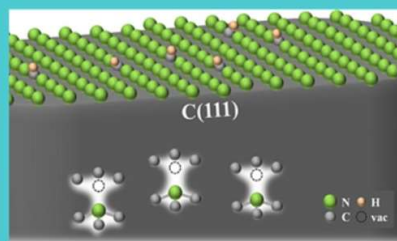
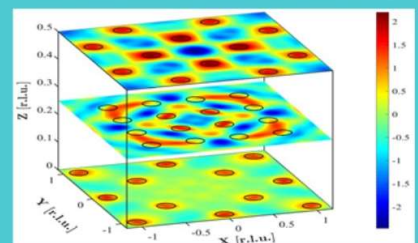
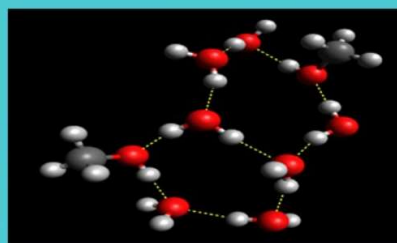
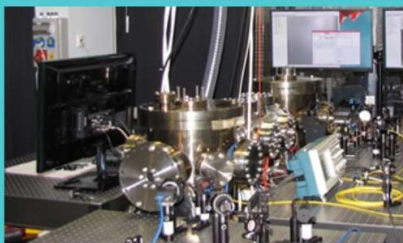
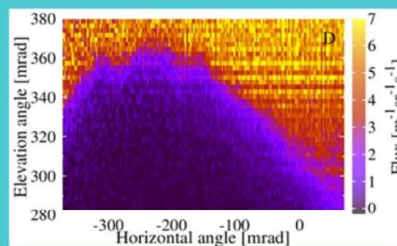




WIGNER 2017



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

Wigner RCP 2017

Annual Report

Wigner Research Centre for Physics
Hungarian Academy of Sciences
Budapest, Hungary
2018

Wigner Research Centre for Physics
Hungarian Academy of Sciences
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FOREWORD

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



Among the deepest human desires is the passion to uncover secrets, embarking one on the path toward the joy of discovery. Such joy is the privilege of scientists who manage to pioneer something unprecedentedly new, and are gifted with such an experience for their endeavours. The joy of the discovery of the unknown, this experience compensates for all the hard work leading to novelty. There are numerous walks of life, many where it is simpler to gain material wealth and financial prosperity; but the multifarious lifestyle of a scientist, the participation in symposia and conferences, the enriching discussions, the many international collaborations and fascinating encounters with great intellectuals, make the life of a scientist exciting and rich.

When this scientific lifestyle is realized in a collegial, supportive and creative atmosphere, one which we aim to maintain at our institute, then all these factors combine to form an especially exciting and rewarding environment, where we recognise that we belong to a community contributing to the promotion of science and technology and thus to the development of the society.

Perhaps this pleasant atmosphere contributed to our being especially successful during the past few years. Based on our achievements, we have been awarded a series of national and international project grants and started a number of research projects which could serve as solid foundations for our scientific and economic development in the coming years. Furthermore, these projects enable opportunities to better financially honour the work of our leading researchers, as well as to broaden our academic and industry partnerships.

In the present brief introduction, we only mention a selection of our results from the last year. First of all, we must mention the National Quantum Technology Program which offers 3.5 billion HUF budget for the participating partners. This program was initiated by our scholar Péter Domokos, who also acts as the coordinator of this impressive program. Under the coordination of the Institute of Solid State Physics and Optics of Wigner RCP, eight outside institutions also participate in the consortium: Budapest University of Technology and Economics, Eötvös Loránd University, Hungarian Academy of Sciences Centre for Energy Research, ERICSSON Hungary, Nokia Bell Labs, Bonn Hungary Electronics Ltd., and Femtonics Ltd.

During the 4-year duration of the project, the consortium partners aim to integrate Hungary into the European quantum internet network currently under development, maintain and improve the competitiveness of Hungarian researchers in the field of quantum technology, and to increase the number of experts in quantum technology in Hungary both as scientists and in engineering fields.

Within the framework of the consortium, the goals to be achieved include quantum communication between two quantum encrypted points, and execution of quantum bit operations – the foundations of quantum computation. The first year of the program is the preparatory phase, this includes setting up the required laboratories. The test experiments will begin in the second year, and the instrumentation developed by the experts will be deployed in the third year. Investigating practical applications of the developments will be emphasized in the final phase of the program.

