigate the phase transition between the low and high

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confinement modes, limit cycle oscillations, edge localized modes and other phenomena. This collaboration is funded by the EUROFUSION consortium.

EAST installation. — A new Lithium beam emission spectroscopy diagnostics has been installed at EAST tokamak, which is located in Hefei, China. In this development all the previous experience was included so a cutting edge technology beam and observation system was shipped and installed (Fig. 2). In this collaboration the Chinese partners purchased the diagnostics and we will partly be responsible for the operation as well as the scientific exploitation. The system design and production was mostly at Wigner RCP where both the beam and the observation system was carefully tested. After the tests the systems have been disassembled, packed and shipped. The system was assembled in Hefei in the lab first and then installed on the tokamak. The installation was successful, however a lot of technical problems had to be solved on the site. Proof of principles measurements were also carried out, but in 2014 there was no physics measurement campaign, only engineering campaign. This limited our measurement possibilities as well. A longer physics campaign is envisaged for 2015 where the diagnostics can show its capabilities. A fairly unique feature of this superconducting device, that Lithium coating is applied on the plasma facing components. The lithium coating significantly changes edge plasma characteristics, which can studied and with Lithium beam diagnostic. The lithium coating also means risk as it covers the vacuum windows and it can block the beam emission. The Chinese fusion program is developing rapidly and the centre of this program is the EAST tokamak now, which means a great potential for the future collaboration options.
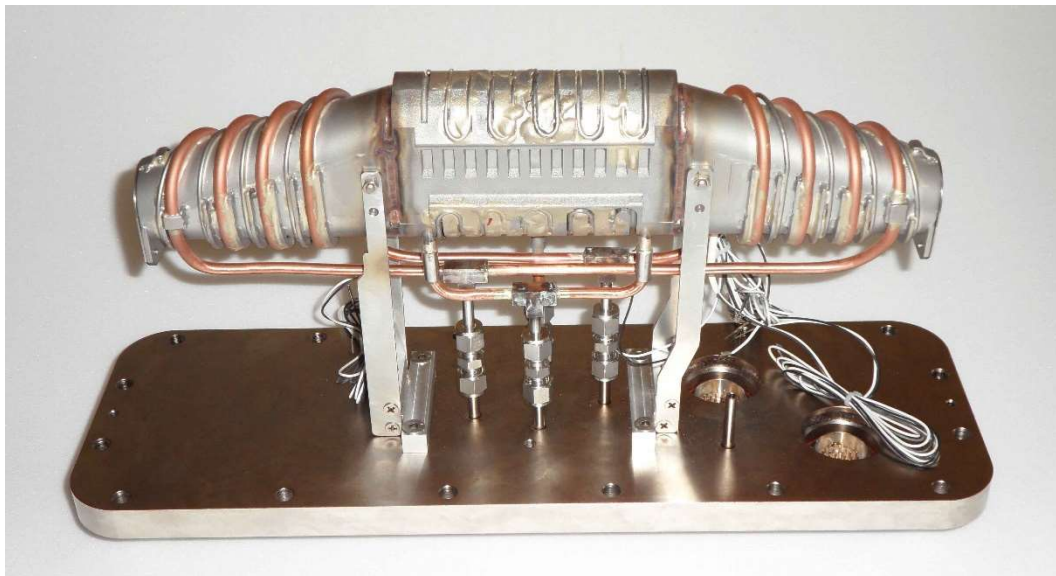
Figure 2. *Sodium neutralizer of the EAST lithium beam diagnostics.*

Grants

EUROFUSION Consortium grants:

Enabling research project on geodesic acoustic modes (A. Bencze, 2014-2014)

Enabling research project on turbulent transport (D. Dunai, 2014-2014)

Enabling research project on scrape off layer turbulence studies (S. Zoletnik, 2014-2014)

WPMST2 on Fast-ion loss detector developments (S. Zoletnik, 2014-2016)

WPJET BES diagnostic operation (S. Zoletnik, 2014-2014)

WPSA- JT60-SA BES diagnostic feasibility study (D. Dunai, 2014-2016)

Korean-Hungarian joint laboratory program of Korea Research Council of Fundamental Science and Technology (S. Zoletnik, 2012-2014)

Institute of Plasma Physics, Chinese Academy of Sciences EAST tokamak Diagnostic Li-beam BES contract (S. Zoletnik, 2013-2014)

International cooperation

Institute of Plasma Physics, Chinese Academy of Sciences

National Fusion Research Institute in Daejon, South Korea.

INSTITUTE OF PLASMA PHYSICS, Academy of Sciences of the Czech Republic

Max-Planck-Institut für Plasmaphysik, Garching, Germany

Culham Centre for Fusion Energy, Culham, United Kingdom

Joint European Torus, Culham, United Kingdom

ITER & Fusion for Energy, Cadarache, France

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See also: R-O.2, R-O.9, R-O.11, R-R.1, R-R.2, R-R.7, R-R.8

JET EFDA Contributions

Due to the vast number of publications of the large collaborations in which the research group participated in 2014, here we list only a short selection of appearances in journals with the highest impact factor. Wigner scientists participating in this collaboration are Cseh G, Dunai D, Gál-Hobirk K, Kálvin S, Kocsis G, Mészáros B, Petravich G, Réfy D, Szabolics T, Szepesi T, Zoletnik S.

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See also: R-R: ASDEX Upgrade Team

R-R. Pellet and video diagnostics

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

Reliability study of pellet ELM pace making on ASDEX Upgrade and JET. — The injection of cryogenic solid hydrogen isotope pellets has been proven as a powerful tool for edge localized mode (ELM) pace making in devices where at least parts of the plasma-facing components have carbon surfaces. In modern, more reactor-relevant machines with all-metal walls, significant changes of the pedestal conditions and the ELM dynamics were observed that are due to the wall material. This implies that the reliability of the pellet ELM pace making technique should be reconsidered as well. In the last campaigns of the all-metal wall ASDEX Upgrade and JET, there was special emphasis on the investigation of the reliability of pellet ELM triggering, with remarkable contributions from HAS scientists. The experiments revealed that – despite similar perturbations caused by the pellets – the pellet ELM triggering potential was reduced in certain plasma scenarios. In general, the probability of a pellet triggering an ELM is dependent on the time elapsed since the previous ELM. Even lag times were observed where this probability drops to zero. It was found that when using nitrogen-seeding for confinement improvement, some of the pellet trigger potential was recovered also.

Pellet penetration depth database analysis at ASDEX Upgrade. — Cryogenic pellet injection is one of the most successful ways to fuel fusion plasmas. The goal of pellet fuelling is that the pellet material penetrates into the plasma as deep as possible. In the last five years our research group has set up a pellet penetration depth database, in order to derive a scaling law describing penetration depth as the function of pellet mass and speed, and plasma temperature and elongation. In 2014, the database was extended to clarify the effect of the toroidal magnetic field on pellet penetration depth. It is important to understand this effect because the next large fusion experimental machine – ITER – is planned to operate with a much higher magnetic field. Preliminary results show that the pellet penetration depth is increases slightly with the magnetic field.

Video diagnostics development for Wendelstein 7-X stellarator (W7-X). — Our group is developing a ten-channel overview video diagnostic system for W7-X (based on self-developed Event Detection Intelligent Cameras [EDICAM]), with the aim to monitor almost the entire inner wall and detect dangerous events. In 2014, seven out of the ten channels were delivered; three of them in a modified set-up: two channels are using PCO Pixelfly cameras, while the third channel was changed due to a leak in the housing AEQ port. As a result, in this third channel an image guide is used, enabling (for example) a commercial ultra-fast camera. A special software VIDACS (Video Diagnostics Data Acquisition and Control Software) was developed for the simultaneous control of the ten camera channels. The beta version of VIDACS, delivered to W7-X, only supports EDICAMs, but adding another

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camera type (for example PCO) requires only the development of the camera-side software, with a minor modification in VIDACS itself. Additionally, the development of special video analysis software, EDVIS (EDICAM Visualisation Software), was also started. EDVIS will be able to visualize up to ten movies simultaneously on one screen, four of which can be viewed at larger resolution on another screen. Videos can be processed to generate time signals (for example, average brightness within a user-defined area), and these can be compared to other measurements (to be read from the experiment data archive by EDVIS).

Table-top pellet injector (TATOP) development. — In 2014 there were two major upgrades to the TATOP system. In the first upgrade, the pellet reservoir capacity was modified to 3×1000 pellets, instead of the 1×5000. This allows the user to change pellet material without opening the vacuum system. The second upgrade is a new stop cylinder design, addressing the problem of pellets becoming stuck inside the accelerator. To test the new design, a test-bed installation was also designed and manufactured.
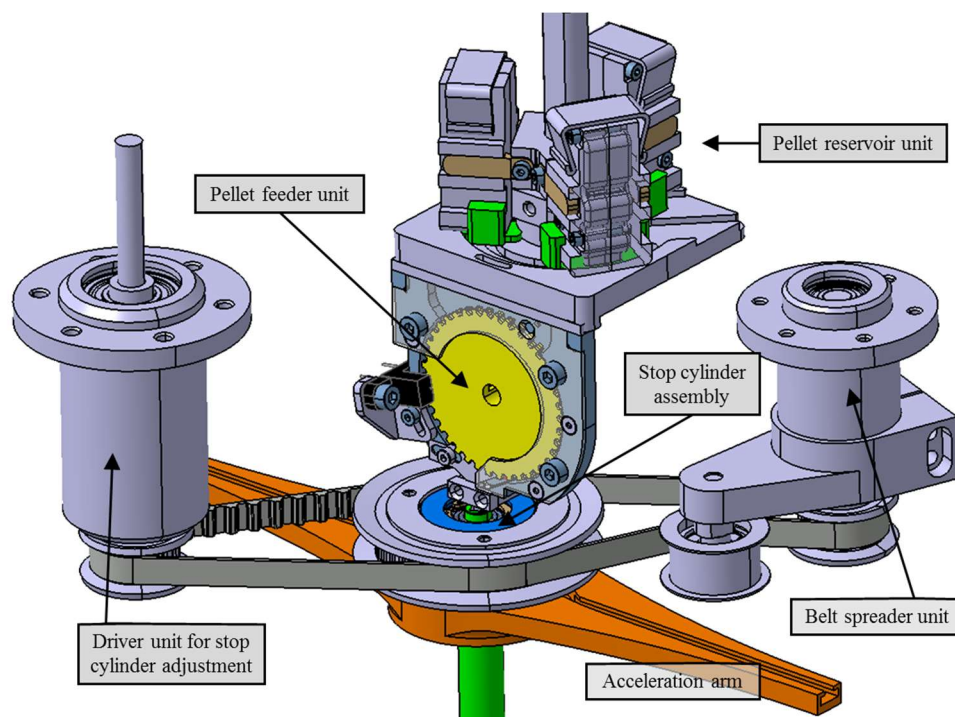
Figure 1. *CAD design of the TATOP with the new pellet reservoir unit.*
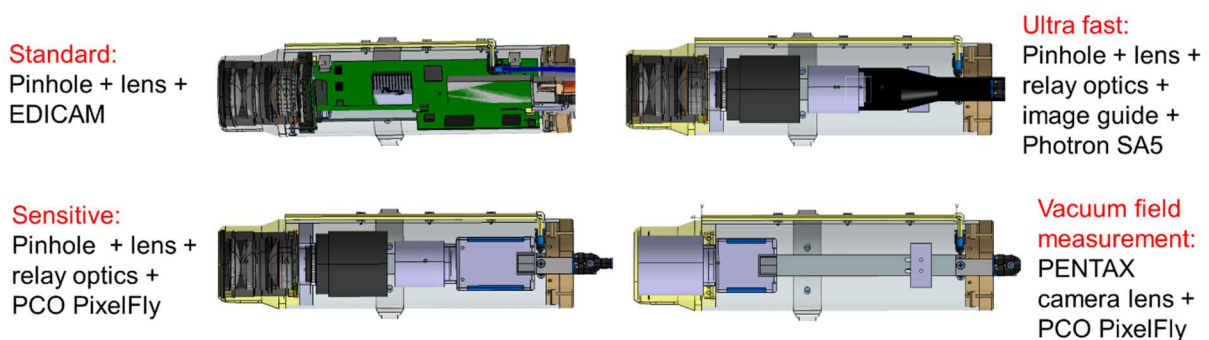
Figure 2. *Different camera head set-ups for the W7-X overview video diagnostic system.*

Grants

EUROfusion: WP Medium-Size Tokamak 1 (G. Kocsis, 2014-2014)

EUROfusion: WP Stellarator 1 (T. Szepesi, 2014-2014)

EUROfusion: WP SA (T. Szepesi, 2014-2014)

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)

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ASDEX Upgrade Team

Due to the vast number of publications of the large collaborations in which the research group participated in 2014, here we list only a short selection of appearances in journals with the highest impact factor. Wigner scientists participating in this collaboration are Gál-Hobirk K, Kálvin S, Kocsis G, Szepesi T.

1. Ayten B, Westerhof E et al. [ASDEX Upgrade Team]: Non-linear effects in electron cyclotron current drive applied for the stabilization of neoclassical tearing modes. **NUCL FUSION**, 54:(7) Paper 073001. 13p. (2014)

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See also: R-Q: JET EFDA Contributions

R-T. Space Technology

János Zoltán Nagy, Kálmán Balajthy, András Balázs, Attila Baksa, László Hevesi, István Horváth, Zoltán Pálos, Bálint Sódor, Sándor Szabó, Sándor Szalai, Lajos Szalai, Gábor Tróznai, Pál Gábor Vizi

Our research group was involved in the development of the on-board control and data acquisition computer for the Philae lander of the Rosetta spacecraft in the nineties. Rosetta was launched on its ten-year journey through space on 2 March 2004 with the goal of arriving at the comet 67P/Churyumov-Gerasimenko and landing on the surface to examine the nucleus directly.

Comets carry material that has remained in an unaltered state for billions of years. Consequently, their investigation supports research on the formation of the Solar System and evolution of life on the Earth.

The hardware and software of the failure-tolerant Command and Data Management Subsystem (CDMS) of the Philae lander were developed jointly by our institute staff and the Hungarian SGF Ltd. We developed the on-board computer that autonomously controls the operation of the Philae probe after its separation from the Rosetta orbiter. After separation, CDMS controls ten scientific instruments on the lander and regulates the energy balance and temperature conditions. The fault-tolerant computer establishes radio contact with the orbiter to receive commands and transmit scientific data to Earth.
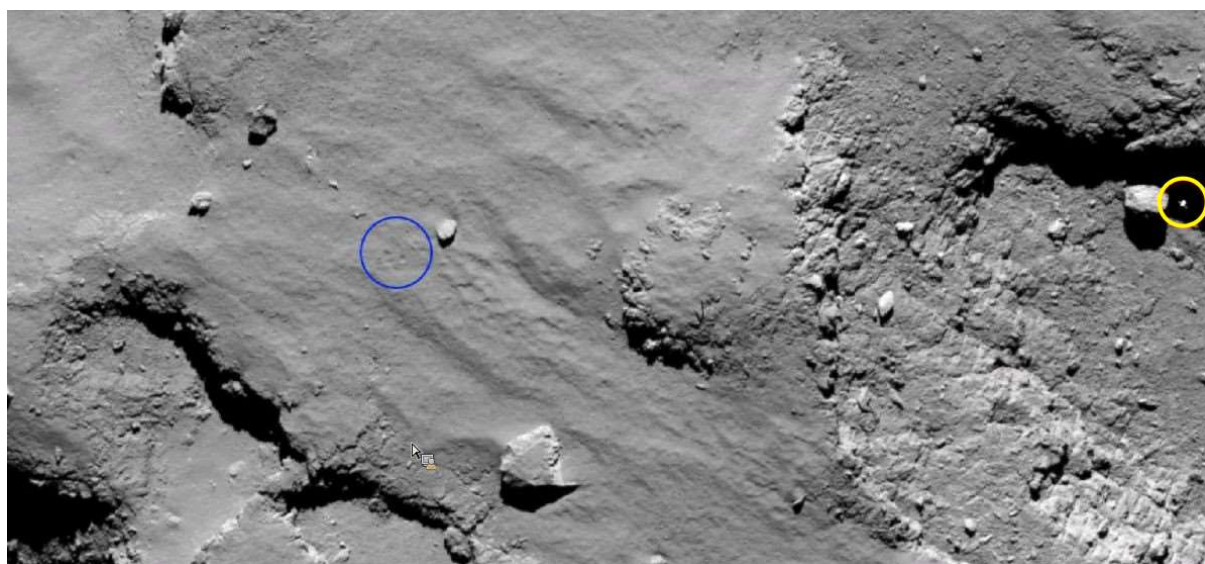
Figure 1. *Photos taken from 67P/Churyumov-Gerasimenko by Rosetta. The first landing site is indicated by the left circle. After collision it bounced and then landed again in the area indicated by the right circle.*

We are taking part in the *Obstanovka* experiment on the Russian Orbital Segment of the International Space Station, for which we developed and manufactured the onboard data acquisition and control system. It contains three processors and has been operational for

more than a year. As the telemetry capacity is limited, the entire first-year research data was returned to Earth by astronauts on a removable disk (Fig 2, Fig 3).

Figure 2. *Astronauts make assembly of Obstanovka during spacewalk.*

Figure 3. *The transport container in which data returned on Earth.*

We are also developing and manufacturing DC/DC power supply units for the following future missions: the PEP experiment of the Juice mission and for the Plasma Ion Camera of the BepiColombo mission. This year we performed stress tests and delivered the second flight DC/DC power supply unit for BepiColombo. The unit is shown in Fig 4.
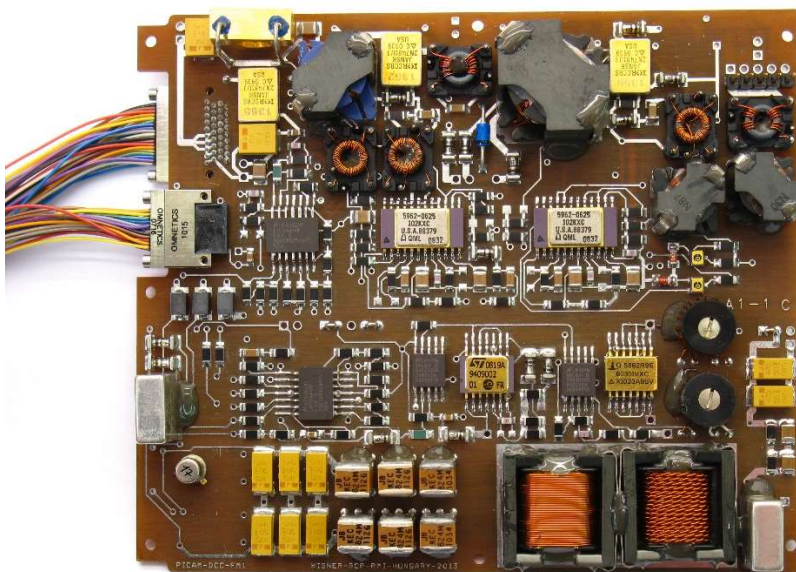
Figure 4. *Power supply unit for BepiColombo*

International cooperation

IRF (Swedish Institute of Space Physics), Juice (K. Szegő)
Imperial Colleague, London (S. Szalai)
IKI Moszkva (J. Nagy)
DLR Köln (S. Szalai)
ESOC Darmstadt (S. Szalai)
MPA Lindau (S. Szalai)
CNES Toulouse (S. Szalai)
IWF Gratz, FMI Helsinki (S. Szalai)

Publications

Articles

1. Kuwahara T, Hirn A, Apathy I, Bodnar L, Csoke A, Deme S, Pazmandi T, Szanto P, Troznai G, Zabori B: TRITEL-JMS: A three-dimensional silicon detector telescope dedicated for operation on board microsatellite RISESAT. **T JPN SOC AERONAUT S**, 12:(29) pp. Tr_13-Tr_17. (2014)

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3. Vizi PG, Bérczi Sz, Horváth I, Horváth AF, Vizi JCs: Modern Analytical Methods Applied to Earth and Planetary Sciences for Micro, Nano and Pico Space Devices and Robots in Landing Site Selection and Surface Investigation. In: Workshop on The Modern Analytical Methods Applied to Earth and Planetary Sciences, Sopron, Hungary, 01.11.2014, Lunar and Planetary Institute, Houston, Texas, USA, Paper 4007. 2 p.

Computational Sciences Research Group

Gábor Vattay, István Csabai, Sándor Laki, József Stéger, László Dobos,
Gábor Gombos

This group was established in late 2013 to foster research in data and computation intensive research areas. The last two decades have seen an unprecedented change in almost all areas of sciences. Before that most disciplines were determined by the scarcity of experimental data. The exponential pace of microelectronics development has changed this, on one hand by making available high throughput sensors and digital instruments and on the other by providing high speed computers with large storage and fast interconnecting network. Beyond the almost limitless opportunities there are demanding challenges, too: how to handle the data avalanche from experiments, how to get out the most from information technology in various scientific disciplines, and also how to understand and manage the ever growing complexity of the computational system itself. We study computer networks and systems like it was a "natural phenomena" and also with continuously following the technologies, we use them for analyzing science data in various fields from genomics to cosmology.

In January 2014 the group won its first EU FP7 ICT project within the Future Internet Public Private Partnership (FI-PPP). The XIFI project will establish federated infrastructure components, with functional components that satisfy the interoperability requirements for the European Future Internet core platform. Though computer networks are man-made, the Internet does not have a blueprint, so in some sense it is very much similar to complex dynamical systems in physics and a similar methodology is required to analyze and understand it. The XIFI open federation will leverage existing public investments in advanced infrastructures and support advanced large-scale deployment of FI-PPP early trials across a multiplicity of heterogeneous environments and sector use cases that should be sustained beyond the FI-PPP programme. In cooperation with the project partners we have integrated the Wigner cloud node, and installed and tested the virtualization framework and the flexibly configurable modules. We have organized the annual consortium workshop in Budapest, which strengthened the group's position in the collaboration and won further support for development.