Researchers of the institute started 8 new OTKA projects worth a total of 185.85 million HUF. Two of the grants are postdoctoral fellowships, from the remaining six grants 3 are in the field of experimental physics: one of them aims at *Ultrafast processes research*. The second one studies *Soft matters*, while the third project investigates *Chemical changes in low dimensional materials using electron spectroscopy*. The other 3 projects are theoretical in nature: one of them belongs to the quantum computer research, the other one investigates the *Dynamics of coherent and open quantum optic networks*, the third one studies the *Questions of merger of magnetism and topology in quantum insulations*. In 2017, three previous OTKA grants were completed, thus the number of currently running OTKA projects is 30 with a 785.77 million HUF total budget.

In 2017, after a longer gap, the researchers of the institute became very successful concerning the EU co-founded national R+D+I grants. The most significant winning research proposals were:

NVKP_16-1-2016-0043: *Development of fluorescent dyes and high resolution, fast scanning 3D microscope for the treatment of epilepsy* (327 million HUF for 3 years), VEKOP-2.3.3-15-2016-00001: *Determination of atomic structure of nanosystems* (121.4 million HUF for 2 years), VEKOP-2.3.2-16-2017-00015: *Research on ultrahigh-speed molecular and nanooptical switches* (440.3 million HUF for 4 years); VEKOP-2.3.2-16-2016-00011: *Strategic workshop for the technological challenges of renewable energy systems* (150 million HUF for 3.5 years).

Besides the above projects, the Institute for Solid State Physics and Optics won 2 new intergovernmental mobility grants (TÉT). One of them is the „*New technologies in agriculture based in cold gas discharge plasmas*” in cooperation with Croatia, the other one is with Slovenia: „*Structure of aqueous solutions of sugars and alcohols*”

Currently 4 significant EU projects are running: the “NEURAM – Visual genetics: establishment of a new discipline to visualize neuronal nuclear functions in real-time in intact nervous system by 4D Raman spectroscopy” EU H2020 FET-Open, the “VISGEN – Transcribing the processes of life: Visual Genetics” EU H2020 MSCA-RISE and 2 big research infrastructure projects. In 2017, researchers of the institute joined two COST collaborations COST CA16101: *MULTI-modal Imaging of FOREnsic SciEnce Evidence - tools for Forensic Science*. The other one is COST OC-2017-1: *Lithium niobate nanoarchitectures: From quantum level to cross-disciplinary applications* (LN2020). This latter COST Action already organized two preparatory conferences, the first one on February 24-26 2017 and second one on May 26-28 2017, where the researchers of the institute were among the participants.

Overall, we can conclude that the Institute was able to attract significant third-party financing for its scientific budget in 2017. These programs are expected to bring outstanding achievements primarily in the fields of quantum optics and quantum electronics, modern

optics (nanooptics, fluorescent dyes) and developments in solid state physics (new type solar cells combined with perovskite-based coal nanostructures).

In addition to their research activities, our colleagues contribute greatly to university level education and recruiting young researchers. Related indicators of the institute are improving. The above summary fills us with optimism, looking forward to the future ahead as our institute is on track with both the human resources and the infrastructural background required for sustainable development.

Aladár Czitrovsky

director of the Institute for Solid State Physics and Optics
of the Wigner Research Centre for Physics

AWARDS AND PRIZES

Awards of the State of Hungary and Government of Hungary

J. Sólyom: Officer's cross of the Order of Merit of Hungary (civil division)

Awards of the Hungarian Academy of Sciences

Z. Donkó: Prize of the Hungarian Academy of Sciences

G.G. Barnaföldi: Physics Prize of the Hungarian Academy of Sciences

D. Beke, Hungarian Academy of Sciences Award for the youth attendees of International Conference (Hungarian Academy of Sciences)

M. Veres: Honourable Mention of the Secretary General of the Hungarian Academy of Sciences

A. Derzsi: Award for Young Scientists of the MTA 2017



International professional awards

Z. Németh, ESA outstanding contribution certificate (Outstanding contribution to the Rosetta mission)

T. Csörgő, Distinguished Referee (2017), by the Editors in Chief of European Physical Journal C

F. Nemes, TOTEM Performance Award (2017), Proposed by A. Scribano, Chairman of the TOTEM Collaboration Board, awarded by S. Giani, Spokesperson of the TOTEM Collaboration

K. Szegő: ESA outstanding contribution certificate (Outstanding contribution to the Rosetta mission)

I Hagymási: Alexander von Humboldt research fellowship

L. Rózsa, Alexander von Humboldt research fellowship

National professional awards

M. Varga-Kőfaragó: György Ferenczi Memorial Prize

János Nagy: Albert Fonó Prize

Pál Vizi: Ernő Nagy Prize

B. Török: Béla Julesz prize in Cognitive Science, Technical University of Budapest

R. Ünneper, Jenő Ernst Award

A. Czitrovsky: Nándor Bárány Award of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology

L. Oláh, Géza Györgyi Award of the Wigner RCP RMI

G. Hamar, Géza Györgyi Award of the Wigner RCP RMI

R. Szipócs: Applied Research Award of the Wigner RCP SZFI

L. Himics: Applied Research Award of the Wigner RCP SZFI

L. Bencs: Publication Award of the Wigner RCP SZFI

Conference awards

Viktor Ivády, MRS Spring Meeting Conference Award

Viktor Ivády, Knut and Alice Wallenberg Foundation Conference Award

Bolyai János Scholarship of the HAS granted in 2017

D. Barna

A. Derzsi

P. Rácz

Z. Zimborás

Other award

Á. Takács: "30 Under 30" 2017 by Forbes Hungary 2017

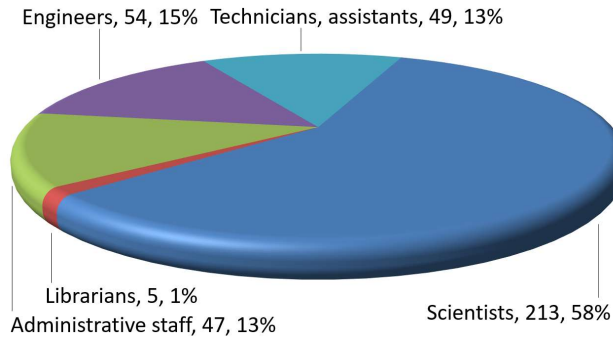
Other scholarship

L. Kocsor, Scholarship of the Márton Áron Research Program (Ministry of Foreign Affairs and Trade)