In December 2014 in the new framework programme H2020 the group won a new project in which bioinformatics tools would be used for outbreak detection. The health of humans and animals around the world is increasingly under threat due to new and recurring epidemics and foodborne disease outbreaks, which place pressure on health services and the production of livestock. These epidemics also reduce consumer confidence in food and negatively impact trade and food security. The longer it takes from the start of an outbreak of a disease, for example Ebola, influenza or salmonella until it is detected and stopped, the greater the consequences are. The most important factor in being able to limit the consequences and costs of such outbreaks is the ability to quickly identify the disease-causing microorganisms that are causing the disease. Also there is the need to gather knowledge about the mechanisms that cause the disease, and how the bacteria are transmitted to and between humans. The goal of the COMPARE project is the development of a better surveillance system for infectious diseases, to speed up the detection of, and response to, disease outbreaks among humans and animals worldwide through the use of

new genome technology. Our group is primarily responsible for the advanced database system which will store and share the genomic data collected by researchers worldwide, and for the development of tools which will enable fast and efficient analysis of the data. We have organized a kickoff workshop in Budapest and invited Danish and British collaborators.

Grants

XIFI: European Public-Private-Partnership on Future Internet, GA604590: "eXperimental Infrastructures for the Future Internet" (Node coordinator G. Vattay, 2014-)

Compare: Horizon 2020 program (GA 643476:"COllaborative Management Platform for detection and Analyses of (Re-)emerging and foodborne outbreaks in Europe") (I. Csabai, 2014-)

Laboratory of Speech Technology for Rehabilitation (LSTR)

András Arató, József Laczkó, Norbert Márkus, Szabolcs Malik

Development of the MObile SlateTalker (MOST) was continued for new devices and operating system versions. A Braille typewriter-style input module was created for tablets and phones. New users were trained to use MOST on their devices. A full tactile Braille-Morse version for deaf-blind users was created that also included the possibility for use with email. The TalkPad program was further developed for nonspeaking autistic children. A multi-layer table can be generated for them with special music and text possibilities. 43 people use MOST and 20 people use the TalkPad system.

In the field of rehabilitation of people with movement disorders, cooperation with the National Institute for Medical Rehabilitation has been developed and strengthened. Paraplegic patients use rehabilitation techniques based on functional electrical stimulation. The biomechanics and neural control of movement have been analysed, based on kinematic and bioelectric data assessed from impaired individuals.

These results are being applied in medical rehabilitation protocols. Such protocols and trainings comprise bicycling movements of spinal cord injured patients of the National Institute for Medical Rehabilitation. We continued the preparation for organizing and hosting the conference of the International Society of Motor Control in 2015 in Budapest.
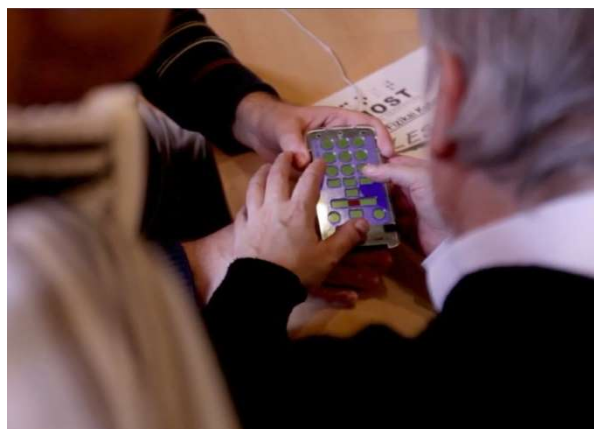
A presentation with a hands-on demonstration was given at the on the international conference for deaf-blind people, which was organised by the Hungarian Association for Deaf-Blind People SVOE in Visegrád.

A lecture was presented at the Hungarian Association of Rehabilitation Pedagogy (Magyar Gyógypedagógiai Társaság MGYT) in Vác about the activity of LSTR.

A demonstration was given for the Hungarian Association for the Blind about newly developed devices. Internet media informed about the event:

Index.hu: http://index.hu/video/2014/11/20/lesek/

Zugloilapok: http://zugloilapok.hu/web/guest//hirmegjelenito?view_article_3s2C=a-latasserulteket-segito-eszkozokrol-tartottak-konferenciat-zugloban

Publications
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resistance on hamstrings and quadriceps muscle activities during cycling. ACTA PHYSIOL HUNG, 101 (4), pp. 505–516 (2014)

2. J Laczko, P Katona, A Valy: Muscle co-activation as function of crank angle when cycling on an ergometer with altered power output. Neuroscience Meeting Planner. Soc. for Neuroscience . Program No. 630.06 (2014)

3. M Mravcsik, J Laczkó: Muscle co-activation during arm cycling against altering crank resistances. 7th World Congress of Biomechanics, Control Number 3864 (2014)

4. L Simo, D Piovesan, J Laczko, C Ghez, RA Scheidt: Submovements during reaching movements after stroke. Accepted at the36th Annual International IEEE EMBS Conference (2014)

INSTITUTE FOR
SOLID STATE PHYSICS AND OPTICS

S-B. Complex Systems

Ferenc Iglói, Róbert Juhász, István Kovács, Gergely Roósz[#], Attila Virosztek, András Sütő[E], Péter Szépfalusy[E†]
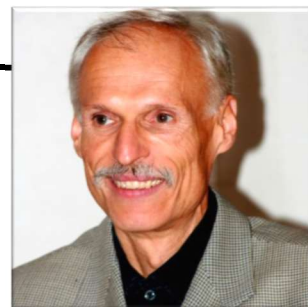
The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Critical behavior of disordered quantum systems. — By means of a strong-disorder renormalization group method, we have shown that the (imaginary-time) spin-spin autocorrelation function of the random transverse-field Ising chain and the survival probability in the disordered contact process and in the problem of random walks in random environments exhibit *multiscaling* in the critical point, with an exponential distribution of scaling exponents in the case of a semi-infinite lattice.

We considered the zero-temperature random transverse-field Ising model on a star-like network composed of M semi-infinite chains connected to a common central site. By the strong-disorder renormalization group method, the scaling dimension x_M of the local order parameter at the junction has been calculated.

We studied the low-energy properties of the long-range random transverse-field Ising chain with ferromagnetic interactions decaying as a power α of the distance. Using variants of the strong-disorder renormalization group method, the critical behavior is found to be controlled by a strong-disorder fixed point with a *finite* dynamical exponent $z_c = \alpha$. Approaching the critical point, the correlation length is found to diverge exponentially. In the critical point, the magnetization shows a square-logarithmic finite-size scaling and the entanglement entropy satisfies the area law. These observations are argued to hold for other systems with long-range interactions, even in higher dimensions. In the case of stretched exponentially decaying interactions, the critical behavior is controlled by *infinite-disorder* fixed points different from that of the short-range model.

Corner contribution to cluster numbers in percolation and in the Potts model. — We considered the Q-state Potts model as well as the percolation process at criticality and study the number of Fortuin-Kasteleyn (and spin) clusters, N, which intersect a given contour. To leading order, N is proportional to the area of the contour; however, there occur logarithmic contributions related to the corners. These are found to be universal and their size in two-dimensional systems can be calculated by employing techniques from conformal field theory.

In the random-bond Potts model in the large-Q limit, N represents the excess entropy and its prefactor is proportional to the central charge of the model. Our results indicate that there are logarithmic finite-size corrections in the free-energy in three-dimensions, too.

[#] Ph.D. student

[E] Professor Emeritus

[†] Deceased

Galilean invariance in confined quantum systems. — We clarified the meaning of Galilean invariance of N-particle quantum systems in confined geometries, and proved some interesting spectral consequences of this invariance. Implications for ground state superfluidity and periodic ordering were also discussed.

Grant

Publications

Articles

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2. Juhász R: Critical behavior of models with infinite disorder at a star junction of chains. **J STAT MECH-THEORY E,** 2014:(8) Paper P08005. 14 p. (2014)

3. Juhasz R: Distribution of dynamical quantities in the contact process, random walks, and quantum spin chains in random environments. **PHYS REV E**, 89:(3) Paper 032108. 14 p. (2014)

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5. Juhász R, Kovács IA, Iglói F: Random transverse-field Ising chain with long-range interactions. **EUROPHYS LETT**, 107:(4) Paper 47008. 6 p. (2014)

6. Kovacs IA, Elci EM, Weigel M, Igloi F: Corner contribution to cluster numbers in the Potts model. **PHYS REV B**, 89:(6) Paper 064421. 8 p. (2014)

7. Kovács IA, Iglói F: Corner contribution to percolation cluster numbers in three dimensions. **PHYS REV B**, 89:(17) Paper 174202. 9 p. (2014)

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9. Roósz G, Divakaran U, Rieger H, Iglói F: Nonequilibrium quantum relaxation across a localization-delocalization transition. **PHYS REV B**, 90:(18) Paper 184202. 10 p. (2014)

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Article in Hungarian

11. Iglói F, Kovács I: Végtelenül rendezetlen kritikus viselkedés (Infinitely unordered critical behaviour, in Hungarian). **FIZIKAI SZEMLE**, 64:(11) pp. 366-371. (2014)

See also: S-F.20

S-C. Long range order in condensed systems

Balázs Újfalussy, Péter Balla[#], Gábor Csire[#], Pawel Kamasa[A†], Krisztina Kádas, Annamária Kiss, Karlo Penc, István Tüttő[A], Lajos Károly Varga, Levente Vitos

Berry phase effects in spin nematics. — How quantum fluctuations melt a classical order and create novel quantum states is a fundamental question of modern condensed matter physics. Among many phenomena, mechanisms involving topological effects have been studied in great detail in one-dimensional spin chains. In particular, the Berry phase associated with rotation of spins plays a crucial role, as its presence discriminates between antiferromagnetic Heisenberg chains with half-integer and integer spins, making the excitations in the former gapless and in the latter gapped.

A similar Berry phase appears for the spin quadrupoles (nonmagnetic spin states). We studied its effect in the spin-1 Heisenberg model with bilinear and biquadratic couplings, which was conjectured to support nematic (quadrupolar) order, a question that remained open for many years.
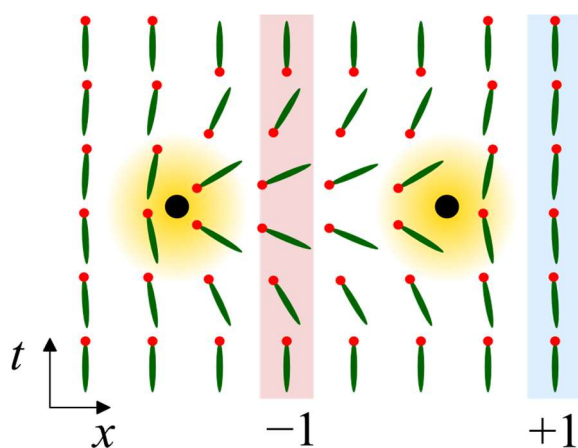
Figure 1. *World lines of directors in 1+1-dimensional space time. The directors tend to align with adjacent ones in space, and they can rotate in time. Rotations of a director as a function of time lead to a Berry phase. Directors can either rotate by an angle 0 or π, as shown in the two highlighted world lines, picking up a phase pi in the latter case. This causes destructive interference when the distance between the vortices (black dots separating domains of different windings) is odd, eventually leading to dimerization.*

Starting from an effective low-energy model, we showed how a Berry phase leads to dimerization and obliterates the nematic order and we derived scaling relations of the correlation length and the dimerization strength. Subsequently, we used a density-matrix renormalization-group approach to verify these predictions. We further explored in detail the entanglement spectrum for which we derive exact expression at particular points.

High-entropy alloys. — A new high-entropy alloy composition ($Ti_{20}Zr_{20}Hf_{20}Nb_{20}X_{20}$ (X = V or Cr) was developed for high-temperature applications. The V-containing alloy has a single-phase bcc structure, whereas the Cr-containing alloy contains a small amount of Cr_2Nb and Cr_2Hf intermetallic compounds. The

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[#] Ph.D. student

[A] Associate fellow

[†] Deceased

calculated Young modulus E is in good agreement with the experiments. The $Ti_{20}Zr_{20}Hf_{20}Nb_{20}X_{20}$ (X = V or Cr) alloys show large elastic and plastic strain limits and the bcc phase is stable against heating for 600 s up to 1173 K.

Bulk Amorphous Alloys. — Clear correlation was found between the amorphous nature of the newly developed bulk amorphous $Mg_{54}Cu_{28}Ag_7Y_{11}$ alloy and its hydrogen charging - discharging capacity. The fully crystallized alloy does not desorb hydrogen and can be excluded from hydrogen storage applications.

The validity of the Steinmetz law (P = KBn) elaborated for modelling ferromagnetic hysteresis has been analyzed using the *tanh* model, by splitting the minor loops in three or two components, corresponding to different magnetization processes at different excitation levels. It is shown that the original Steinmetz law with the exponent n = 1.6 is valid only at and above the coercive field - for intermediate and high induction values - where all the three magnetization processes are present. At small magnetization levels, the exponent is about 3, much higher than the original proposed value.

Interface Physics. — The work of separation and interfacial energy of the Ni(1 1 1)/Cr(1 1 0) interface were calculated via first-principles methods. Both coherent and semi-coherent interfaces are considered. We found that magnetism has a significant effect on the interfacial energy; that is, removing magnetism decreases the interfacial energy of the semi-coherent interface by around 50%. Electronic, magnetic and atomic structures at the interface were discussed. An averaging scheme was introduced and used to estimate the work of separation and interfacial energy of semi-coherent interfaces based on the results of coherent interfaces.

f-electron systems. — Peculiar heavy-fermion behavior has attracted recent attention in certain samarium compounds with large specific heat coefficient which is insensitive to external magnetic field. In addition, clear Kondo-like logarithmic temperature dependence is observed in the resistivity in several cases. It has been suspected that charge degrees of freedom are important because of the field-insensitivity, in striking contrast to the ordinary Kondo effect which is easily damaged by magnetic field.

Motivated by these experimental observations, we searched for a charge-fluctuation mechanism that gives rise to an energy scale much smaller than bare hybridization. As the minimal model, we have studied the (spinless) multichannel interacting resonant level model by means of the continuous-time quantum Monte Carlo method. The numerically derived thermodynamical and dynamical properties show rich phenomena including quantum critical points and a composite lineshape of the single-particle spectrum, in contrast to a simple scaling description of the charge susceptibility, and a surprisingly wide-ranged perturbation description of the accurate numerical data from the strong-coupling Fermi-liquid fixed point.

Mechanical properties of materials. — Within the same failure mode, iron has the lowest ideal tensile strength among the transition metals crystallizing in the body-centered cubic structure. We have demonstrated that this anomalously low strength of Fe originates partly from magnetism and is reflected in unexpected alloying effects in dilute Fe(*M*) (*M* = Al, V, Cr, Mn, Co, Ni) binaries. We employed the structural energy difference and the magnetic pressure to disentangle the magnetic effect on the ideal tensile strength from the chemical

effect. We found that the investigated solutes strongly alter the magnetic response of the Fe host, which is explained based on the single-particle band energies.

RKKY interaction on alloy surfaces. — We studied the coupling between magnetic impurities on surfaces of Cu_xAu_{1-x}, Cu_xPd_{1-x} random substitutional alloys. Our main result was to numerically link the surface state properties on the surfaces of these alloys to the RKKY-type interaction between two magnetic impurities. While this can be done analytically for bulk materials, it can not be done for surfaces, let alone for alloy surfaces. We found that similarly to pure material surfaces, the properties of the interaction are determined by the properties of the surface state if it exists. We obtained an oscillatory part of the interaction, which behaves similarly to that of pure surfaces. The decay, however, is faster, due to a new exponential term coming from the disorder. By numerical comparison, we showed that the exponent of the decay is proportional to the electron coherence length at the Fermi surface, which can be calculated from the half width of the surface state spectral function. We demonstrated on the example of Cu_xPd_{1-x} alloys that if the Fermi surface of the host is distorted by alloying in such a way that the surface state disappears or becomes unoccupied, the oscillatory interaction also disappears in a particular way. Interestingly we also found that in Pd-rich alloys the interaction reappears due probably to an entirely different mechanism.

Grants and international cooperation

OTKA K84078: Magnetic, mechanical and thermal properties of alloys and their surfaces (B. Újfalussy, 2011-2015)

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, multicomponent metallic alloys (L. Vitos, 2013-2016)

OTKA IN 83114: Complex functional magnetic materials (participant, B. Újfalussy, 2010-2014)

OTKA K7771: Multiscale investigations of magnetic heterostructures based on first principles (participant B. Újfalussy, 2009-2014)

Marie Curie grant PIRG-GA: Numerical study of dynamics and magnetic properties of strongly correlated electron systems (A. Kiss, 2011-2015)

STINT Swedish-Hungarian joint project, Atomic-scale investigation of steel materials by first principles method (L. Vitos, 2009-2014)

Hitelap Zrt, "Meta-materials", (L.K. Varga, 2014)

Progen Kft, "Methods and technologies for nanocrystalization", (L.K. Varga, 2014)

Oak Ridge National Laboratory, "Beyond Rare-Earth Magnets", (B. Újfalussy, 2013-2014)

Publications

Articles

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See also: S-D.5, S-F.14

S-E. Non-equilibrium alloys

Judit Balogh, László Bujdosó, Dénes Kaptás, Tamás Kemény[A], László Ferenc Kiss, Imre Vincze[E]

The accuracy of measuring the saturation magnetic moments of some **Heusler alloys** with the help of a superconducting quantuminterference device (SQUID) magnetometer is crucial for the confirmation or rejection of their half-metallic nature. A simple method has been described which reduces those systematic errors of a SQUID magnetometer that arise from a possible radial displacement of the sample in the second-order gradiometer super-conducting pickup coil. By rotating the sample rod (and hence the sample) around its axis into a position where the best fit is obtained to the output voltage of the SQUID as the sample is moved through the pickup coil, the accuracy of measuring magnetic moments can be increased significantly. The fit is based on a nonlinear least-squares regression which is characterized by a regression value R (being unity for a perfect fit). With this method, the accuracy could be increased over the value given in the specification of the device and in the cases of pure iron and nickel samples, the literature values were reproduced by the best fits. The suggested method is only meaningful if the measurement uncertainty is dominated by systematic errors – radial displacement in particular – and not by instrumental or environmental noise. Fig. 1 shows the saturation magnetization M_0 (obtained from extrapolation according to the law of approach to saturation) and $M_{5K,5T}$ (measured at 5 K and 5 T) and moment m_0 and $m_{5K,5T}$ for one of our Heusler alloy sample, $Co_{1.9}Fe_{1.1}Si$, as a function of the regression value R. The correlation between the saturation magnetization (saturation moment) and the regression is evident. The apparently different values of the saturation moments obtained for $Co_{1.9}Fe_{1.1}Si$ is an artefact related to the differences in the regression value.
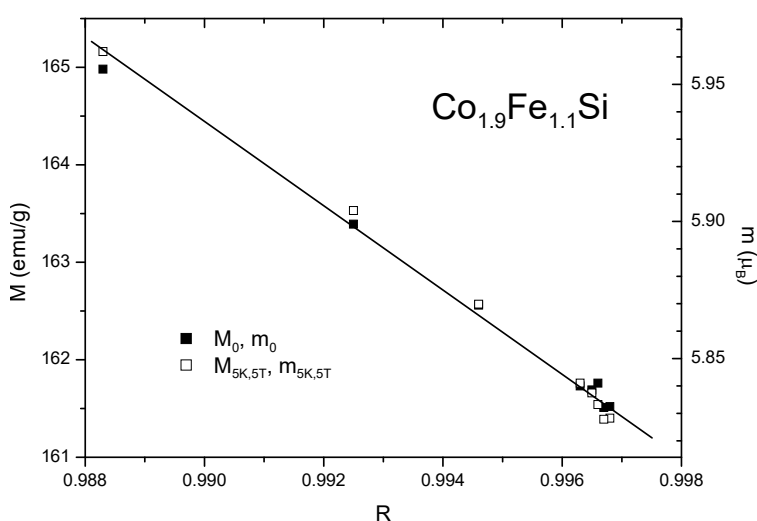
Figure 1. *Saturation magnetization M_0 and $M_{5K,5T}$ (definitions: see text) and moment m_0 and $m_{5K,5T}$ for $Co_{1.9}Fe_{1.1}Si$ as a function of the regression value R.*

The electronic, thermodynamical, and transport properties of **ordered Fe$_3$X (X=Al,Si) alloys** were studied from first principles in an international collaboration. We present here a unified approach to the phase stability, the estimate of the

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[A] Associate fellow
[E] Professor Emeritus

Curie temperature, the temperature dependence of sublattice magnetizations, magnon spectra, the spin-stiffnesses and residual resistivities. An important feature of the present study is that all calculated physical properties are determined in the framework of the same first-principles electronic structure model combined with the effective Ising and Heisenberg Hamiltonians used for studying the thermodynamical properties of alloys. Curie temperatures, spin-stiffnesses, and magnon spectra are determined using the same calculated exchange integrals. Finally, the transport properties are calculated using the linear-response theory. Our theoretical estimates compare well with available experimental data. In particular, calculations predict (in agreement with experiment) the ordered $D0_3$ phase as the ground-state alloy structure, demonstrate that a correct relation of Curie temperatures of Fe_3Al/Fe_3Si alloys can be obtained only by going beyond a simple mean-field approximation, provide reasonable estimates of spin-stiffnesses, and give resistivities compatible with structural disorder observed in the experiment. Although the calculated temperature dependencies of the Fe magnetization on different sublattices are similar, they nevertheless deviate more than in the experiment, and we discuss a possible origin.

Grants

OTKA K101456 Mössbauer and Magnetic Study of Intermetallic Compounds (I. Vincze, 2012.03.01-2016.02.29)

TéT 10-1-2011-0579 Magnetic interactions in multilayer heterostructures (Greek-Hungarian bilateral collaboration, J. Balogh, 2012.10.01-2014.09.30)

International cooperation

National Center for Scientific Research "Demokritos" (Athens, Greece), Magnetic interactions in multilayer heterostructures (J. Balogh)

Department of Condensed Matter Physics at the University of Seville (Seville, Spain) (L.F. Kiss)

Institute of Physics, Academy of Sciences of the Czech Republic, (Prague, Czech Republic) (I. Vincze)

Publications

Article

1. Kiss LF, Kaptás D, Balogh J: Reducing systematic errors in measurements made by a SQUID magnetometer. **J MAGN MAGN MATER**, 368: pp. 202-206. (2014)

See also: S-C.14, S-F.10
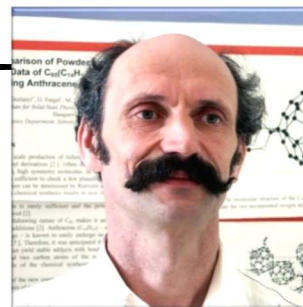
S-F. Laboratory for advanced structural studies

Gyula Faigel, Gábor Bortel, László Gránásy, Zoltán Jurek, Katalin Kamarás, Gyöngyi Klupp, Bálint Korbuly[#], Éva Kováts, Katalin Németh[#], Gábor Oszlányi, Áron Pekker, Sándor Pekker, Frigyes Podmaniczky[#], Tamás Pusztai, László Rátkai, Zsolt Szekrényes[#], Hajnalka Mária Tóháti[#], Gyula Tóth, György Tegze, Miklós Tegze

The laboratory for advanced structural studies 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 the first two fields. We also carried out single-molecule x-ray imaging measurements at LCLS (Stanford); however, the evaluation of these measurements is quite involved and results are expected in the next year only.

Carbon based systems. — Lately, various carbon based materials have become the center of intensive research. Earlier, we concentrated on fullerenes and related compounds, whereas recently, metal organic framework materials (MOF), carbon nanotubes and nanotube-based hybrid systems have been our center of interest.

Metal-organic frameworks. — Metal-organic frameworks (MOFs) are high-porosity crystalline solids based on the coordination polymers of transition and rare-earth metals. They are composed of two structural units: metal-containing clusters (secondary building units, SBUs) at the vertices and organic moieties (linkers) at the edges. The topologies of MOFs are controlled by the local symmetries and the functionalities of the SBUs and the linkers, resulting in the formation of 3D frameworks and also lower-dimensional structures. MOFs are highly modular systems: more than one hundred types of SBUs and several thousand linkers can be combined to a huge number of individual structures with finely-tuned lattice parameters and properties. A spectacular characteristic of the family is the unusually low space filling: these materials have the highest inner surface area among all pore systems. The uniform shape and size of the ordered pores allow high rates of diffusion of gases. The supramolecular interactions with the guest molecules result in selective absorption. These properties make MOFs suitable hosts for effective storage of gases and for effective separation of mixtures of gases. Various chemical reactions can be performed in MOFs with significant topochemical control. The majority of the linkers are composed of rigid aromatic molecules with remarkable photophysical activities like fluorescence. Some SBUs have magnetic moments, making a group of MOFs to interesting molecular magnets. Based on the above properties, MOFs and related architectures became the most intensively studied crystalline systems in material science in the last decade. This year we started to develop a new family of MOFs with Zn-based SBUs and cubane-dicarboxylate linkers. We successfully synthesized four new frameworks of different compositions, and determined their structures by single-crystal X-ray diffraction. The following new MOF structures formed: i): three interpenetrated networks with 4-connected, mononuclear SBUs; ii): a 2D network with 4-connected, dinuclear SBUs (paddle-wheels); iii): a cubic network with 6-connected, tetranuclear SBUs; iv): a double-layered architecture with 7-connected, tetranuclear SBUs. The detailed characterization of the physical properties and the activation of the new MOFs are in progress. To study the supramolecular properties of

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[#] Ph.D student

MOFs, we also prepared various fullerene cocrystals of basic Zn-benzoate, the monomer precursor of the well known MOF-5.

Infrared spectroscopy on carbon-based systems. — A significant part of our research this year involved carbon nanotubes and nanotube-based hybrid systems. We studied the optical properties of separated metallic and semiconducting carbon nanotubes, and the mechanism of their sidewall functionalization reactions. Our most important results concerned carbon nanotubes filled with various small molecules, and the effect of the encapsulation on their fluorescent properties. Research on potential solar-cell materials involved surface modification of silicon quantum dots and nanowires of lead-methylamine iodide.

Theory of phase transformations. — We have investigated various aspects of crystalline freezing within atomistic and coarse-grained continuum models. Along this line, we studied the (precursor-mediated) homogeneous and heterogeneous nucleation of nanocrystals using a simple dynamical density functional theory, the phase-field crystal (PFC) model. It has been shown that the mismatch between the lattice constants of the nucleating crystal and the substrate plays a decisive role in determining the contact angle and nucleation barrier, which were found to be non-monotonic functions of the lattice mismatch. We have shown that time-dependent studies are important, as investigations based on equilibrium properties often do not find all of the preferred nucleation pathways. We have investigated the structural aspects of the amorphous precursors in homogeneous nucleation mediated by an amorphous precursor (Fig. 1). Modelling of these phenomena is essential for designing materials on the basis of controlled nucleation and/or nano-patterning. The same atomistic continuum model has been used to evaluate the anisotropy of the body-centred cubic crystal-liquid interface as a function of orientation and temperature: The Euler–Lagrange equation of the phase-field crystal model has been solved under appropriate boundary conditions for 18 orientations at various reduced temperatures. The orientation-dependent results were fitted with an eight-term Kubic harmonic series. The respective equilibrium (Wulff-) shapes vary with increasing reduced temperature from a nearly spherical shape to a polyhedral form (Fig. 2). We have investigated the anisotropy

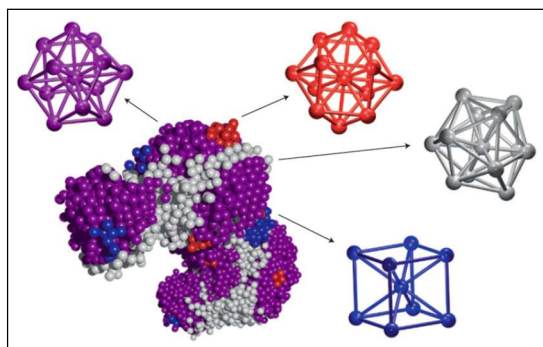**Figure 1.** *Local order in the amorphous precursor assisting crystal nucleation in colloidal suspensions: fcc-, bcc-, hcp-like and liquid-like short range orders all appear.*

Figure 2. *Wulff shapes computed from the Kubic harmonic expressions fitted to 18 interface free energy values evaluated at each reduced temperature [ε = 0.0, 0.1, 0.2, 0.3, 0.375, and 0.5 for panels (a)–(f), respectively].*

of the free energy for the crystal-liquid interface within a Ginzburg-Landau model, and have shown that remnant anisotropy exists at the critical point. We developed a nonlinear hydrodynamic theory of crystallization working on the atomic scale. The model recovers appropriate behaviour of acoustic phonons, the capillary wave spectrum, and steady-state growth with velocity inversely proportional to viscosity. Finally, we reviewed recent advances we made in using orientation-field-based phase-field approaches, and illustrated/discussed the possibility of making quantitative modelling of (a) complex polycrystalline growth morphologies and (b) the manipulation of the crystallization process (Fig. 3).
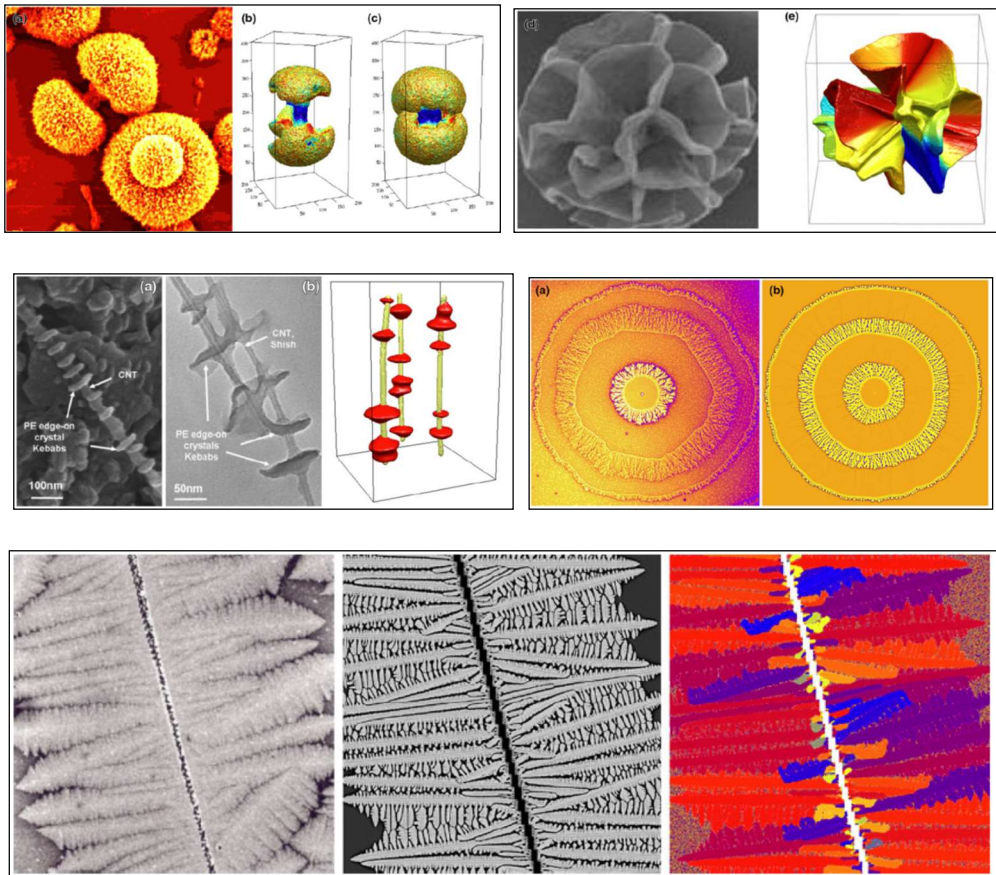
Figure 3. *Orientation-field-based phase-field approaches to exotic growth morphologies: The results are presented in blocks: experiment is on the left, simulation(s) on the right. 1ˢᵗ row: dumbbell shape (left) and "floral" (right) spherulites; 2ⁿᵈ row: 'shish-kebab' structure (left) of polymer disks on fullerene nanotube, and the effect of oscillating temperature (right); 3ʳᵈ row: the effect of scratching on the crystallization of a polymer film.*

Grants

ESA PECS Contract No. 4000104330/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2011–2014).

ESA PECS Contract No. 4000105034/11/NL/KML: MAGNEPHAS III – Modelling of growth and transformation kinetics (L. Gránásy, 2011–2014).

EU FP7 NMP-2011-LARGE-5/280421: EXOMET – Physical processing of molten light alloys under the influence of external fields (L. Gránásy, 2012–2016).

TÉT_12_FR-2-2014-0034: Phase-field modelling of polycrystalline and multi-phase solidification (T. Pusztai, 2014–2015).

OTKA NK- 105691, Science in nanolaboratories (K. Kamarás 2013-2017)

OTKA ANN-107580, Nanoscale investigation of molecular scaffolding (K. Kamarás 2013-2016)

OTKA K-81348, Ultrafast diffraction imaging of single particles (Tegze Miklós 2010- 2015).

International cooperation

Cooperation with colleagues at the École Polytechnique, Paris, France in the framework of the TÉT_12_FR-2-2014-0034 project (T. Pusztai, L. Gránásy, B. Korbuly, L. Rátkai).

Department of Chemistry, University of Nottingham, Prof. Andrei N. Khlobystov

Faculty of Physics, University of Vienna, Prof. Jannik C. Meyer (joint OTKA - FWF project)

Department of Chemistry, Durham University, Prof. Kosmas Prassides

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See also: S-D.30, S-D.31

S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Bernadette Sas[A], Kálmán Tompa[E], Tamás Verebélyi[#], Francis Ian Bickford Williams[A]

Water rotation barriers on protein molecular surfaces. — The experimental characterization of hindered-rotation barriers and mapping the energetic heterogeneity of water molecules bound to the molecular "surface" of proteins are critical for understanding the functional interaction of proteins with their environment. To achieve this goal, we introduced an original wide-line NMR procedure which is based on the spectral motional narrowing following the melting (thawing) of interfacial ice. The procedure highlights the differences between globular and intrinsically disordered proteins. It enables us to delineate the effect of solvent on protein structure, to distinguish between point mutants, monomeric and oligomeric states, as well as to characterize the molecular interactions taking part in different cellular processes. This is a unique experimental approach introducing novel physical quantities and quantifying the heterogeneous distribution of motional activation energy of water in the interfacial landscape (Fig. 1).
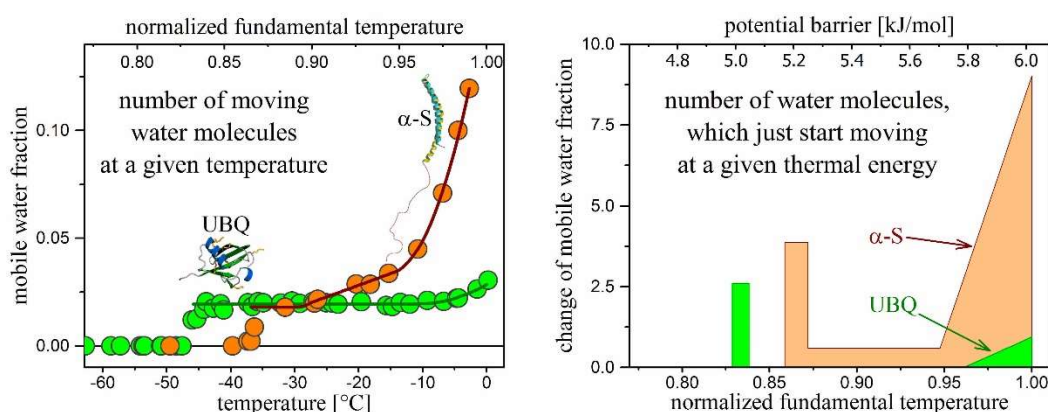
Figure 1. *Hydration properties and water rotation barriers at the molecular surface of a globular protein (ubiquitin, UBQ) and an intrinsically disordered protein (α-synuclein, α-S) both dissolved in water. Mobile water fraction as a function of normalized temperature (left panel) determined by wide-line NMR and its differential quotient; i.e., the number of water molecules which start moving at the given temperature (right panel).*

Hydrogen skeleton and mobility in polycrystalline lysozyme. — Hen egg white lysozyme is considered as a globular-protein standard. The hydrogen mobility parameter (HM) was determined from wide-line ^{1}H-NMR spectra at 4 K $\leq T \leq$ 298 K (Fig. 2). The parameter HM is a quantitative measure of the structural dynamics (inner mobility) of protein molecules. The HM parameter values measured at 4 K and at room temperature were used as the rigid-

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lattice and the mobile-state reference, respectively, for a globular protein. The thermal evolution of HM is connected with qualitative changes in protein dynamics.
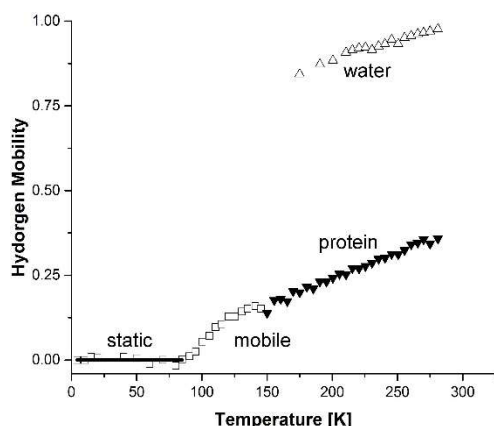
Figure 2. *Hydrogen mobility determined from ^{1}H-NMR spectra of hen egg white lysozyme. The polycrystalline sample were described by a single HM value below 150 K. The protein molecules and the water content of the sample show markedly different dynamics above 150 K.*

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)

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See also: S-D.28.

S-I. Electrodeposited nanostructures

László Péter, Imre Bakonyi, Kata Berkesi, Bence Lázár, Katalin Neuróhr, Lajos Pogány[A], Bence Tóth, Sándor Zsurzsa[#]

Electrodeposition of magnetic/non-magnetic nanowires. — NiCo/Cu nanowires of 240 nm diameter have been prepared by electrodeposition with the help of anodic alumina templates. The layer thickness of the NiCo layer was kept constant (at about 20 nm), while the Cu layer thickness was varied between 0.2 and 5.2 nm. Electrodeposition parameters were chosen so that the composition of the magnetic layer was $Ni_{0.5}Co_{0.5}$ for maximizing the magnetoresistance effect. After the synthesis of the multi-layered nanowires, the template was dissolved selectively, and individual nanowires were treated in the subsequent experiments. The average composition of the nanowires was checked in a transmission electron microscope where the composition modulation was also verified. The magnetoresistance and the magnetothermopower were measured with a lithographically prepared multi-contact probe. A maximum of 14% was found for the giant magnetoresistance effect at 3.5 nm Cu layer thickness both in external magnetic field parallel and perpendicular to the nanowire axis. A linear relationship between the magnetic-field-dependent Seebeck coefficient and the electrical conductivity was found where the magnetic field was an implicit variable during the experiments. These results verified the dominating diffusive thermopower contribution, as expected from the Mott formula. (This work was performed in co-operation with the Institute of Applied Physics, University of Hamburg.)

Many attempts have been made to obtain Co-Bi multi-layered films and nanowires. Besides the usual aqueous solutions, deposition experiments from dimethysulfoxide were also performed. It was found that the nucleation of bismuth on cobalt requires such a high overvoltage that makes impossible to produce a layered material. According to the X-ray diffraction study of the samples prepared, granular mixtures could only be obtained. (This work was performed in co-operation with NCSR "Demokritos", Athens.)

Fabrication of nanoporous anodic aluminum oxide templates. — A home-built workstation for the preparation of nanoporous anodic alumina templates has been extensively tested. The electropolishing conditions of as-received high-purity aluminum discs were optimized. It was established that the electropolishing procedure always leaves behind a damaged zone near the edge of the electropolished area which zone tends to be seriously over-etched in the subsequent sample preparation steps. A preparation protocol adopted from the relevant literature could be adapted. In oxalic acid solutions, the pore diameter was obtained as 40 nm, and the 10 % porosity of the membranes was in good agreement with literature data. Scanning electron microscopic images showed that the nanopores were nearly completely separated from each other.

[A] Associate fellow
[#] Ph.D student

Electrodeposition of metals from nonaqueous solutions. — Electrodeposition from methanolic solutions can lead to deposit compositions that are not available from aqueous solutions. In our experiments, metallic Ni-Mn deposits could be obtained up to about 50% Mn molar ratio, while deposits of higher manganese content were dominantly oxide precipitates. The morphological characterization of Ni-Mn deposits prepared with methanol as solvent revealed the solution composition – deposition potential regime where metallic deposits can be obtained.

Industrial activities. — An upscaling of the former experimental setup for the production of large-surface-area amorphous nickel-phosphorus coatings has been performed. The workstation implemented will be capable of producing 500 cm^2 coatings for fine-polishing and serving subsequently as sputtering targets to prepare multi-layered coatings for neutron mirror applications.

A risk analysis of a specific type of corrosion failure occurred in the Nuclear Power Plant of Paks has been performed in connection with the service lifetime extension of the power plant. A detailed electrochemical corrosion study of the stainless steel samples provided was performed. While the pitting corrosion resistance of the samples studied proved to be sufficient, the mechanism of the cavity formation after the initial pitting corrosion was found to be partly of microbiological origin. Several risk factors of this corrosion mechanism have been identified.

Grants, contracts

OTKA K 104696: Electrodeposition of special magnetic materials from nonaqueous solutions (L. Péter, 2012-2015)

Corrosion tests and literature survey to support the lifetime extension analysis of the Nuclear Power Plant of Paks - Contract by Trapus és Társa Kft. (L. Péter, 2014)

Project KMR_12-1-2012-0226 Development of components for new-generation neutron physics devices (Contractor: L. Rosta; subcontractor: L. Péter, 2013-2015)

International cooperation

NIH TéT 10-1-2011-0555 (Hungarian-Greek bilateral project): Magnetotransport phenomena in ferromagnetic/semimetal nanowires (L. Péter, 2012-2014)

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, 2014-2018)

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See also: S-C.29

S-L. Nanostructure research by neutron scattering

László Almásy, Katalin Pánczél-Bajnok, Gergely Eszenyi, Margit Fábián, György Káli, Adél Len, Gergely Nagy, László Rosta, Noémi Kinga Székely, Gyula Török[A], Renáta Ünnep[#], Tamás Veres
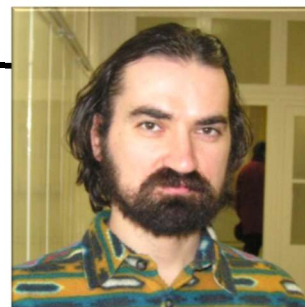
We study the microscopic structure of materials using methods of neutron diffraction and neutron spectroscopy. These techniques allow us to asscess the interatomic and intermolecular structure and interactions which in turn determine the macroscopic properties and behavior of the materials. We operate a couple of instruments which are installed at the national large-scale facility - Budapest Research Reactor. Besides our own projects, we work in open cooperation with external scientists who require these methods for their research.

Polymers. — Bulk polymer materials properties change with time, which is usually unfavourable and means degradation of the materials properties. Thermoplastic polyurethanes gain their hardness and flexibility from the interdigitated hard and soft domains of nanometer size. Small-angle neutron scattering on sample materials treated by accelerated thermal and humidity aging revealed microstructural changes: the migration and the rearrangement of the hard domains and the soft domains, as a result of the polymer chain breaks induced by hydrolysis, the extent of which depends on weathering conditions. These rearrangements lead to the loss of hardness and further the complete degradation of the material. Structure-property relationship can be constructed on the basis of the experimental data.

Liquid mixtures. — Aqueous solutions exhibit a great variety of behaviors, many of which are still not fully understood. Simple aqueous solutions of small amphiphilic molecules (such as ethanol) most often show a moderate tendency to phase separation on nanometer length scales, which are hardly detectable except when the thermodynamic state of the mixture is close to the phase-separation boundary line. In simple cases, this behavior can be accurately described by the competing hydrogen bonding and hydrophobic interactions. A new phenomenon has been observed on aqueous solutions of cyclic amines, piperidine being an example. While the thermodynamics of these solutions resembles that of many other non-ideal aqueous solutions, their structure is completely different on the nanometer length scales. Scattering measurements indicate that instead of showing the traditional concentration fluctuations, the molecules here form relatively strong water-amine pairs and, by hydrogen bonding to other water molecules, adopt a molecular microemulsion-like arrangement, never before observed in molecular solutions.

Biomagnetic materials. — Magnetoferritin, a synthetic derivative of the iron-storage protein (ferritin), has a potential for perspective applications in drug delivery and as a

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[A] Associate fellow
[#] Ph.D student

contrast agent. Its strict monodispersity and capability of being loaded by varied amount of iron oxides is counterbalanced by the structural instability at high pH and excessive iron loading. The direct influence of the iron on the structure of the protein shell is, however, hard to assess. Contrast-variation small-angle neutron scattering and X-ray scattering showed that at high iron loadings the protein shell becomes partly destroyed and opened, which leads to some aggregation of the magnetoferritin particles above a certain loading factor threshold, which is about the half of the theoretical loading capacity of magnetoferritin.

Grants

EU-FP7-INFRASTRUCTURES-2011-1-283883: NMI3-II —Neutron Scattering and Muon Spectroscopy Integrated Initiative (L. Rosta, 2012-2015)

Polish-Hungarian Joint Research Project: Structural and thermodynamic studies of ternary mixtures with ionic liquids (L Almásy, 2014-2016)

International cooperation

JINR (Dubna, Russia), PNPI (Gatchina, Russia), Kazan Federal University (Kazan, Russia), PSI (Villigen, Switzerland), Institute of Chemistry (Timisoara, Romania), Institute of Macromolecular Chemistry "Petru Poni" (Iasi, Romania), A.I. Cuza University (Iasi, Romania), Pharmaceutical Faculty, Comenius University, (Bratislava, Slovakia),

Institute of Experimental Physics (Kosice, Slovakia), LLB (Saclay, France), ILL (Grenoble, France), INPC (Mianyang, China).

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See also: R-M.4

S-M. Neutron optics

János Füzi, László Cser[A], Zoltán Imre Dudás, Zoltán László[#], Márton Markó, Ferenc Mezei[E], János Orbán[#], Alex Szakál[#]

Neutron instrumentation development. — Serving the quest of neutron spectroscopy research for understanding the structure and dynamics of solid state matter on nano- and picometric scale, the main task of the Neutron Optics Research Group is the ongoing improvement of the neutron delivery system and spectrometer suite deployed around the 10-MW Budapest Research Reactor (BRR), central element of the Budapest Neutron Centre (BNC). One of the key and largest research facilities in Hungary, it is the base for a significant domestic and international user community to serve for exploratory and applied research in many fields of science and technology as well as for methodological developments in neutron beam techniques. The flux on sample of the BNC neutron reflectometer has been significantly increased by the installation of the new double monochromator system. In the frame of the NMI3-II Detectors JRA, we have designed and tested the prototype of a novel type of thin solid boron converter detector with gas amplification and delay-line encoding, intended to replace the expensive ^{3}He isotope in future large-area detector arrays.

Neutron holography. — As an efficient tool to investigate the local structure around a specific nucleus embedded in a crystal lattice, successful holographic imaging of nuclei was demonstrated with neutrons based on the short-range strong interaction. Neutrons are unique in the sense that they possess magnetic moment and interact with the magnetic moments of the atoms in a crystal. This interaction opens the possibility of holographic imaging of magnetic moments. As a first step towards magnetic holography, we performed model calculations of a magnetic hologram taking into account the magnetic form factor and the polarization factor. We found that the form factor significantly reduces the measurement domain and the polarization factor modulates the hologram. A reconstruction method was developed which utilizes the properties of the polarization factor to separate the three components of the magnetization vectors and provide the spatial distribution of the magnetic moments around a specific atom in a crystal.

Design of metamaterial structures. — Metamaterials show unusual electromagnetic properties not found elsewhere in nature. Their negative permittivity and permeability over the same frequency range results in negative refractive index. Besides the intriguing problems of fundamental research, this new class of materials allows innovative technical applications. A fishnet structure with zero refractive index has been designed with impedance matching, to enhance the gain and directivity of patch antennas. The finite-element simulations show that the gain of the antenna is increased from 4dB to 15 dB by applying two layers of the designed metamaterial above the antenna.

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

Structural investigations of hybrid silica gels. — The sol-gel technique has been employed to synthesize crystalline Willemite and amorphous silica gels. Rare-earth-metal-doped Willemite has been characterized by neutron and X-ray diffraction, thermal analysis, photoluminescent and FT-IR Spectroscopy. To achieve the best luminescence, the effect of the concentration of the activator ion (Eu^{3+}, Ce^{3+}, Tb^{3+}) and the presence of the charge compensator (Li^+ and K^+) have been investigated. The gels will be used to incorporate porphyrins or rare-earth metals. The obtained hybrid materials can be applied in the development of gas sensors or in photodynamic therapy of cancerous cells.

Grants and international cooperation

KMR_12-1-2012-0226 Development of components for new-generation neutron research instrumentation (L. Rosta, 2012-2015)

EU-FP7-INFRASTRUCTURES-2011-1-283883, NMI3-II — Neutron Scattering and Muon Spectroscopy Integrated Initiative – Detectors JRA (L. Rosta, 2012-2015)

Institute of Nuclear Physics and Chemistry of the China Academy of Engineering Physics (INPC – CAEP) Mianyang: commissioning of neutron spectrometers (high-resolution neutron diffractometer, cold triple-axis spectrometer) delivered and installed by Mirrotron Ltd., Budapest.

Chinese 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.

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S-N. Laser applications and optical measurement techniques

Aladár Czitrovszky, Kárpát Ferencz, Zoltán György Horváth[A], Péter Jani[A], Attila Kerekes[#], Szilvia Kugler, Attila Tibor Nagy, Dániel Oszetzky, Lénárd Vámos

Aerosol drug delivery/deposition in human lungs. — Within the project our aerosol laboratory was equipped with a number of new instruments (Raman spectrometer, Pharmaceutical cascade impactor, light scattering and aerodynamic aerosol sizer, laser Doppler anemometer, temperature- and humidity-controlled measurement chamber, etc.). In this laboratory, we performed a number of measurements about aerosol deposition: we determined the ratio of deposited particles from an air flow in different segments of 3D airway models consisting of different number of generations of the human lung, for different particles sizes and at different flow rates (Fig. 1). This information gives an experimental input to the numerical stochastic lung deposition model developed by a group in the Centre for Energy Research of HAS. We developed also different optical methods to quantify the amount of deposited particles on cascade impactor catch plates, based on Raman and luminescence spectroscopy, optical microscopy and interferometry. These results can be used to determine the size distribution, the median diameter and other physical properties of aerosol drugs applied in metered dose and dry-powder inhalers. These results were used in 3D lung model deposition experiments, where small silicon plates were installed into the realistic 3D-printed airway models. With Raman spectroscopy, we measured the active agent of the drug, with optical microscopy the surface coverage was determined, and by the interferometric method the volume of the deposited material was measured. The aim of this experimental work is to obtain enough data for the goal of the project, to increase the efficiency of aerosol drugs and decrease the harmful side effects.

EXMET - LIPS – RAMAN spectroscopy and Interferometry project. — In cooperation with the Budapest University of Technology and Economics –BUTE and University of Miskolc – (UM), we studied the properties of specific samples at different excitation levels using laser induced plasma spectroscopy and micro-Raman spectroscopy methods, and compared the benefits and disadvantages of these methods. On the basis of these results, we started the design of a combined spectroscopic instrument having ampliative features, especially in case of high-fluorescence samples. In cooperation with UM, we started the development of Michelson-type interferometer, using a frequency stabilized laser and high-quality optical elements for the investigation of vibrations.

Optical thin-film structures consisting of nanoscale laminated layers. – We have continued our research towards the development of optical thin-film structures containing nano-optically thin layers for advanced applications in laser physics and information technology. Using the latest multiple target thin-film optimization method, we have developed high-

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[A] Associate fellow
[#] Ph.D student

efficiency low-dispersion thin-film polarizer coatings for high-power femtosecond Ti:sapphire lasers (ELI project in Czech Republic), fast dielectric scanner mirrors, wide-band output coupler mirrors, HR 267 nm/0° type low-dispersion high reflectors for femtosecond UV application, Gauss-filter type correlators for Ti:sapphire amplifiers, AR 266 nm & 638 nm/0° double-band antireflective coatings for photoacoustic analyzers, etc.

Surface diagnostics. — We have continued the study of the profile and the quality of large-diameter high-quality optical surfaces with a white-light interferometric surface profiler. Laser-induced damage threshold measurements have also been performed. A novel method is under development that would combine surface diagnostics with aerosol science: drug samples of a next-generation impactor are investigated by the interferometric surface profiler to determine the exact volume of deposited species. Such a new method would give us much faster results than the existing and known analytical processes.

Participation in TAMOP Educational Program for ELI. – in the frame of this project, we elaborated 2 lecture notes related to ELI-ALPS for students and PhD students and organized an educational course and laboratory practice at College of Mechanical Engineering and Automation (GAMF) in Kecskemét.

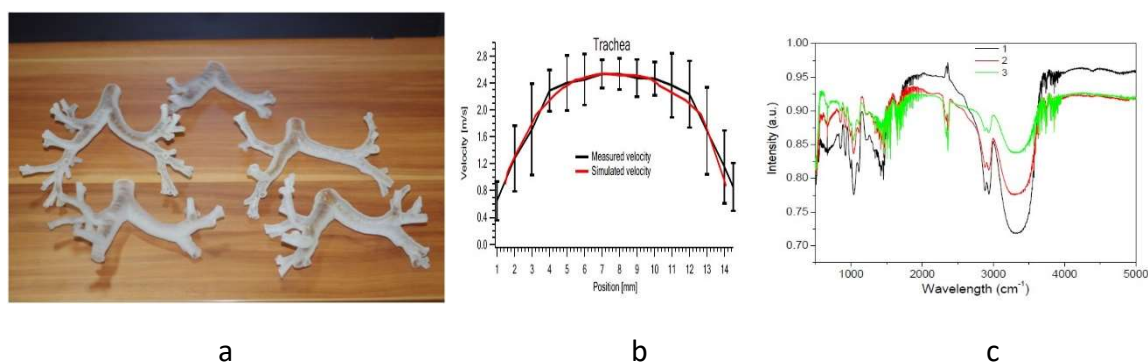a   b   c

Figure 1. *Realistic 3D-printed human hollow airways (a), measured air flow profile in a cross-section of lung tract compared with model calculations (b) and luminescence spectra of deposited aerosol particles (c).*

Grants

HOYA - Wigner RCP: Measurements of industrial indoor aerosol pollution (A. Czitrovszky, 2014)

EXMET 903010-14: Development of LIPS-Raman and interferometric measurement methods (A. Czitrovszky, 2014- 2015)

HAS – Wigner RCP 81018-13: Infrastructural Developments, establishing a service laboratory for optical measurements (A. Czitrovszky, 2014-2015)

HAS – Wigner RCP 81033-14 – MTA: Deposition of aerosols (supplement) (A. Nagy, 2014)

International cooperation

University of Vienna – Wladyslaw Witold Szymanski, Study of optical properties of aerosols and their climate relevance with dual wavelength optical particle spectrometer

Max Planck Institute of Quantum Optics (Garching, Germany) - Ferenc Krausz, Study of ultrafast light-matter interactions.

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See also: R-P.1, S-P.4, S-P.6, S-P.19, S-R.11, S-R.12

S-O. Femtosecond lasers for nonlinear microscopy

Róbert Szipőcs, Attila Csákányi, Dóra Haluszka[#], Attila Kolonics, Zoltán Várallyay

Femtosecond lasers. — For our hand-hold 3D nonlinear microscope system (*FiberScope*), we have developed 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. The repetition rate of the laser can be optimized for nonlinear processes taking place in the specially designed fiber delivery system, which results in an optimized excitation spectrum of our pulsed laser source and a high signal to noise ratio of our handhold microscope (compared to nonlinear microscopes comprising industry standard, 80 MHz Ti:sapphire lasers). This fact is demonstrated in Fig. 1, where two SHG images of the collagen fibers in an *ex vivo* murine skin sample are displayed. For both pictures, the same microscope setup was used. It is clearly seen that our novel Yb-fiber laser generates a considerably higher SHG signal than the Ti:sapphire laser having the same average power of 5 mW. Based on our recent results of laser safety investigations, we can say that the whole, cost-efficient, fiber-laser-based *FiberScope* hand-hold microscope system can be safely used for basal cell carcinoma (skin cancer) detection, *in vivo* monitoring of penetration of nanomedicine or different cosmetics through the skin, for instance.
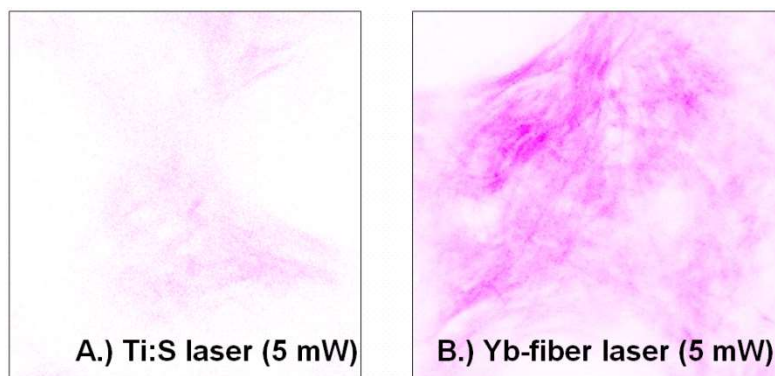
*Figure 1. Comparison of SHG imaging performance of different mode-locked lasers having the same average power of 5 mW (on the sample) for nonlinear microscopy. Ex-vivo murine skin sample, imaging depth: z = 30 µm, same microscope settings. Collagen distribution measured by **A)** an industry standard, 80 MHz Ti:sapphire laser, and by **B)** our newly developed Yb-fiber oscillator and amplifier system (with a variable repetition rate).*

Non-linear microscopy. — In parallel with our cutting-edge non-linear microscope developments (such as the *FiberScope* system or a gradient-index-lens-based coherent anti-Stokes Raman scattering (CARS) microendoscope system), we performed a high number of experiments using our (in-house made) CARS imaging system. The measurements were

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[#] Ph.D student

related to *in-vivo* optical disease diagnosis in dermatology (such as characterization of obesity, for instance), or in neurology (such as characterization of animal models developed for studying sclerosis multiplex, for instance), in collaboration with our scientific partners: Semmelweis University, Department of Dermatology and University of Szeged, Department of Neurology, respectively. In neurology, as a first step, we demonstrated that this novel CARS-imaging setup allows for label-free imaging of the brain (Figure 2.). For instance, tuning the CARS setup to CH_2 vibration of myelin lipids, we could record high quality 3D CARS images of the myelin. Since myelin loss and axonal degeneration are the pathological hallmarks of several inherited and acquired neurological disorders, a method that allows simultaneous visualization of the two inter-related processes in live tissues may have great research utility.
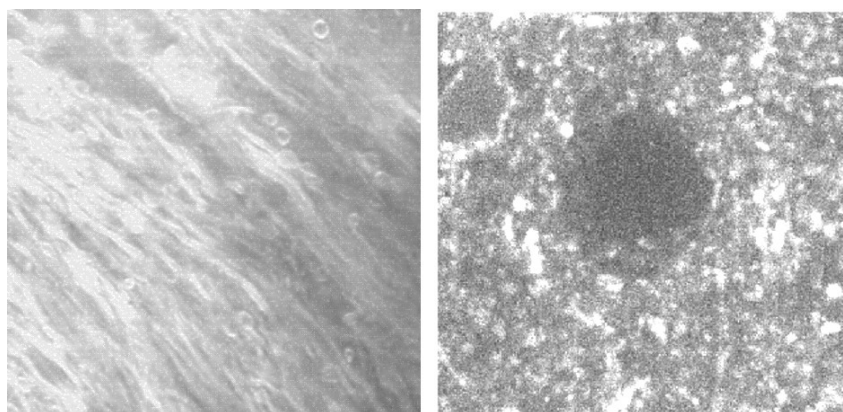
Figure 2 Left: *CARS image of myelin fibers in the white matter of rat brain slice,* **Right:** *autofluorescence image of the cytoplasm in the gray matter of a rat brain slice.*

Optical fiber theory and technology. — Dispersive properties of optical fibers play an important role in long-distance, high-speed optical data transmission systems and in ultrashort (ps or fs) pulse optical fiber laser systems. We showed that the group delay (τ) of a relatively narrow-band optical pulse transmitted through a piece of optical fiber of unit length is proportional to the energy (U) stored by the standing-wave electromagnetic field at the same (central) frequency, as long as the confinement loss is small. We found that having this relationship in mind we can construct higher-performance "dispersive" optical fibers, such as hollow- or solid-core photonic bandgap (PBG) fibers. In collaboration with the University of Szeged, Department of Quantum Electronics, we performed a comparative study to find the most accurate spectral-phase retrieval method that is suitable for measuring higher-order chromatic dispersion of optical fibers. We tested the stationary phase point, the minima–maxima, the cosine function fit, the Fourier transform, and the windowed Fourier transform methods, and found that out of these five techniques, the Fourier-transform method provided the dispersion coefficients with the highest accuracy, and it could also detect rapid phase changes in the vicinity of leaking-mode frequencies within the transmission band of the PBG fiber sample for instance.

Grants

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See also: R-P.1

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 stoichiometric lithium niobate. – High-quality Mg-doped stoichiometric lithium niobate (sLN:Mg) just above the Mg threshold concentration has been grown by the high-temperature top-seeded solution growth (HTTSSG) technique from K_2O–Li_2O–Nb_2O_5–MgO mixtures for nonlinear optical applications in the THz frequency range. In a series of growth experiments, crystal quality and dopant distribution along the boules were investigated by UV absorption edge, OH band position and Mg concentration measurements, and a correlation between the OH vibrational frequency and the Mg concentration was found. The data can be used to achieve uniform dopant distribution in high-quality sLN:Mg crystals by using a semi-continuous feeding HTTSSG technique with adequate feeding composition.

LiNbO₃ crystals doped with optical-damage resistant ions. – The IR spectra of stoichiometric LiNbO₃ crystals containing photorefractive damage resistant ions (M = Mg, Zn, Sc, In, Hf, Zr or Sn) above their threshold concentration revealed OH⁻ absorption bands absent in undoped crystals (Fig. 1, left). The higher the valency of the dopant ion the lower the observed frequency of the hydroxyl vibration, and the closer the O – H bond direction to the oxygen plane perpendicular to the crystallographic c axis of the crystal. The bands were attributed to stretching vibrations of hydroxyl ions in $M_{Nb}^{n+} - OH^-$ (n = 2, 3 or 4) type defect complexes (Fig. 1, right).
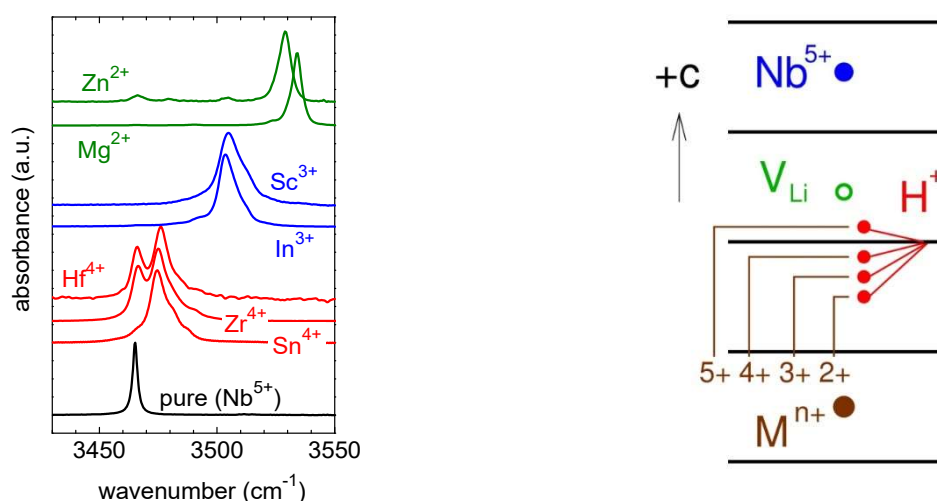

Figure 1. *Left: Infrared absorption spectra of stoichiometric LiNbO₃ crystals doped with photorefractive damage resistant ions M^{n+} above their threshold concentrations, **Right**: Schematic drawing of the $M_{Nb}^{n+} - OH^-$ defect models for various values of n.*

Coherent radiative processes in rare-earth doped LiNbO₃. – A simple, pulsed or CW pump probe measurement scheme developed to measure the homogeneous linewidth of an atomic transition in an inhomogeneously broadened spectral line of a dopant ion in a single crystal was applied to the $^4I_{11/2} - {}^4I_{15/2}$ Er transition in $LiNbO_3:Er^{3+}$ crystals. A comparison of population relaxation and dipole relaxation times (T_1 and T_2) for the split absorption line components due to slightly different crystallographic environments has been carried out. Observed differences in T_1 and T_2 remained within experimental error. The effect of magnetic field on the homogeneous linewidth has also been studied. A magnetic induction of approximately 50 mT increased T_2 from 7 to 8 ns.

Phase transition of potassium lithium niobate (KLN) crystals. – Raman spectra, UV absorption edge and phase transition measurements have been performed on Ta^{5+} and Ti^{4+} doped KLN crystals. The observed differences indicate that Ti^{4+} ions, in addition to Nb may also occupy Li sites, thereby decreasing the number of Nb_{Li} antisites while Ta^{5+} substituting only Nb suppresses the relaxor characteristics of KLN more effectively.

Lithium yttrium orthoborate ($Li_6Y(BO_3)_3$, LYB) single crystals doped by rare-earth ions. – Low temperature EPR spectra of LYB:Yb grown by the Czochralski method show the presence of a dominant Yb^{3+} centre which can be clearly identified by the fully resolved hyperfine structures due to the ^{171}Yb and ^{173}Yb isotopes. Such centres are substituted at Y sites, and due to their weak interaction with the lattice are suitable for resonant nonlinear optical experiments. The Stark levels of the $^2F_{7/2}$ and $^2F_{5/2}$ multiplets of the Yb^{3+} ion in $Li_6Y(BO_3)_3$ crystals have been determined by optical absorption and luminescence measurements. For LYB containing 5 mol% Yb, an additional line originating either from Yb pairs or from unwanted rare-earth ions present in the crystal has been detected.

Undoped LYB single crystals have been investigated by polarized UV absorption spectroscopy. Two bands near the UV absorption edge, at about 220 and 240 nm, were tentatively attributed to Fe^{3+} impurities. This could be supported by heat treatments of the air-grown crystals in a reductive atmosphere expected to result in a $Fe^{3+} \rightarrow Fe^{2+}$ conversion. After a 3-h-treatment at 500 °C, the intensity of these bands decreased, while a new, broader one appeared between 350-500 nm, which may correspond to Fe^{2+} centres.

Energy levels of Eu and Tb doped polytypic $GdAl_3(BO_3)_4$ crystals. – Electronic transitions of the Eu^{3+}, Tb^{3+} and Gd^{3+} rare-earth ions in rhombohedral and monoclinic GAB crystals were assigned using temperature and concentration dependent absorption measurements in the 16000–32000 cm^{-1} wavenumber range. An effect due to the symmetry reduction (R32 - C2/c) was revealed in some of the absorption bands of Tb^{3+}, Eu^{3+} and Gd^{3+} ions. Using polarization-dependent absorption measurements the energy levels of the low-energy part of ^7F and ^5D states of the Eu^{3+} ion were successfully determined in both structural modifications.

$Li_2B_4O_7$-based dosimeters and detectors. – Transition metal-doped $Li_2B_4O_7$ tissue-equivalent thermoluminescent dosimeter and neutron detector materials have been characterised by luminescence methods. In the case of Mn-doped ceramics and single crystals the thermoluminescence was essentially identified with Mn photoemission having photon energies at 2 eV easily discernible from the luminescence of self-trapped excitons and possible co-dopants Cu and Ag, all emitting at higher energies.

Yttrium oxyorthosilicate scintillators. – Polycrystalline, cerium-doped yttrium oxyorthosilicate ($Y_{1.99}Ce_{0.01}SiO_5$, YSO:Ce) scintillator materials have been synthesized and characterized. The samples have been prepared using a mixed-powder route with LiF and NaF additives. The final reaction products have been analyzed for phase purity by X-ray powder diffraction (XRD) and Raman spectroscopy. The concentration of the additives and the temperature of the thermal treatment have strongly affected the formation of the desired X2-YSO phase. The best yield for X2-YSO has been obtained with the application of 18 mol% LiF at 1400 °C. Samples obtained in this way also showed the highest luminescent efficiency which was attributed to the effect of Li^+ on the formation of the X2-YSO phase.

Analytical methods for environmental control and advanced materials. – Atmospheric concentrations, fluxes and emission sources of a few C3-C9 alkyl nitrates (ANs) at the coast of the Belgian North Sea were determined. The daily levels of ANs ranged in 0.03-85 pptv, and consisted primarily of nitro-butane and nitro-pentane isomers. Shorter-chain ANs were the most abundant in Atlantic/Channel/UK air masses, while longer chain ANs prevailed in continental air. The AN-fluxes were higher for summer than for winter and spring. ANs originated from traffic/combustion, secondary photochemical formation, biomass burning and marine sources.

High-resolution flame- and graphite-furnace atomic absorption spectrometry methods (solid sampling and solution-based) were optimized and applied to the determination of different constituents in $LiNbO_3$ optical crystals (Mg, Rh), in SiC nano-materials (Al, Si), as well as to quantify/screen the Cu content of various alcoholic beverages. The latter method is cost-effective, since it works with the injection of 20 μL samples, without any chemical modifier. Due to the fast furnace-heating program, one analytical cycle is shorter than 1 min.

Grants
OTKA K 83390: Resonant optical processes in solids (L. Kovács, 2011-2015)

OTKA K101819: Design, fabrication and analysis of luminescent silicon carbide nanocrystals for in vivo biomarker applications (Á. Gali, participant: L. Bencs, 2012-2015)

MTA Infrastructural Developments: Development of analytical systems for the analysis of environmental and advanced nano-materials (L. Kovács, 2013-2014)

International cooperation
Tartu University (Estonia), Recombination luminescence of doped borates: origin and application in dosimetry (G. Corradi)

Osnabrück University (Germany), Small polarons in luminescent $LiNbO_3$: From bulk to nanocrystals (G. Corradi)

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10. <u>Tichy-Rács É</u>, Komlai K, <u>Mandula G</u>, <u>Lengyel K</u>, <u>Kis Zs</u>, <u>Kovács L</u>, <u>Corradi G</u>: Ritkaföldfém ionok spektroszkópiai tulajdonságai lítium-ittrium-ortoborát egykristályokban (Spectroscopic properties of rare-earth ions in lithium-yttrium-orthoborate single crystals, in Hungarian). In: Ádám P, Almási G (szerk.) In: Kvantumelektronika 2014: Proc. of the VII. Symposium on the results of domestic quantum-electronics research. Budapest, 28.11.2014, Eds.: Ádám P, Almási G, University of Pécs, Hungary, 2014.Paper P77.

Others

11. Hartmann E: A krisztallográfia forrásainál (At the sources of crystallography, in Hungarian). **FIZIKAI SZEMLE** 64:(10) pp. 330-333. (2014)

12. Kovács L: Miért jó a kristály, ha hibás? (What is a crystal good for, if it is faulty? in Hungarian). **FIZIKAI SZEMLE** 64:(10) pp. 351-354. (2014)

13. Mandula G, Kis Zs, Tichy-Rács É, Komlai K, Kovács L, Lengyel K, Corradi G: Spectroscopic properties of Yb3+ ions in $Li_6Y(BO_3)_3$ single crystals. In: Eurodim 2014, Kent, Great Britain, 13.07.2014-19.07.2014, Paper A4.

See also: S-S.10

S-R. Nanostructures and applied spectroscopy

Miklós Veres, Tamás Demján[#], László Himics[#], Margit Koós[A], István Rigó[#], Sára Tóth, Tamás Verebélyi[#]

Color centers in nanodiamonds. — Diamond nanoparticles (DNPs) are very promising materials for many new applications in different fields such as bio-marking, quantum computing and sub-diffraction imaging. The majority of these applications is based on the single-photon emitter defect centers formed in DNP crystals. A novel technological method has been developed for the creation of this type of color centers in DNPs with an average size of 5-20 nm by using a simple and widely available technique, like plasma-immersion ion implantation (PIII) or focused ion beam (FIB) implantation with low-energy ions. Nitrogen-related defect centers have been prepared successfully using these techniques.

Among the color centers created in nanocrystalline (nc) diamond films, the silicon vacancy (SiV) center is of particular interest due to its stable, intense and narrow zero-phonon line (ZPL) at 738 nm for the utilization of in-vivo biosensing. Unfortunately, its emission could be affected by the neutral vacancy-related general radiation (GR1) center having doublet emission structure with ZPLs at 741 and 744 nm and being present in the top layer of chemical vapour deposited (CVD) nc diamond films. For high-quality applications, it is important to clarify the role of the GR1 defect center. The contribution of GR1 defect center emission to the red shift of the peak position and the considerable broadening of the SiV center's ZPL (Fig. 1a) have been verified by intense laser excitation in nc diamond films.
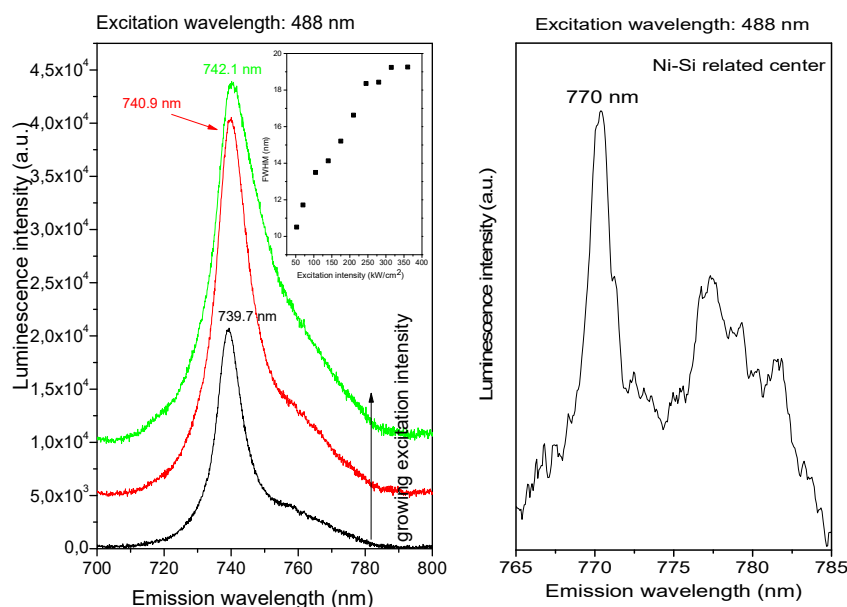
Figure 1. (a) Zero-phonon line shape of SiV center in nc diamond films (average grain size <50 nm) measured using 488 nm laser excitation. The insert shows the change of line broadening with excitation intensity. (b) Emission of Ni-Si related complex defect center in a nc diamond film sample measured with 488 nm laser excitation.

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[A] Associate fellow

Ni-Si related complex color center was successfully created in nc diamond films with different grain sizes. This Ni-Si defect center has a zero phonon line centered at around 770 nm with a FWHM of 3 nm (Fig. 1b), which makes it a possible candidate for biomedical applications. This center is an efficient single-photon emitter with short luminescence lifetime.

Grants

OTKA PD-106130: Generation of highly luminescent color centers in nanocrystalline diamond (S. Tóth, 2012-2015)

TÁMOP-4.1.1.C-12/1/KONV-2012-0005: Preparation for educational and R&D activities related to the Hungarian ELI project in the concerned sectors (M. Veres, 2014-2015)

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

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)

Publications

Articles

1. Csarnovics I, Nemec P, Nazabal V, <u>Veres M</u>, Csik A, Allix M, Kokenyesi S: Stimulated structural changes of Se in nanolayered composite films. MATER CHEM PHYS, 143:(2) pp. 889-893. (2014)

2. <u>Himics L</u>, <u>Tóth S</u>, <u>Veres M</u>, Balogh Z, <u>Koós M</u>: Creation of deep blue light emitting nitrogen-vacancy center in nanosized diamond. APPL PHYS LETT, 104:(9) Paper 093101. 5 p. (2014)

3. Mitsa V, Holomb R, Kondrat O, Popovych N, Tsud N, Matolín V, Prince KC, Lovas G, Petretskiy S, <u>Tóth S</u>: Synchrotron XPS studies of illuminated and annealed flash evaporated a-Ge2S3 films. J NON-CRYST SOLIDS, 401: pp. 258-262. (2014)

4. Oláh N, <u>Veres M</u>, Sulyok A, Menyhárd M, Gubicza J, Balázsi K: Examination of nanocrystalline TiC/amorphous C deposited thin films. J EUR CERAM SOC, 34:(14) pp. 3421-3425. (2014)

5. Shpotyuk O, Kozyukhin S, Shpotyuk Y, Demchenko P, Mitsa V, <u>Veres M</u>: Coordination disordering in near-stoichiometric arsenic sulfide glass. J NON-CRYST SOLIDS, 402: pp. 236-243. (2014)

Books

6. <u>Borossáné Tóth S</u>, <u>Himics L</u>, <u>Nagyné Szokol Á</u>, <u>Veres M</u> (eds.): Az ELI-ALPS és a jövő természettudományi kutatásai (The ELI-ALPS and the natural science research of the future, in Hungarian), Kecskemét, Hungary, 12.12.2014, College of Kecskemét, 2014, 86p.

7. <u>Nagyné Szokol Á</u>, <u>Borossáné Tóth S</u>, <u>Veres M</u> (eds.): Optikai méréstechnikai módszerek az optikai alkatrészek és felületek minősítésére (Optical measurement methods for qualifying optical parts and surfaces, in Hungarian), Budapest, Hungary, 21.11.2014, College of Kecskemét, 2014, 60 p.

8. <u>Veres M</u>, <u>Borossáné Toth S</u>, <u>Nagyné Szokol Á</u> (eds.): Az ELI-APS felépítése, lehetőségei és alkalmazási perspektivái (Structure, possibilities and application perspectives of ELI-ALPS, in Hungarian), Kecskemét, Hungary, 05.12.2014, College of Kecskemét, 2014, 86 p.

Conference proceedings

9. Mitsa V, Holomb R, Lovas G, <u>Veres M</u>, Ivanda M, Kovach T: Spectroscopic evidence of coexistence of clusters based on low (α) and high temperature (β) GeS2 crystalline phases in glassy germanium disulfide matrix. In: 37th International Convention on Information and Communication Technology, Electronics and Microelectronics (MIPRO), Opatia, Croatia, 26.05.2014-30.05.2014, eds.: Biljanovic P, Butkovic Z, Skala K, Golubic S, Cicin-Sain M, Sruk V, Ribaric S, Gros S, Vrdoljak B, Mauher M, Cetusic G, Rijeka: MIPRO, 2014. pp. 7-10.

10. <u>Veres M</u>, <u>Himics L</u>: Belső feszültség lokális változásának vizsgálata optikai anyagokban pásztázó Raman-spektroszkópiai mérésekkel (Inestigation of local change of internal stress in optical materials by scanning Raman-spectroscopy measurements). In: Optikai méréstechnikai módszerek az optikai alkatrészek és felületek minősítésére (Optical measurement methods for qualifying optical parts and surfaces, in Hungarian), Budapest, Hungary, 21.11.2014, eds.: Nagyné Szokol Á, Borossáné Tóth S, Veres M, College of Kecskemét, 2014. pp. 41-60.

See also: S-Q.2, S-Q.3, S-L.19, S-N.12, S-N.13

WIGNER DATACENTER

Gábor Pető, Kármen Almási, Balázs Bagó, Péter Bányai, Ferenc Cseh, László Erdélyi, Szabolcs Hernáth, László Kovács, Miklós Madurovicz, Viktória Mészáros, Dezső Mihalovics, Imre Molnár, Zoltán Nagy, János Sajben, Benjámin Somhegyi, Domokos Szabó, Péter Szabó, Gábor Szentiványi, Endre 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-O 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 decisive role – in international and domestic research, development and innovation (R & D & I) projects that require high level, extensive IT background.*

The Datacenter has already started its second year of operation, and in the framework of its mission it has been providing hosting services to the Geneva based European Organization for Nuclear Research (CERN) as well as infrastructure services to the National Information and Communication Services Ltd, for governmental purposes. The Datacenter has been able to supply the installed equipment a hundred percent during the uninterrupted operation, all the while maintaining the strict technical service level (Service Level Agreement, SLA), which fact was partly due to the heroic efforts of the staff who kept on carrying out all their tasks even in the extreme weather conditions which led to an environmental disaster in December 2014. In 2014 the main task of the Datacenter was to provide high level hosting services on one hand, and on the other hand to lay the foundation and execute the preparatory work for the infrastructure necessary for the expansion of the service activities. For this reason, the staff of the Datacenter conducted three public procurement procedures in the value of 260 million HUF, and they also finished the preparatory work for another five public procurement procedures. Since November 2014 the Datacenter has achieved outstanding results in the development of the redundancy of the datacenter insurance services, with the active support of the Hungarian Academy of Sciences.

The Datacenter infrastructure. — In 2014, one of the main challenges for the staff of the Datacenter was the fine-tuning of the infrastructure; by setting and fine-tuning the optimum parameters they were able to achieve significant increase in efficiency under the present circumstances. The average annual PUE (Power Usage Effectiveness) value of the Datacenter decreased significantly in 2014. Since the annual aggregate net IT energy consumption of the Datacenter exceeded the 3 GWh in 2014, the improvement of PUE alone resulted in significant cost rationalization. To this end, the technical education and the training of the staff was continuous. Moreover, further progress has been made in order to increase the redundancy of the infrastructure to an even higher level, and another project, related to the expansion of the power capacity available for the Datacenter, is also in an advanced state. In addition to all these the ISO auditing of the operational processes of the Datacenter has also begun. The Datacenter has plans to join to further efficiency increasing green projects.

The IT services of the Datacenter. — In 2014, the most important service area of the Wigner Datacenter, the CERN@WIGNER Tier-0 hosting, also achieved considerable increase in quantity, and improvement in quality. At the beginning of the year the equipment delivered to the Datacenter by the CERN occupied only one computer room, with 50% utilisation rate (filling only 41 rack cabinets); by the end of the year the first and the second rooms operated on 90% and the third room on 30% (filling 183 rack cabinets altogether). The net value of the installed CERN equipment increased from HUF 1.5 billion in January 2014 to HUF 4.5 billion by the end of December 2014. This huge capacity also significantly increased the number of tasks in the area of the value-added IT hosting activity. Just to give an example, the colleagues belonging to the IT support team fixed or replaced defective parts in the installed equipment for more than 150 times during the year, as part of their daily operational tasks. Naturally, the center fulfilled its contractual obligations to CERN a 100% at all times during the hosting activity. In order to support the data processing processes of the LHC experiments the data network connections of the Tier-0 center also had to be developed: as a result, from now on the Wigner Datacenter will provide the redundant connection points for the new Russian Tier-1 center to the CERN network.

Wigner Cloud infrastructure. — While keeping up the continuous provision of the CERN@WIGNER hosting services, the Wigner Datacenter has begun to develop its own value-added IT service system as well. The Wigner Cloud infrastructure is capable to serve a significant part of the computing capacity needs of the institute's research teams. The foundation to this work is the constant technological and knowledge transfer between the CERN and the Wigner Datacenter which also provides the opportunity to our staff to quickly and efficiently acquire and apply the knowhow and the experience accumulated in the course of the work of the CERN IT. Starting out from a concept, having gone through planning, market survey and tests the Wigner cloud arrived to the installation phase in 2014; at the end of the year the equipment for the first phase of the cloud infrastructure arrived, and it will be ready to serve real-world applications from March 2016, following the installation, test operation and trial run. Short-term expansion plans for the cloud infrastructure also include the installation of significant tape storage capacity.

THE RESEARCH LIBRARY

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) located at the Csillebérc Campus, Budapest. Although it is jointly financed by all the user Institutes, it is developed and managed by the Wigner Research Centre.

Collections. — On 31 December 2014, the library held 66767 monographs and conference proceedings, 40095 journal issues, and 40 893 research reports. In 2014 it held 78 important periodicals, and was enriched by 203 printed monographs including 110 books purchased from the project "Knowledge Base Development". 23 books had been purchased and provided to the library at the expense of research projects, and a further 70 books were donated.

Services. — All library services (excluding circulation) are available on an improved and completely redesigned website that was launched in November 2013. Its English version became operational in 2014. Due to the importance of Open Access, a new page was added in the main menu of the website that provides useful links related to that topic.

Electronic resources. — As a consortium member of the Electronic Information Service (EISZ) national programme, the library has access to the most important academic databases and platforms including Science Direct, Springer Link, Journal Citation Report, EBSCOhost, and we also have an institutional subscription to the American Chemical Society Publications and IOPScience.

In 2014 the accessible information services were broadened with electronic books. To meet the users' needs and in response to incoming requests, a total of 63 e-books have been purchased including 11 e-books within the aforementioned "Knowledge Base Development" project, 50 e-books were purchased from our savings on the Science Direct journal database subscription, and 2 additional books were financed by research projects. All e-books are accessible from everywhere within the institute's IP network, and their contents can be transfered to any storage device. The e-books are available in the online catalogue and through the E-library link on the library website. A user manual was created and made accessible to provide help with using the EBSCOhost e-book services. Library staff attended the 'Electronic book' training, organised by the Informatics for Public Service and Libraries Foundation (INKA).

The online catalogue has been developed and re-designed making electronic search easier. The number of books accessible in the catalog was broadened: by re-cataloging a total of 1000 records, 95% of the materials in the reading room are now searchable.

Events. — The library hosted a workshop of the Association of the Hungarian Librarians, Research and Special Libraries Section on 17 October 2014 as part of the series "New services marketing", with 40 delegates attending.

To familiarize new researchers and scholars of the institute with the library and its services, a training session was held in October 2014 for 17 participants.

SUPPLEMENTARY DATA

Education

Budapest University of
Technology and Economics

Eötvös Loránd University

Óbuda University

Pázmány Péter
Catholic University

Semmelweis University

National University of
Public Service

Szent István University,
Gödöllő

University of Miskolc

Budapest

University of Debrecen

College of Kecskemét

Pannon University,
Veszprém

University of Pécs

University of Szeged

Graduate and post-graduate courses
Eötvös Loránd University, Budapest

— Advanced experimental particle physics (G. Vesztergombi)
— Algebraic Field Theory I. (P. Vecsernyés)
— Budapest semester in cognitive science (M. Bányai)
— Cognitive neuroscience (L. Négyessy)
— Detector systems in particle and nuclear physics (G. Pásztor)
— Electrodeposition of metals (L. Péter)
— Electrons in solids (J. Sólyom).
— Experimental gravitational wave physics (G. Debreczeni)
— Introduction to gravitation and high energy physics (M. Vasúth)
— Laser cooling of neutral atoms (P. Domokos)
— Low temperature plasma physics (Z. Donkó)
— Macromolecules (S. Pekker)
— Magnetism (J. Balogh)
— Many-body problems 1-2. (G. Szirmai)
— Metastable metallic materials (T. Kemény)
— Modeling of the neural system (G. Orbán, M. Bányai)
— Nanomagnetism (J. Balogh)
— Neural modeling (Z. Somogyvári, D. Cserpán)
— Neuroinformatics, (L. Négyessy, Z. Somogyvári, L. Zalányi, F. Bazsó)

- Nuclear solid state physics I (D.L. Nagy)
- Nuclear solid state physics II (D.L. Nagy)
- Optics and relativity theory (D. Varga, Gy. Dávid, J. Cserti)
- Pattern formation in complex systems (Á. Buka and T. Börzsönyi)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Plasma physics of the Solar System (K. Szegő)
- Renormalization methods for strongly correlated systems (Ö. Legeza).
- Solid state physics I (I. Tüttő)
- Statistical learning in neural systems (Z. Somogyvári)
- Statistical learning in the neural system (G. Orbán, M. Bányai)
- Structure investigation methods in materials science (L. Rosta)
- Superconductivity (I. Tüttő)
- Topological insulators 1-2. (J. Asbóth)

Budapest University of Technology and Economics

- Chapters from high-temperature experimental plasma physics (G. Kocsis, T. Szepesi)
- From femtosecond lasers to attophysics (P. Dombi)
- Group theory in solid state research (G. Kriza)
- Infrared and Raman spectroscopy (K. Kamarás)
- Interacting spin systems (K. Penc)
- Introduction to category theory (G. Böhm)
- Introduction to fusion plasma physics (S. Zoletnik)
- Introduction to general relativity (M. Vasúth)
- Introduction to theoretical plasma physics (A. Bencze)
- Introductory physics (A. Gilyén)
- Low temperature plasma physics (Z. Donkó)
- Magnetohydrodynamics in low dimensional systems (A. Bencze)
- Modern solid state physics (A. Virosztek)
- Neutron scattering I, part of the course Experimental methods in material science (B. Nagy, L. Bottyán)
- Nuclear solid state physics I (D.L. Nagy)
- Nuclear solid state physics II (D.L. Nagy)
- Physics 1 (A. Gilyén)
- Quantum entanglement (Sz. Szalay)
- Spectroscopy and the structure of matter (K. Kamarás)
- Superconductivity (G. Kriza)
- Theoretical solid state physics (A. Virosztek)
- Theory of magnetism II. (A. Virosztek)
- Trends in materials science (Á. Gali)

College of Kecskemét

- ELI-ALPS related technologies (A. Czitrovszky, A. Nagy, D. Oszetzky, Sz. Kugler, A. Kerekes)

Óbuda University, Budapest

— Autonomous control of Philae (A. Balázs)
— Chemistry and Physics of Polymers (S. Pekker)

Pannon University, Veszprém

— Landing on a comet with Hungarian participation (A. Baksa, A. Balázs, Z. Pálos Pannon)

Semmelweis University, Budapest

— Networks and stability (I. Kovács, SE)
— Neuroinformatics, (L. Négyessy, Z. Somogyvári, L. Zalányi, F. Bazsó, Semmelweiss University, ELTE)

Szent István University Gödöllő

— Biophyics (Z. Szőkefalvi-Nagy, both in Hungarian and in English, two courses)
— Biophysics (I.F. Barna)

University of Debrecen

— Experimental Particle Physics (D. Horváth, University of Debrecen)

University of Miskolc

— The description of weak gravitational waves in general relativity (I. Rácz)

University of Pécs

— Biorobotics (J. Laczkó)
— Control theory (J. Füzi)
— Digital control (J. Füzi)
— Electronics (J. Füzi)
— Introduction to algebra and number theory (J. Laczkó)
— Linear algebra (J. Laczkó)
— Mathematical methods in Physics III. (B. Kollár)
— Mathematical methods in Physics IV. (P. Ádám)
— Neuro-biomechanical programming (J. Laczkó)
— Numerical methods (P. Ádám)
— Open quantum systems (P. Ádám)
— Optical measurement technique (A. Czitrovszky)
— Probability theory (P. Ádám)
— Resonant light-matter interaction (P. Ádám)
— Statistical physics (Szlachányi Kornél)
— Stochastic processes in the economy(P. Sinkovicz)
— Theoretical mechanics (Szlachányi Kornél)
— Theoretical physics III. (P. Ádám)

University of Szeged

— Applications of statistical physics (F. Iglói)
— Calculus for informatics students (G. Pusztai)
— Calculus for physics students (G. Pusztai)
— Disordered systems (F. Iglói)
— Introduction to the physics of laser plasmas (I. Földes)
— Introduction to statistical physics (F. Iglói)
— Introduction to the theory of Lie groups (G. Pusztai)
— Linear spaces and operators (G. Pusztai)
— Quantum integrability: from sigma models to AdS/CFT (J. Balog)
— Representations of topological groups (G. Pusztai)
— Statistical physics (F. Iglói)
— Strongly correlated electron systems (I. Hagymási).
— Theory of nonlinear processes in strong laser fields. Introduction to attophysics II. (S. Varró)
— Theory of open quantum systems (L. Diósi)

Laboratory practices and seminars
Eötvös Loránd University, Budapest

— Inner Structure of Compact Stars (G.G. Barnaföldi)
— Introduction to Gravitational Theory and High-Energy Physics (G.G. Barnaföldi, M. Vasúth)
— Electronics and Measurement Technology laboratory (G. Kiss et al)
— Experiments on liquid crystals (Á. Buka, N. Éber, T. Tóth-Katona)
— IT Tools for Research Work (Sz. M. Harangozó)
— IT Basics (Sz. M. Harangozó)
— Laboratory practice in solid state physics and materials science (M. Bokor)
— Laboratory practice - MHD (Z. Németh)
— Nuclear Techniques & X-ray Spectroscopy (Z. Németh)
— Phases of the Strongly Interacting Matter (P. Lévai)
— Particle and Nuclear Physics Detectors laboratory (G. Hamar, D. Varga)
— Particle and Nuclear Pysics seminar (D. Varga, M. Csanád)
— Physical chemistry laboratory practice (K. Neuróhr)
— Raman spectroscopy, part of the part of the Biophysics laboratory practice (M. Veres)
— Solar-terrestrial relation for astrophysics students (M. Tátrallyay)
— Solid-state physics seminar (J. Sólyom)

Budapest University of Technology and Economics

— Artificial polymers laboratory (D. Beke)
— Chemical and medical biological measurement technics (B. Sódor)
— Engineering practice (D. Beke, 2 semesters)
— General and inorganic chemistry laboratory, autumn semester, (Gy. Károlyházy)

- Inertial Confinement Fusion, part of the course Introduction to the fusion plasma physics (I. Földes)
- Infrared and Raman spectroscopy (K. Kamarás)
- Introductory physics (D. Szemes, on 2 faculties)
- Laboratory practice (M.A. Kedves, B. Raczkevi)
- Laboratory practice on experimental methods in materials science (B. Nagy)
- Laboratory practice on investigation methods in materials science (K. Tompa and M. Bokor)
- Medical biological computer practices (B. Sódor)
- Physics 1 (D. Szemes)
- Physics lab for physics BSc students (B. Somogyi)
- Polymer physics laboratory (D. Beke)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)
- Solving problems in physics: practice 1 (B. Somogyi, G. Thiering)
- Structure investigation methods in materials science (A. Len, L. Almásy)
- Thermodynamics (P. Ván)
- Variational methods in the basic laws of physics, (T.S. Biró)

College of Kecskemét

- Experiments on interferometry and light scattering (A. Nagy, A. Czitrovszky, D. Oszetzky, A. Kerekes)

Linköping University (Sweden)

- Quantum mechanics (Viktor Ivády)

University of Pécs

- Control theory seminar (J. Füzi)
- Electronics laboratory practice (J. Füzi)
- Modern Physics (practice, M.A. Pocsai)
- Numerical analysis (A. Kovács)

University of Szeged

- Calculus practical course (G. Pusztai)
- Digital laboratory (A. Barna)

IPP Prague

- Summer training course in experimental plasma physics (A. Bencze)

Diploma works
Eötvös Loránd University, Budapest

- Zs. Benkő: Causal analysis of action potential related micropotentials (Supervisor Z. Somogyvári)

- B. Cziráki: The application of noise filtering methods in analysing gravitational wave data, (Supervisor: I. Rácz)
- B. Csengeri: Investigation of flow patterns using digital image processing (BSc, Supervisor T. Börzsönyi)
- B.A. Fekete: Patterns generated by DC electric field in nematic liquid crystals (BSc, Supervisor N. Éber)
- V. Herczeg: Density functional theory study of spin state transitions in Fe(II)-based molecular systems (Supervisor: Gy. Vankó)
- J. Horváth: Investigation of fulleride anions by infrared spectroscopy (Supervisor: K. Kamarás)
- P. Magyar: Response functions of strongly coupled plasmas (Supervisor: Z. Donkó)
- B. Megyeri: Investigation of field theories with locally finite degrees of freedom (Supervisor: P. Vecsernyés)
- D.G. Nagy: Statistical model of the episodic memory (Supervisor: G. Orbán)
- M.A. Pocsai: Particle acceleration by lasers (MSc, Supervisor: I.F. Barna)
- B.M. Powell: Laser pulse selection and laser-matter interactions (BSc, Supervisor: I. Földes)
- T. Rakovszky: Localization and delocalization in quantum walks (BSc, J. Asbóth)
- P. Udvarhelyi: Spintronics at ambient temperature: investigation of the nitrogen-vacancy center by means of quantum-mechanical simulation (BSc, Supervisor: Á. Gali)
- L. Vanó: Edge plasma turbulence studies on MAST with beam emission spectroscopy (BSc, Supervisor: D. Dunai)
- L. Varga: Renovating the CMS pixel detector (Supervisor: V. Veszprémi)
- D. Vech: Investigation of planetary space weather effects at Venus (Supervisor: K. Szegő)

Budapest University of Technology and Economics

- P. Balla: The equation of motion method for spin systems with multipolar Hamiltonians (Supervisor: K. Penc)
- A. Czopf: Design of optical coupling system for the ASDEX Upgrade tokamak (Supervisor: S. Zoletnik)
- A. Csóré: Biomarkers and third generation solar cells: examination of semiconductor nanocrystals with modern computational methods (BSc, Supervisor: Á. Gali)
- G. Dósa, Study of ODS steels by time-of-flight neutron diffraction (Supervisor: L. Rosta)
- Gy. Károlyházy: Fabrication and analysis of SiC nanocrystals doped by metals (MSc, Supervisor: Á. Gali)
- R. Kovács: Thermodynamic conditions of wave propagation, dispersion and damping (Supervisor: P. Ván)
- D.Á. Major: Examination of reduction of silicon carbide nanoclusters (BSc, Supervisor: Á. Gali)
- D.Á. Major: Determination of pKa values for silicon carbide nanoclusters (BSc, Supervisor: Á. Gali)
- A. Szekeres: Modelling of thermodynamic systems, (Supervisor: P. Ván)
- M. Timár: Investigation of strongly correlated systems by renormalization methods (Supervisor: Ö. Legeza)

— P. Vermes: Measurement of self-diffusion coefficient of nickel by neutron reflectometric study of 62Ni/natNi multilayers (Supervisor: L. Bottyán)

University of Pécs

— G. Mogyorósi: Realization of non-classical quantum states of light by linear optical processes (MSc, P. Ádám)

University of Szeged

— Á. Galzó: Grouptheoretical methods in physics (Supervisor: G. Pusztai)
— I. Magashegyi: Lie theory and its applications (Supervisor: G. Pusztai)

University of Erlangen

— Di Zhang, Carrier-Envelope Phase Effect in Photoelectron Emission from Plasmonic Nanostructures (Supervisors: P. Dombi and P. Hommelhoff[*])

Ph.D students
Eötvös Loránd University, Budapest

— G. Barcza: Nonlocal density matrix renormalization group applied to strongly correlated systems (Supervisor: Ö. Legeza)
— D. Barta: Change of gravitational wave signals from compact binaries in interstellar medium (Supervisor: M. Vasúth)
— Gy. Bencédi: Investigation of the identified hadron spectra at high momentum (Supervisor: P. Lévai)
— D. Berényi: Strongly interacting matter (Supervisor: P. Lévai)
— G. Csire, Quasiparticle spectrum of superconductor-metal heterostructures (Supervisor B. Újfalussy)
— Z. Darázs, Quantum control with measurements (T. Kiss and A. Csordás)
— T. Demján: Investigation of semiconductor nanostructures by means of atomistic simulations (Supervisor: Á. Gali)
— M.M. Dolgos: Metastable structures in stratified systems (Supervisor L. Bottyán)
— A. Dombi: Quantum dynamics of atomic motion in multimode optical resonator fields (P. Domokos)
— G. Hamar: Experimental study of high momentum particle production in heavy ion collisions (Supervisors: P. Lévai and D. Varga)
— I. Hagymási, Heavy-fermion behaviour in the periodic Anderson model (Supervisor J. Sólyom)
— Sz.M. Harangozó: Nuclear effects at high transverse momenta in the CERN LHC's heavy-ion collisions (Supervisors: G.G. Barnaföldi, G. Papp)
— L. Holló: AdS/CFT correspondence, (Supervisor: Z. Bajnok)
— G. Homa: Quantum information and irreversibility (Supervisor: L. Diósi)
— G. Kiss: Microstructure gaseous particle detectors (Supervisor: D. Varga)
— J. Konczer: Integrable methods in the AdS/CFT correspondence (Supervisor: Z. Bajnok)

- B. Korbuly: Phase-field modeling of complex polycrystalline patterns (supervisor: L. Gránásy)
- G. Kónya: Many-body physics in cavity QED (P. Domokos)
- N. Laczai: Preparation and study of polycrystalline scintillator materials (Supervisor: L. Bencs)
- 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: Optimal integration of declarative and semantic memories (Supervisor: G. Orbán)
- F. J. Nemes: (Supervisors: M. Csanád and T. Csörgő)
- K. Németh: Chemical modification and optical spectroscopy of single-walled carbon nanotubes (Supervisor K. Kamarás)
- N. Német: Theory of hybrid systems formed by nanomechanical oscillator and superconducting qubit (Supervisor: L. Diósi)
- É. Oláh: Particle physics teaching in secondary school (within the Teacher's PhD program of ELTE, Supervisors D. Horváth and D. Varga)
- L. Oláh: Analysis of identified particles by ALICE HMPID (Supervisors: G. G. Barnaföldi, D. Varga)
- M. Pápai: Theoretical Characterization of Electronic States of Iron Complexes (Supervisor: Gy. Vankó)
- S. Pochybová: High energy quark and gluon jets in proton-proton and heavy ion collisions (Supervisor: P. Lévai)
- P. Pósfay: Application of functional renormalization group method in compact stars, (Supervisors: G.G. Barnaföldi, A. Jakovác)
- D. Réfy: Beam emission spectroscopy measurements to support understanding of H-mode in fusion plasmas (Supervisor S. Zoletnik)
- L. Rátkai: Dynamics of crystalline self-organization within continuum theory (supervisor: T. Pusztai)
- P. Salamon, Extraordinary properties of bent-core and rod-like nematic liquid crystals, (Supervisor: N. Éber)
- A. Ster: Electron-nucleus, proton-nucleus and nucleus-nucleus collisions at very high energies (Supervisors: B. Lörstad, L. Lönnblad (University of Lund, Sweden) and T. Csörgő)
- B. Szabó, Shear zones in dry granular materials (Supervisor: T. Börzsönyi)
- K. Szász: Identification of point defects in semiconductors by calculating the hyperfine tensor (Supervisor: Á. Gali)
- É. Tichy-Rács: Synthesis, crystallization and spectroscopic investigation of rare-earth alkali borate scintillator materials (Supervisor: K. Lengyel)
- R. Ünnep: Study of self-assembly functional nano particles by neutron scattering (Supervisor F. Mezei)
- M. Vargyas: Jet modification/narrowing in relativistic heavy ion collisions (Supervisor: J. Rak (University of Jyvascyla, Finnland), T. Csörgő),
- T. Verebélyi, NMR and DSC study of protein solutions (Supervisor K. Tompa)
- M. Verebélyiné Dósa: Planetary space weather around Venus (Supervisor: G. Erdős)

— A.J. Zsigmond: Study of high energy QCD matter in Pb+Pb and p+Pb collisions in the CMS experiment at the LHC (Supervisors: F. Siklér and G.I. Veres[*])
— S. Zsurzsa, Electrodeposited magnetic nanowires (Supervisor: I. Bakonyi)

Budapest University of Technology and Economics

— P. Balla, Optical properties of magnetic materials (Supervisor K. Penc)
— Á. Bácsi: Theoretical study of gapless low-dimensional systems: grapheme and the Luttinger model (Supervisor: A. Virosztek)
— D. Beke: Synthesis and analysis of SiC based nanoclusters (Supervisor: Á. Gali)
— G. Cseh: Investigation of transient processes in hot plasmas (G. Kocsis), BME
— D. Cserpán: Neural cells' current source density exploration based on sCSD analysis of experimental data and simulations (Supervisor: Z. Somogyvári, BME)
— M. Horváth: Generalized boltzman equation (Supervisors: T.S. Biró, A. Janovác) BME
— Gy. Károlyházy: Controlled formation of point defects in silicon carbide (Supervisor: Á. Gali)
— M. Lampert: Comparative study of plasma turbulence and zonal flows in various tokamaks (Supervisor S. Zoletnik)
— B. Nagy: Study of inverse proximity effect in ferromagnet/superconductor heterostructures (Supervisor: L. Bottyán, BME)
— J. Orbán: Investigation and development of signal processing electronics for position sensitive particle counters (Supervisors: L. Rosta and Cs. Sükösd)
— F. Podmaniczky: Dynamics of solidification, pattern and defect formation in phase-field crystal theories (supervisor: L. Gránásy)
— B. Somogyi: Ab initio study of semiconductor nanocrystals (Supervisor: Á. Gali)
— A. Szakál: Extension of applicability of atomic resolution neutron holography (Supervisor: L. Cser)
— J. Szalai: Development and associated thermo-mechanical analysis of diagnostic component of fusion powerplants (Supervisors, A. Piros and G. Veres, BME)
— D. Szemes: Dynamics of light-activated functional molecules studied with ultrafast spectroscopy (Supervisor: György Vankó, BME)
— G. Thiering: Investigation of semiconductor nanostructures by means of atomistic simulations (Supervisor: Á. Gali)
— B. Tál: Measurement of transient events in hot magnetized plasmas (Supervisor G. Veres)

Óbuda University, Budapest

— J. Nagy: Working out the on-board data acquisition system and on-board communications system of a small satellite making scientific measurements in the vicinity of Earth (Supervisor A. Molnár)
— Zs. Szekrényes: Study of complex nanostructures by infrared spectroscopy (Supervisor K. Kamarás)

Semmelweis University, Budapest

— M. Ashaber: Wiring functional tactile cortical representations, combined optical imaging, light- and electron microscopic track tracing studies in the primate somatosensory cortex (Supervisor: L. Négyessy)

— Zs. Benkő: Exploring causality for understanding dynamical behaviour of cortical areas based on multichannel electrode system measurements (Supervisor: Z. Somogyvári)

— P. Katona: Computer modelling of limb movements (Supervisor: J. Laczkó)

— E. Pálfi: The role of somatosensory cortical inhibition in tactile functions of primates (Supervisor: L. Négyessy)

Pázmány Péter Catholic University, Budapest

— B. Jákli, Control of biomechatronic robotic arm (Supervisor L. Négyessy)

— Á. Vály: Biomechanical modelling (Supervisor: J. Laczkó)

National University of Public Service

— P.G. Vizi: Micro- and nanorobots in military, space and security technics (Supervisor:)

University of Debrecen

— M. Bartók: Search for supersymmetry at the Large Hadron Collider (Supervisor: V. Veszprémi)

University of Szeged

— A. Barna, Investigation of contrast and stability of ultrashort KrF laser pulses (Supervisors: I. Földes and Z. Gingl)

— D. Haluszka, Nonlinear microscopy for Dermatology (Supervisor: R. Szipőcs)

— L. Himics, Nanocrystalline diamonds for advanced applications (Supervisor M. Koós)

— I. Rigó, Preparation and characterization of plasmonic diamond-gold nanostructures (Supervisor M. Veres, University of Szeged)

— 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)

University of Pécs

— M. Aladi: High harmonics generation in gases and clusters (Supervisor I. Földes)

— R. Bolla: Spectroscopy with high harmonics radiation (Supervisor I. Földes)

— V. Csajbók: Inducing ultrafast currents in dielectrics (Supervisor: P. Dombi)

— A. Kerekes: Aerosol deposition of drugs within human lung models, (Supervisor: A. Nagy)

— B. Kollár: Quantum information in quantum-optical networks (T. Kiss)

— A.Zs. Kovács: Collective and transport processes in Yukawa Systems (Supervisor: P. Hartmann)

— I. Márton: Ultrafast photoemission from plasmonic structures (Supervisor: P. Dombi)

— G. Mogyorósi: Realization of unphysical processes for qubit systems (P. Ádám)

— E. Molnár: Conditional realization of non-classical quantum states of light by linear optical processes (P. Ádám)

— M. Mravcsik: Biological movement control and man-machine connection (Supervisor: J. Laczkó)

⸺ B. Nagy: Controlling photoelectrons on the nanoscale with plasmonic nanoparticles (Supervisor: P. Dombi)

⸺ M.A. Pocsai: Ionization studies in Rb vapor (Supervisor: I.F. Barna)

⸺ P. Sinkovicz: Exotic magnetic phases and quantum phase transitions in ultracold atoms (G. Szirmai)

⸺ Á. Varga: Quantum state discrimination (P. Ádám)

⸺ K. Varga-Umbrich: Study of coherent excitation and ionization of alkali atoms by strong laser pulses. (Supervisor: M.A. Kedves)

Szent István University Gödöllő

⸺ Z. László, Magnetic bearings for neutron beam phase space tailoring equipment (Supervisors J. Nagy, J. Füzi)

University of Granada, Spain

⸺ E. López Centella: Weak (multiplier) Hopf algebras (Supervisors: J. Gómez Torrecillas, G. Böhm)

University of Linköping

⸺ V. Ivády: Investigation of point defects for quantum bit applications (Supervisor: Á. Gali)

Dissertations

Ph.D

Á. Bácsi: Theoretical study of gapless low-dimensional systems: grapheme and the Luttinger model, 108p. 2014

K. Berkesi, Radioaktív kontamináció vizsgálata sima és megnövelt felületű nemesfém elektródokon (Investigation of radioactive contamination on smooth and rough noble metal electrodes), 110 p. 2013

K. György, Atomabszorpciós spektrometriai kutatások optikai egykristályok vizsgálatára (Atomic absorption spectrometric studies for the analysis of optical single crystals), 110p, 2013

I. Hagymási, Heavy-fermion behaviour in the periodic Anderson model, 104p, 2014

Sz. Kugler, The determination of nitrogen exchange between the atmosphere and lake Balaton

L. Radnay: Investigation of steel structure critical stiffness: strengthening by posttensioning and stressed skin diaphragm design, 2014

P. Salamon, Extraordinary properties of bent-core and rod-like nematic liquid crystals, 147p. 2013

D.Sc

T. Pusztai: A polikristályos megszilárdulás fázismező modellje - nukleáció és növekedés (Phase-field modeling of polycrystalline solidification - nucleation and growth), 104p, 2014.

F. Siklér, Új kiértékelési módszerek és alkalmazásuk az erős kölcsönhatás vizsgálatában (New analysis methods and their application in the study of the strong interaction), 199p. 2014.

Memberships

A. Arató	— National contact of the Association for the Advancement of Assistive Technology in Europe (AAATE)
	— Program committee member of the International Conference on Computers Helping People with Special Needs (ICCHP)
P. Ádám	— Member of the Laser Physics Committee of MTA.
K. Bajnok	— Member of the Archeomerical Subcommittee of Geochemical and Mineralogical Scientific Committee of the H.A.S.
Z. Bajnok	— Member of the ESF Holograv Steering Committee
	— Member of the ESF Holograv Executing Committee
	— Member of the Particle Physics Committee of the H.A.S.
I. Bakonyi	— Member of the Solid State Physics Committee of MTA (2011-2014)
	— Member of the Editorial Advisory Board (from 2005), Journal of Materials Science and Technology (Bulgaria, Sofia)
	— Member of the European Board (from 2006), European Academy of Surface Technology (EAST)
	— Member, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
Judit Balogh	— Int. Board on the Application of the Mössbauer Effect (IBAME), 2012-2017
József Balogh	— Member of the Particle Physics Committee of the H.A.S
G.G. Barnaföldi	— Editor of The European Physics Journal A: Hadrons and Nuclei Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
	— Member of Physics PhD School at Eötvös Loránd University, Budapest
	— Hungarian representative, Board Member of the CERN LHC ALICE Collaboration,
	— Group Leader of the Hungarian ALICE Group
	— Member of the Eötvös Loránd Physical Society (ELFT)
	— Member of the European Physical Society (EPS)
	— Hungarian representative, rapporteur, WG2 QCD Topic Leader of the New Compstar COST MP1304 action (2013-2017)
	— IAC member of the ISOTDAQ International School on Trigger and Data Acquisition
	— LOC member of the ISOTDAQ 2014 International School on Trigger and Data Acquisition 2014
	— LOC member of the 7th FIKUT – Workshop of Young Researchers in Astronomy and Astrophysics 2014, Budapest
	— LOC member of the CompStar 2015 Meeting, Budapest
	— IAC member of the International Conference of the High-pT Physics for the RHIC/LHC Era
	— Member of the general assembly of the Hungarian Academy of Sciences

F. Bazsó	— Programme Committee Member, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
L. Bencs	— Editorial Board member of ISRN Analytical Chemistry
	— Member of the Work Committee for Environmental Chemistry of MTA
T.S. Biró	— Vice director of MTA Wigner FK RMI (Sept.01.2013-)
	— Editor-in-Chief (theory) (Oct.01.2013-) of the European Physical Journal A: Hadrons and Nuclei;
	— Member of IAC for Sigma Phi 2014 (held in Rhodos, Greece)
	— Member of International Advisory Board for Strangeness in Quark Matter (SQM2015 Dubna, Russia);
	— Member of the Physics PhD School at TU Budapest (BME)
	— Member of the Physics PhD School at Eötvös University (ELTE) Budapest
	— External member of the ELTE TTK PhD Council
	— Member of the Nuclear Physics Committee at the Hungarian Academy of Science
	— Member of the Eötvös Loránd Physical Society (ELFT),
	— Chairman of the Zimányi Foundation for Physics,
	— Editor of the Wigner Yearbook 2014,
	— IAC member of the Sigma Phi 2014, Rhodos
	— IAC member of the SQM2015, Dubna
	— LOC member of the Zimányi School 2014
L. Bottyán	— Member of MLZ Review Panel Magnetism and Spectroscopy, Elastic Application
G. Böhm	— Member of Expert Panel W&T1: Mathematical Sciences, Fonds Wetenschappelijk Onderzoek – Vlaanderen (Scientific Research Fund – Flanders, 2012 -- 2018)
Á. Buka	— Electronic-Liquid Crystal Communications, Editorial Board
	— International Liquid Crystal Conference, International Advisory Board
	— Solid State Physics Committee of MTA, Member
G. Cseh	— Member of the Hungarian Nuclear Society
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L. Csernai	— Member of the Editorial Board, International Journal of Modern Physics E - Nuclear Physics
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T. Csörgő	— Academia Europaea (London), elected member (2011-)
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— Member, physics PhD School, ELTE, Budapest
— Member, Institutional Board, PHENIX Experiment, BNL
— Member, Executive Council, TOTEM Experiment, CERN LHC
— Member, Editorial Board, TOTEM Experiment, CERN LHC
— Member, CERN LHC Resource Review Board
— Member, International Advisory Committee, WPCF 2013 Conference, Acireale, Italy
— Member, International Advisory Committee, ISMD 2013 Conference, Chicago, USA
— Principal Investigator, PHENIX - Hungary sub-collaboration (2003-2013)
— Principal Investigator, TOTEM - Hungary sub-collaboration
— Member of the Editorial Board, TOTEM experiment at CERN LHC
— Member, Section Committee for Physics and Engineering Sciences, Academia Europaea (London)

A. Czitrovszky
— Chairman of the Working Group Instrumentation in EAA
— Member of the Board of International Aerosol Association
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— President of the Hungarian Aerosol Society
— Member of the ELI_ALPS Scientific Advisory Committee
— President of the Hungarian Branch of the European Optical Society
— Head of the Optical Chapter of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology (Budapest)
— Member of the Editorial Board of "Fizikai Szemle"
— Chairman of the Optical Chapter of Roland Eötvös Physical Society
— Chairman of the Committee for the Lasers Physics and Spectroscopy in MTA
— Founding member of Ph.D. school at the University of Pécs

G. Debreczeni
— Computing Coordinator of the Virgo Collaboration (Virgo CC)
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— Member and co-chair of the Ligo - Virgo Joint Computing Comitee (Ligo - Virgo JCC)

L. Diósi
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— Member of the Comitee of Laser Physics of the Hungarian Acedemy of Sciences
— International Conference on Photonic, Electronic and Atomic Collisions, ICPEAC Program Committee Member
— Conference on Lasers and Electro-optics (CLEO Europe 2015), Program Committee Member

	— SPIE Optics and Optoelectronics Conference (Prague 2015), Program Committee Member
P. Domokos	— Editor of the European Physical Journal D
	— Liaison Committee representative of the International Union of Pure and Applied Physics (IUPAP)
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Z. Donkó	— Member of International Scientific Committee, Conference series "Symposium of the Phenomena in Ionized Gases", from 2006
	— Member of International Advisory Board, Conference series "Strongly Coupled Coulomb Systems", 2007-
	— Member of International Scientific Committee, Conference series "Symposium on Application of Plasma Processes," from 2008
	— Member of the Laser Physics Committee of MTA
	— Member of OTKA Council on Natural Sciences and Engineering
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N. Éber	— Member of The Open Crystallography Journal, Editorial Board
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	— Member of the Editorial and Programme Advisory Board of the Springer Complexity publishing program
	— Member of the Executive Committee of the European Neural Network Society
	— Member of the Editorial Board of the Journal of Applied System Studies
	— Member of the Editorial Board of the Cognitive Neurodynamics
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G. Faigel	— XFEL In-kind Review Committee member
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	— Member of EPS and ELFT, also of the Laser Physics Committee of the Roland Eötvös Physical Society
	— LASERLAB Europe: Users' Representative
	— General Assembly member, LASERLAB Europe
	— Member of COST Action MP 1208, management committee
	— Substitute member of the COST Action MP 1203, management committee
	— Member of the Euratom, Inertial Fusion Energy Working Group
T. Fülöp	— Member of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)
J. Füzi	— International Scientific Advisory Council of BNC (Budapest Neutron Centre)
	— Editorial Board Member, Pollack Periodica
	— Editor, IEEE Transactions on Magnetics, SMM21 Budapest issue
L. Gránásy	— Member of the ESA Topical Team "Solidification of Containerless Undercooled Melts", SOL – EML
	— Member of The Minerals, Metals, and Materials Society, USA
	— Solid State Physics Committee of MTA
	— Mathematics and Science Committee of AKT
	— Elected member of the Academia Europae (London)
P. Hartmann	— Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" Member of International Scientific Committee, 2008-2014
D. Horváth	— Member of the Editorial Board of "Fizika Szemle"; member of the CMS Publication Committee; member of the "M-T Szakbizottság", "INKP Kuratórium", "MTA Fiz. Osztály", "MTA Részecskefizikai Bizottság"
F. Iglói	— Coeditor – Europhysics Letters
J. Janszky	— Member of the Laser Physics Committee of MTA
K. Kamarás	— Editorial Board Member, European Physical Journal B

Z. Kis	— Member of the Editorial Board of the Physical Review A
T. Kiss	— Member of the Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP) — Member of the Management Committee of COST Action MP1006 — Member of the Laser Physics Committee of ELFT
G. Kocsis	— Member of the Hungarian Nuclear Society — Member of the Nukleon Editorial Board — Member of the EUROfusion JET CDT2 Project Board — Member of the EUROfusion S1 Project Board — Member of the Roland Eötvös Physical Society
L. Kovács	— Member of the Hungarian National Committee, International Union of Crystallography — Member of the International Advisory Committee of EURODIM and ICDIM Conference series — Member of the Program Committee of the OMEE Conference series — Member of the Laser Physics Committee of H.A.S.
P. Kovács	— Member of the general assembly of the Hungarian Academy of Sciences
G. Kriza	— Member of the Solid State Physics Committee of MTA (from 2007) — Member of Ph.D. School of Physics, BME (from 2008) — Member of Bolyai Fellowship Board, MTA (from 2010) — Member of MTA Domus Hungarica Scientiarum et Artium Fellowship Board (from 2008)
N. Kroó	— Chair of the Governing Council of the Hungarian Research Infrastructure Program — Chair of the Rátz High School Prize — Member of the Hungarian UNESCO Committee — Chair of the Dennis Gabor International Prize Committee — Chairman of the Research Infrastructure Expert Group of ERA (EC) — Member of the High Level Expert Group on Digital Libraries and Scientific Publications (EC) — Member (former Chair) of the Section of Physical and Engineering Sciences of Academia Europaea — Member of the Advisory Group on ESOF — Member of the ELI_ALPS Scientific Advisory Committee — Editorial Board, Laser Physics Letters
K. Kutasi	— Member of International Scientific Committee, Conference series "International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment," from 2006 — Member of International Scientific Committee, Conference series of "Central European Symposium on Plasma Chemistry" 2013-
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	— Member of the CERN Council
	— Member of the ESFRI (European Strategy Forum on Research Infrastructure)
	— Member of the Committee on Research Infrastructure.
	— Member of the Committee on Nuclear Physics.
	— Member of the Committee on Particle Physics.
	— Member of the IAC of the Quark Matter 2012 Conference (Washington, 2012. 08.13-18)
	— Member of the IAC of the 7th International Workshop on High-pT Physics at LHC, (Frankfurt, 2012.03.26-30)
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B. Lukács	— Member of the Astronomical and Space Research Committee of the H.A.S.
F. Mezei	— Chairman of the Physical Society Publication Committe
	— American Physical Society
	— Academia Europaea, London
	— European Neutron Scattering Association (ENSA) Committee
	— Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA
	— International Council for Scientific and Technical Information, University of California, San Diego, USA
D.L. Nagy	— Common Coordination Committee of the Hungarian Academy of Sciences and the Joint Institute for Nuclear Research, Dubna, MTA Representative
	— Joint Institute for Nuclear Research, Dubna, Scientific Council, Member
	— European XFEL, Council, Member
	— FP7 Research Infrastructures Programme Committee, expert
	— International Board of the Applications of the Mössbauer Effect, Chair
	— European Synchrotron Radiation Facility, Consortium CENTRALSYNC, Steering Committee, Member
	— Hyperfine Interactions, Editorial Board, Member
	— International Union of Pure and Applied Physics (IUPAP), Commission on Physics for Development (C13), Member
	— European Physical Society, Council, Member
	— European Strategy Forum on Research Infrastructures, Working Group on Regional Issues, Member

	— European Science Foundation, Member Organisation Forum on Research Infrastructures, Member
	— Program Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research, Dubna, Member
J.Z. Nagy	— Member of the MANT (Hungarian Astronautical Society)
Z. Németh	— Member of the Materials Sicence Work Committee of the Hungarian Academy of Sciences
G. Pásztor	— Member of the Plenary European Committee for Future Accelerators (ECFA)
L. Péter	— Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
	— Representative for Hungary, International Society of Electrochemistry (2011-2016)
	— Council Member of Graduate School of Chemistry, ELTE (2009-)
	— Editor for Electrochemistry (Open Chemistry; formerly Central European Journal of Chemistry; 2009-)
	— Key Reader (Metallurgical and Materials Transactions E, 2014-)
K. Polgár	— Hungarian Advisor of the International Organization for Crystal Growth
	— Member of the International Advisory Committee of the 17th Intern. Conference on Crystal Growth and Epitaxy (ICCGE-17)
	— Member of the International Advisory Board of the Fifth European Conference on Crystal Growth (ECCG5)
L. Rosta	— International Scientific Advisory Council of BNC (Budapest Neutron Centre)
	— European Spallation Source, Steering Committee
	— Hungarian ESS Committee
F. Siklér	— Member of the SPS and PS experiments Committee (SPSC)
	— Institutional representative at the CMS Collaboration Board
	— Member of the CMS Publication Committee, Heavy Ions editorial board
	— Member and secretary of the Particle Phyisics Scientific Committee of the HAS; representative at the general assembly of the HAS
E. Somfai	— IOP member
	— Member of the American Physics Society
J. Sólyom	— Chairman of the Physics Section of the Hungarian Academy of Sciences
Zs. Sörlei	— Member of the Committee of Laser Physics of the Hungarian Academy of Sciences
L. Szabados	— Scientific advisory panel of the journal Classical and Quantum Gravity
T. Szabolics	— Member of the Hungarian Nuclear Society
S. Szalai	— Member of Hungarian Space Research Council
	— Member of ARTEMIS-H steering
	— Member of Rosetta Lander steering

	— Member of the MANT (Hungarian Astronautical Society)
V. Szalay	— CMST COST Action CM1405 Management Committee member
K. Szegő	— Member of Committee on Astronomy and Space Physics of MTA — Member of IAA — Guest Editor of Space Science Reviews
T. Szepesi	— Member of the Hungarian Nuclear Society
E. Szilágyi	— International Committee of the Conference series of Ion Beam Analysis, member
R. Szipőcs	— Member of Optical Society of America
Z. Szőkefalvi-Nagy	— Member of the Editorial Board, International Journal of PIXE — Member of the International Honorary Committee, PIXE
K. Tompa	— Member of the Natural Science Committee of the Hungarian Scholarship Board (2011-2013)
Gy. Török	— Member of IAEA JRC-1575 — Member of JRC-NET
B. Ujfalussy	— President of the Overseeing Committee of Loránd Eötvös Physical society — Secretary of the Materials Science Group of Loránd Eötvös Physical society — Member of the Solid State Physics committee of the HAS
G. Vankó	— Member of the Committee on Atomic and Molecular Physics and Spectroscopy, MTA — Secretary of the Hungarian Synchrotron Committee, MTA — Management Committee, EU COST Action MP1203 Advanced X-ray spatial and temporal metrology
L.K. Varga	— Member of the International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM) — Member of Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)
S.Varró	— Member of the Commitee of Laser Physics of the Hungarian Acedemy of Sciences — Member of the Committee of the Quantumelectronics Division of the Lóránd Eötvös Physical Society
P. Ván	— Editor of the Continuum Mechanics and Thermodynamics, Springer, — Secretary of the Society for the Unity of Science and Technology — Scientific Advisory Board member of JETC'15 (Joint European Thermodynamics Conference,) — Member of the REPS (Roland Eötvös Physical Society) — Member of the Physics PhD School at TU Budapest (BME)
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 I Upgrade Management Board
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
S. Zoletnik	⸺ European Expert in the EU-Korea fusion collaboration committee;
	⸺ International Tokamak Physics Activities (ITPA) "Diagnostics Topical Group" EU representative
	⸺ EURATOM Science and Technology Advisory Committee (STAC), deputy chair
	⸺ MAST Programme Advisory Committee, Culham, UK
	⸺ International Board of Advisors of the Institute of Plasma Physics, Prague
	⸺ Governing Board of Fusion for Energy, Barcelona, Spain
	⸺ EURATOM Scientific and Technical Committee (STC)
	⸺ Editorial Board of Plasma Physics and Controlled Fusion, IOP
	⸺ International Tokamak Physics Activities (ITPA) diagnostic topical group vice chair

Conferences

"ISOTDAQ 2014", 28 January-5 February 2014, Wigner Data Center

The ISOTDAQ 2014 is the fifth of a series of International Schools dedicated to introduce MSc and PhD students to the "arts and crafts" of triggering and acquiring data for physics experiments. The main aim of the school is to provide an overview of the basic instruments and methodologies used in high energy physics, spanning from small experiences in lab to the very large LHC experiments, spotting the main building blocks as well as the different choises and architectures at different levels of complexity. About half of the school time will be dedicated to laboratory exercises where the students are exposed to most of the techniques described in the lectures. The school was held in English and will have 52 international students, selected according to their CV and a recommendation letter from one of their advisor. Teaching were based on the knowledge of about 20 professionals from all over the world.

"The Future of Many-core Computing in Science – GPU Day 2014, 29 May 2014, Wigner Data Center" MTA Wigner RCP,

A usual 1-day workshop, which takes place at the Wigner Data Center, with about 60-80 participant. It aims to teach student for GPU coding and parallel computing.

"Zagreb – Budapest Meetup 2014 for ALICE" 24 April 2014, Zagreb, Croatia,

The workshop is a bilateral, half-yearly meeting connects the R&D activity of the two ALICE Groups at Budapest and Zagreb.

"Wigner – CCNU Mini Workshop 2014", 7-8 April, MTA Wigner RCP, Budapest

The workshop is a bilateral, yearly meeting connects the activity of the theory groups in Budapest and Wuhan Central China Normal University.

"7th FIKUT – Workshop of Young Researchers in Astronomy and Astrophysics 2014", 17-19 September, Wigner Data Center

The conference is a great opportunity for young PostDoc researchers and PhD students working in astronomy, astrophysics and related topics to present their results. Each sessions will be introduced by a review talk presented by internationally recognized experts of the given topic. In 2014 the main topic was the large databases and Big Data science related to astronomy and astrophysics.

"WPCF 2014: 10th Workshop on Particle Correlations and Femtoscopy", Gyöngyös, Hungary, 25-29 Aug 2014

This conference was organized by a Wigner, ELTE and KRF joint project. It was chaired by T. Csörgő (Wigner), co-chair was T. Novák (KRF) and M. Csanád (ELTE) acted as a conference secretary. WPCF 2014 took place in the main building of the Károly Róbert University College in Gyöngyös, Hungary. The conference attracted 85 participants from 23 countries from 4 continents (Asia, Europa, North- and South-America), we have listened to 73 talks in 5 days. The scientific program was finalized with the help of 14 international conveners and the general structure of the meeting was shaped by 25 members of the International Advisory Committee. We had many (37) young participants and many VIP's including a

Nobel Laureate (presented his talk on skype due to travel difficulties), among others four members of Academia Europaea, the president of the Polish Academy of Arts and Sciences, and the spokesperson (scientific leader) of the CERN LHC experiment TOTEM. The meeting, in particular the participation of students without a PhD and participants from Ukraine (both Kiev and TransCarpathian Regions) were partially supported by 12 sponsors. The web-page of the meeting is archived at http://wpcf2014.karolyrobert.hu/

"Zimányi 2014: 14th Zimányi Winter School on Relativistic Heavy Ion Collisions", Budapest, Hungary, 1-5 December 2014

This conference was organized as an ELTE and Wigner joint project. It was chaired by M. Csanád (ELTE), co-chair was P. Kovács (Wigner) and T. Csörgő (Wigner) acted as a honorary chair. The Zimányi Schools traditionally take place in the building III of Wigner RCP and at the North Building of the ELTE Campus, in Budapest, Hungary. However, in December 2014 the Wigner Campus was a site with catastrophic weather conditions and unforeseen, emergency close-downs, a new venue included the main building of the Hungarian Academy of Sciences. Among exceptional weather conditions, M. Csanád, chair of Zimányi 2014, demonstrated his exceptional organization skills and, with the help of P. Lévai and other co-organizers including T. Csörgő and P. Kovács, we brought the meeting to a successful conclusion.   The Zimanyi 2014 School attracted 80 participants from 16 countries, including 40 students. During the 5 days of the meeting we listened to 63 talks grouped into 16 sections. Due to the exceptionally bad weather conditions, 10 students ended up in an emergency shelter provided by the Hungarian Disaster Protection Authorities and we had to relocate the foreseen sites 6 different times. The meeting, in particular the participation of students without a PhD, were partially supported by 4 sponsors: ELTE, NEFIM, OTKA, and Wigner RCP.

The web-page of the meeting is archived at http://zimanyischool.kfki.hu/14/

Finite-size technology in low dimensional quantum systems workshop, Budapest, 16-27 June 2014 and Integrability in low dimensional quantum systems conference, Tihany, 30 June - 4 July, 2014

This workshop is the continuation of the previous programs I, II, III, IV, V, VI with the same title and aims to discuss ideas and collaborate among the invited participants on the aspects of

- Solvable lattice models and integrable systems

- Bulk, boundary and defect conformal and quantum field theories

- Integrability in the AdS/CFT correspondence

The workshop venue was the Physics Building of the Eötvös University.

The workshop was followed by a conference Integrability in Low Dimensional Quantum Systems in Tihany between 30 June - 4 July of 2014 with the same topic. All over the program lasted for three weeks with 38 foreigner and 13 Hungarian participants.

Workshop "Spacetime-Matter-Quantum Mechanics --- News on Missing Links", 15-29 Sept, 2014 (Castiglioncello)

Following DICE2002, DICE2004, DICE2006, DICE2008, DICE2010, and DICE2012 this workshop addressed researchers in the fields of fundamental interactions, cosmology, general relativity, and quantum mechanics.

JCNS FZ-Jülich – BNC-Wigner Reflectometry Workshop, 22 December 2014

The mini workshop was organized as a joint scientific meeting of JCNS and Wigner RC to prepare for a common (German-French-Hungarian) proposal to build a polarized beam neutron reflectometer "Heritage" at ESS, Lund, Sweden. (15 attendees)

CETS 2014 – 8TH CENTRAL EUROPEAN TRAINING SCHOOL on neutron techniques

Participation in the program with lectures and hands-on practices (http://www.kfki.hu/cets/) (20+ attendees)

Workshop - KSTAR Workshop, 18. 01. 2014. - 19. 01. 2014

The workshop was organized by the BES research group of the Wigner RCP. The main goal of the workshop was to summarize the results of the 2013 measurement campaign on KSTAR and to explore and discuss the main upgrade possibilities and goals for the 2014 measurement campaign.

Workshop - Python applications in fusion, 04. 11. 2014.

The workshop was organized jointly by the Wigner RCP and the BME NTI supported by the Hungarian Nuclear Society. It covered a wide scope of programming techniques, connection of programming languages and fusion applications of python.

International Conference and Workshop on Theoretical Chemistry, "New wavefunction methods and entanglement optimizations in quantum chemistry" 18 - 21 February 2014, Mariapfarr, Austria

The conference was organized by Ö. Legeza and A. Sax. The four-day event which was attended by approx. 65 scientists, boosted the cooperation between researchers from quantum physics and quantum chemistry. (http://tagung-theoretische-chemie.uni-graz.at/en/past-workshops/workshop-2014/)

Annual Fall School of the Material Science group of the Roland Eötvös Physical Society "Material Science in Energetics", Mátrafüred, 8-10 October 2014

"Symposium of the Network of Hungarian Mössbauer Laboratories", Budapest, 7-8 November, 2014

The conference was organized by our group in cooperation with the Eötvös Loránd University. The conference took place in the seminar room of Institute for Solid State Physics and Optics at the Wigner RCP of the Hungarian Academy of Sciences. Guests arrived from Hungary, Germany, Austria, Chech Republic and Slovakia. The two-day meeting was

attended by 38 scientists. The authors presented their newest results in the field of materials science using the method of Mössbauer spectroscopy. The presentations can be viewed at the homepage: http://www.szfki.hu/~baloghj/SNHML2014/index.htm

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. We have started this series by the talk of Beatrix Hiesmayr, from Vienna, who informed us about correspondences between elementary particle physics problems, related to the missing of antimatter in the observed Universe on the one hand and on quantum cryptography on the other hand, on October 21st. This was followed by a talk by Laszlo Veisz from MPI Garching about contemporary, fusion related plasma research on December 18th.

The starting talk for 2015 has been given by Mate Lengyel from Cambridge University about computational neuroscience achievments on the research of spatial orientation of mammals, mainly rats, due to learning in hippocampal neural networks. We still have plans to continue this series by inviting people like Joachim Burgdörfer from Vienna (atomic physics), Ludwig Fadeev from Moscow (mathematical and particle physics) and David Bekenstein from Tel Aviv (cosmology and gravity).

And perhaps more, including the topic of imaginary rarefaction index related phenomena in electronics.

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

http://zimanyischool.kfki.hu/14/agenda

Wigner RCP RMI Seminars

17-01-2014   Ben-Wei Zhang (Central China Normal University, Wuhan): Jet observables in high-energy nuclear collisions

28-01-2014   Dr. Jee Hyun Choi: Functional brain mapping in mice and its application to neuroscience (Biophysics seminar)

29-01-2014   Dr. Attila Gulyás: Egészséges és patológiás aktivitásmintázatok in vitro hippoampusz szeletekben: hogyan generálhat egy hálózat többféle dinamikát? (Healthy and pathologic activity patterns in in vitro hippothalamyc slices: how can a network generate multiple dynamics? Biophysics seminar)

21-02-2014   Gergely Székely (Rényi Institute): Egy axiomatikus út a speciális relativitáselmélettől az általános relativitáselméletig (An axiomatic way from special relativity theory to general relativity theory)

07-03-2014   Ivica Smolić (University of Zagreb): Elusive Effects of Gravitational Chern-Simons Terms

28-03-2014   Ines Aniceto (University of Lisbon) : Resurgent Analysis in Quantum Theories: Perturbative Theory and Beyond

04-04-2014   Simon Ruijsenaars (Leeds University): A recursive construction of joint eigenfunctions for the N commuting hyperbolic Calogero-Moser Hamiltonians

11-04-2014   Gábor Etesi (BME): Gravity as a four dimensional algebraic quantum field theory

09-05-2014   Shen Keming (CCNU Wuhan): The non-extensivity of the Quark-Gluon Plasma and the meaning of the parameter q

16-05-2014   Zoltán Somogyvári (Wigner RCP): Determination of temporal structure of causal effects in time series

30-05-2014   Antonio Ortiz Velazques (UNA, Mexico): Disentangling the soft and hard components of the pp interactions

20-06-2014   János Balog (Wigner RCP) : Relativisztikus pont-mechanika (Relativistic point mechanics)

27-06-2014   Jose Senovilla (Basque Country University UPV/EHU, Bilbao): What is the surface of a Black Hole?

29-08-2014   Barak Kol (Hebrew University, Jerusalem): The effective field theory approach to the two body problem in Einstein's gravity

14-10-2014   Anja Habersetzer (Goethe-Universität, Frankfurt am Main): Tau Vector and Axial Vector Spectral Functions in the Extended Linear Sigma Model

31-10-2014   János Polonyi (Université de Strasbourg): Disszipatív erők elektrodinamikában és ideális gázokban (Dissipative forces in electrodynamics and in ideal gases)

10-11-2014   Kamel Ourabah (University of Algiers): On the Tsallis statistical mechanics approach to the Thomas - Fermi model: Application to quantum plasmas

14-11-2014   Istvan Racz (Wigner Research Centre): The degrees of freedom in general relativity

11-12-2014   Andrew Lowe (Wigner ALICE Group): Quark/gluon jet tagging for ALICE: Machine learning for hadron physics using R

Wigner RCP SZFI Seminars

07-01-2014   Kata Berkesi (Wigner RCP): Radioaktív kontamináció vizsgálata sima és megnövelt felületû nemesfém elektródokon (Investigation of radioactive contamination on precious metal electrodes with both smooth and enhanced surface)

09-01-2014   Imre Hagymási (Wigner RCP): Nehézfermionos és vegyes valenciájú viselkedés kiterjesztett periodikus Anderson-modellekben (Heavy-fermionic and mixed-valence behaviour in extended periodic Anderson models)

14-01-2014   Péter Hartmann (Wigner RCP): Szédítõ porszemcsék, avagy hogyan mérjünk 3000 Tesla-n (Dizzying dust particles,or how to measure at 3000 Tesla)

21-01-2014   Edit Szilágyi (Wigner RCP): Nanostruktúrák vizsgálata ionnyalábokkal (Investigation of nanostructures with ion beams)

21-01-2014   David Dasenbrook (Université de Genève, Switzerland): Electron waiting times in quantum-coherent conductors

28-01-2014   Sándor Varró (Wigner RCP): Extrém elektromágneses hullámok kvantumos tulajdonságai (Quantum properties of extreme electromagnetic waves)

11-02-2014   Gyula Faigel (Wigner RCP): A 2013 évi tudományos teljesítményrõl szóló ismertetés, vagy ami elmaradt a karácsonyi összejövetelen (Review of the scientific performance in 2013, or what was cancelled at the Christmas party)

18-02-2014   Márton Kanász-Nagy (BME): Theory of confinement-induced interlayer molecular resonances

20-02-2014   Jannik Meyer (University of Vienna): Exploring low-dimensional materials by high-resolution microscopy

25-02-2014   András Vukics (Wigner RCP): Az A-négyzet probléma eliminálása a rezonátoros kvantumelektrodinamikából (Eliminating the A-square problem from cavity quantum electrodynamics)

04-03-2014	Zsolt Szabó (BME): Ektromágneses metaanyagok és alkalmazásaik (Electromagnetic metamaterials and their applications)
11-03-2014	János Asbóth (Wigner RCP): Chiral symmetry and Majorana fermions in periodically driven quantum wires
25-03-2014	András Sütõ (Wigner RCP): Galilei-invariancia korlátos kvantumrendszerekben (Galilei invariance in confined quantum systems)
01-04-2014	László Péter (Wigner RCP): Amikor lyuk van a csövön, csak nem ott, ahol kéne (When there is a hole on the tube, just not where it should be)
02-04-2014	Gergely Barcza (Wigner RCP): Nemlokális sûrûségmátrixos renormálásicsoport-algoritmus alkalmazása erõsen korrelált rendszerekre (Application of non-local density matrix renormalization group algorithm on strongly correlated systems)
08-04-2014	Kálmán Tompa (Wigner RCP): Fehérjemolekula modellek és a valóság (Protein models and the reality)
15-04-2014	Anikó Zsuzsa Kovács (Wigner RCP): Dinamikus viszkozitás 2D Yukawa rendszerekben (Dynamic viscosity in 2D Yukawa systems)
22-04-2014	Krisztián Szász (Wigner RCP): Egy potenciális kvantumbit: a foszfor-vakancia pár (A potential qubit: the phosphorus-vacancy pair)
22-04-2014	Dimitrios Charalambidis (FORTH Kreta and ELI scientific director): Non-linear processes in the XUV spectral region: An advanced tool for attosecond pulse metrology and applications
23-04-2014	Róbert Szipőcs (Wigner RCP): Részecskegyorsítás femtoszekundumos szállézer rendszerrel - az ICAN project (Particle acceleration by a femtosecond fiber laser system – the ICAN project)
29-04-2014	István Kovács (Wigner RCP): Rendezetlen kvantum mágnesek összefonódási entrópiája (The entanglement entropy of disordered quantum magnets)
06-05-2014	Sándor Varró (Wigner RCP): Haar Alfréd fizikai matematikája (The physical mathematics of Alfred Haar)
13-05-2014	Tamás Verebélyi (Wigner RCP): Fehérjék szerkezetének vizsgálata a rendezettség ill. rendezetlenség szempontjából széles jelû 1H-NMR és DSC módszerekkel (Lizozim, Növényi stresszfehérjék) (Investigation of the structure of proteins with respect to order-disorder by broad linewidth 1H NMR and DSC methods (Lysosyme, plant stress proteins))
15-05-2014	Attila Szállás (Wigner RCP): Ponthibák vizsgálata AlN félvezetõ kerámiában (Point defects in AlN semiconductor ceramics)
20-05-2014	András Dombi (Wigner RCP): Optical bistability in quantum systems
23-05-2014	Viktor Zólyomi (Wigner RCP): Grafénmentes kétdimenziós anyagok hajnala (Dawn of graphene-free two-dimensional materials)
27-05-2014	Attila Csákányi (Wigner RCP): Pásztázó nemlineáris mikroszkópok optikai leképezõ rendszerének modellezése (Modeling of the optical mapping system of scanning non-linear electron microscopes)
27-05-2014	Norbert Babcsán (Aluinvent Zrt.): Aluhab: egy új anyag (Alu-foam: a new material)
29-05-2014	Balázs Szabó (Wigner RCP): Nyírási lokalizáció kialakulása szemcsés anyagokban (Formation of shearing localization in granular materials)
03-06-2014	Ildikó Némethné Pethes (Wigner RCP): Infravörös optikai üvegek

szerkezetvizsgálata (Structural study of infrared optical glasses)

03-06-2014 László Temleitner (Wigner RCP): A víz szerkezetvizsgálata polarizált neutronokkal (Structural study of water by polarised neutrons)

05-06-2014 László Rátkai (Wigner RCP): Spirális eutektikus dendritek (Spiral euthectic dendrites)

05-06-2014 Márton Markó (Wigner RCP): Szén nanoszerkezetek vizsgálata neutronszórással (Investigation of carbon nanostructures by neutron scattering)

10-06-2014 Nikoletta Laczai (Wigner RCP): Polikristályos ittrium-oxi-ortoszilikátok előállítása és vizsgálata (Preparation and study of polycrystalline Yttrium-oxi-orthosilicates)

10-06-2014 Tamás Demján (Wigner RCP): Tiszta és módosított nanogyémántok elektronikus és optikai tulajdonságai (Electric and optical properties of clean and modified nanodiamonds)

12-06-2014 Alicia Kollar (Stanford University): Exploring strongly correlated matter with multimode cavity QED

17-06-2014 Yutaka Shikano (Institute for Molecular Science, Okazaki, Japan): Solid-state implementation of quantum walk

19-06-2014 Gyula Tóth (Wigner RCP): Atomi szintû fázismezõ-elmélet: Múlt, jelen, jövõ (Atomic level phase field theory: Past, present, future)

24-06-2014 László Himics (Wigner RCP): Kékben és vörösben emittáló színcentrumok kialakítása nanogyémántban (Creating color centers in nanodiamonds that emit in the blue and in the red)

01-07-2014 Sára Tóth (Wigner RCP): GR1 centrum emissziója nano- és mikrokristályos gyémántban (SiV ZPL kiszélesedése) (Emission of GR1 center in nano- and microcrystalline diamond (widening of SiV ZPL))

08-07-2014 Kalliopi N. Trohidou (Institute of Materials Science - NCSR Demokritos): Multiscale modelling of the exchange bias behaviour of bi-magnetic nanoparticle assemblies

10-07-2014 Zsolt J. Bernád (TU Darmstadt, Germany): Entangling remote material qubits by photon exchange

16-07-2014 Sándor Pekker (Wigner RCP): Konjugált kötésû polimerek és szén-nanoszerkezetek (Polymers and carbon nanostructures with conjugated bonds)

29-07-2014 Kenneth R. Elder (Oakland University): Advances in modeling polycrystalline systems: from phase field crystal to complex amplitude models.

30-07-2014 Sándor Pekker (Wigner RCP): Konjugált kötésű polimerek és szén-nanoszerkezetek II. (Polymers and carbon nanostructures with conjugated bonds II.)

26-08-2014 Ulrike Herzog (Nano-Optics, Institute of Physics, Humboldt-University Berlin): Optimal strategies for the discrimination of quantum states

09-09-2014 Ádám Gali (Wigner RCP): A route for integration of classical and quantum technologies operating at ambient conditions

16-09-2014 Gábor Széchenyi (ELTE): Double quantum dots in carbon nanotubes

23-09-2014 Gábor Csire (Wigner RCP): Kvázirészecske spektrum szupravezetõ-fém heteroszerkezetekben (Quasiparticle spectra in superconductor-metal

heterostructures)

30-09-2014	Len Pismen (Dept Chem Eng, Technion, Haifa): Patterns in polarizable active layers: from oscillating tissues to intelligent materials
02-10-2014	Gergely Thiering (Wigner RCP): Ni and Si related point defects in (nano-)diamonds
07-10-2014	Sándor Varró (Wigner RCP): New quantum phase operator and projectors based on SU(1,1) coherent states
09-10-2014	Judit Romhányi (Leibniz-Institute, IFW-Dresden): Thermal Hall effect in SrCu2(BO3)2
14-10-2014	Krisztián Lengyel (Wigner RCP): Kristályok és lézerek (Crystals and lasers)
21-10-2014	Gergely Thiering (Wigner RCP): Ni and Si related point defects in (nano-)diamonds
21-10-2014	Chou Jyh-Pin (Wigner RCP): Proper surface termination for luminescent near-surface NV centers in diamond
21-10-2014	Elisa Londero (Wigner RCP): Characterisation of defect centres in diamond by Density Functional Theory calculations
28-10-2014	Szabolcs Vajna (BME): Topological classification of dynamical phase transitions
04-11-2014	Gergely Szirmai (Wigner RCP): Repulsive self-trapping in a bosonic Josephson Junction with a potential dip in the middle
11-11-2014	Predrag Ranitovic (Lawrence Berkeley National Laboratory, Berkeley, USA): Control of atomic and molecular XUV absorption processes using intense IR fields
18-11-2014	Ervin Hartmann (Wigner RCP): A krisztallográfia forrásainál (At the sources of crystallography)
24-11-2014	Bálint Kollár (Wigner RCP): Disorder and entropy rate in discrete time quantum walks
25-11-2014	Róbert Juhász (Wigner RCP): Hosszú hatótávolságú, rendezetlen rendszerek kritikus viselkedése (Critical behaviour of long-range disordered systems)
09-12-2014	Dan Hüvonen (National Institute of Chemical Physics and Biophysics, Tallinn): Bond disorder in quantum magnets: dynamics and criticality
11-12-2014	Balázs Szabó (Wigner RCP): Nyírási zónák száraz szemcsés anyagokban (Shear zones in dry granular materials)
16-12-2014	Imre Hagymási (Wigner RCP): Szobahõmérsékleti élmágnesség grafén nanoszalagokban (Room-temperature edge magnetism in graphene nanoribbons)
18-12-2014	Zsolt Szekrényes (Wigner RCP): Komplex nanoszerkezetek tanulmányozása infravörös spektroszkópiával (Study of complex nanostructures by infrared spectroscopy)