KEY FIGURES AND ORGANIZATIONAL CHART

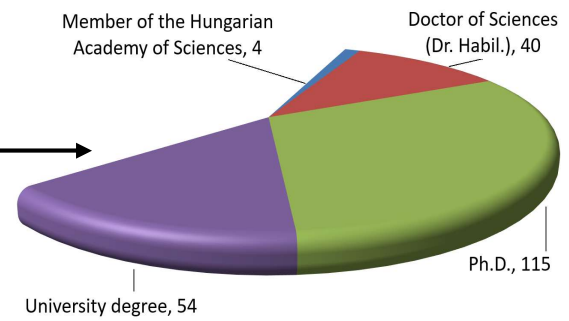
Permanent staff by profession

Total: 368



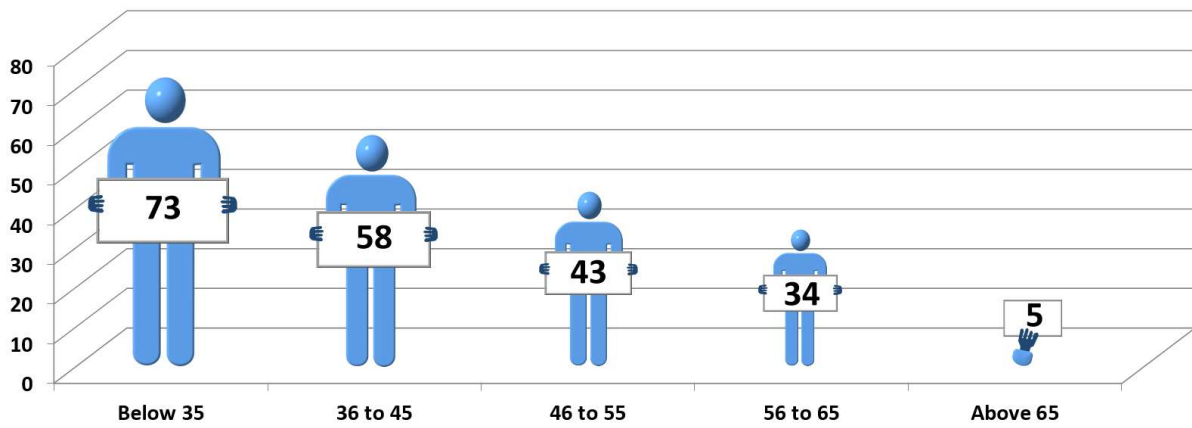
Scientists by degree/title

Total: 213

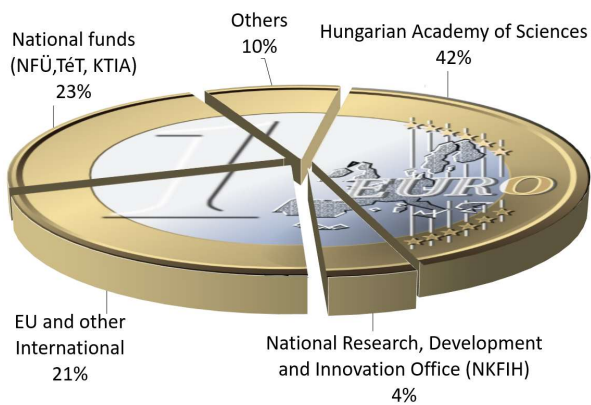


Scientists by age group

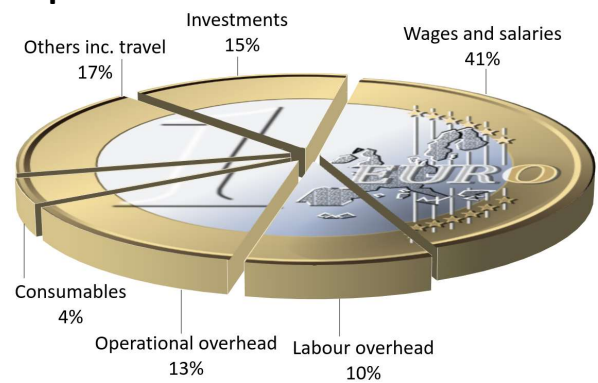
Total: 213



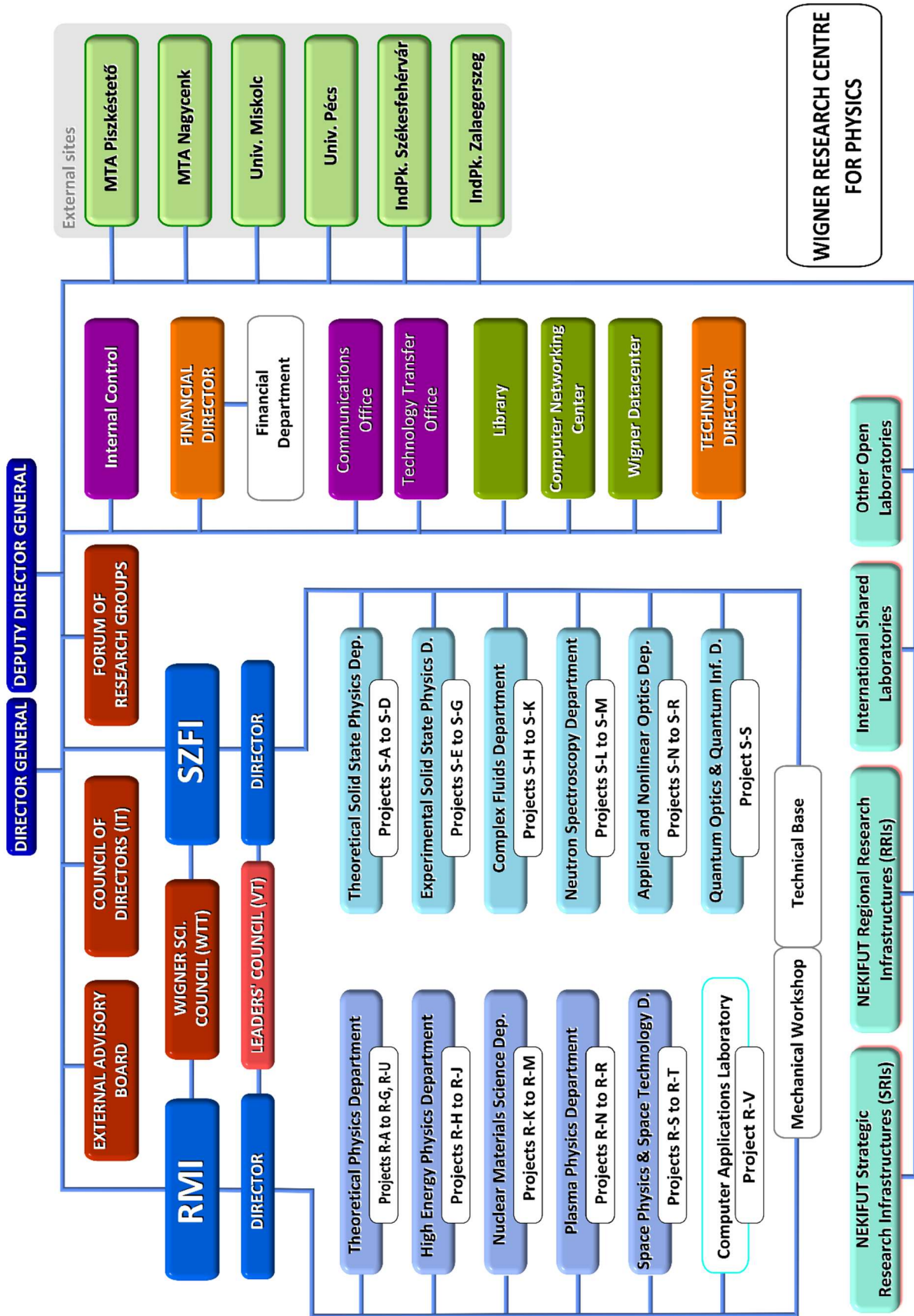
Income*



Expenditure*



*V.A.T not included.



MOST IMPORTANT EVENTS OF THE YEAR 2017

Nóra Szathmáry, communication department

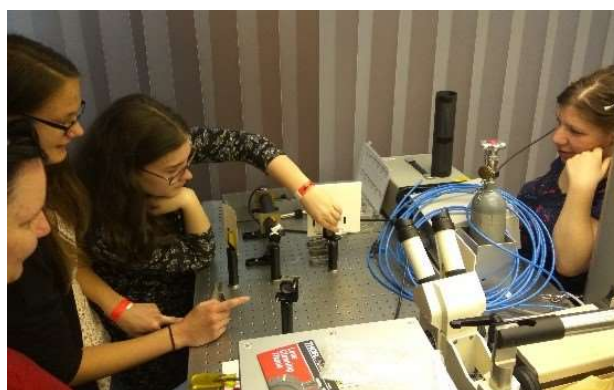


In addition to our core mission, our research centre places a strong emphasis on the dissemination of our research results, including scientific outreach activities aimed at the general public. It is of utmost importance that our most recent and outstanding research achievements should not only be accessible to university students, but also to students at the high school level, in order to inform them about possible career choices at an early stage. Towards this goal, we organise lectures, scientific road shows, and open days. Our colleagues often write expository articles, give interviews, and produce videos and various accessible media to promote their work.

The **Wigner115 Symposium** organized in November on occasion of Eugene P. Wigner's 115th birthday took place at the Conference Hall in the Main Building of the Hungarian Academy of Sciences. Public lectures, invited talks, and poster sessions were curated to showcase the entire range of Eugene P. Wigner's contributions to physics.

All Colours of Physics Roadshow. — This is our interactive program for pupils in primary and secondary schools featuring physics and engineering activities aimed at helping career orientation. The 2017 roadshows had a total of 1700 participants in 12 Hungarian speaking schools in Slovakia.

Our research centre has a long history of organising three different **Open Days** targeting different audiences. This spring, for the fifth consecutive year, we contributed to the international thematic program series **Girl's Day**. 100 girls from different high schools participated in interactive tours at the laboratories, met successful female researchers, and gained insight into scientific and engineering careers.



The **V. CERN-Wigner Open Days** weekend in September provided occasion for our research groups collaborating with CERN to present their work to the general public. The 2-day program series featured stands with exhibits, lectures, and a live connection to the CERN headquarters in Geneva, among many other programs, giving participants an insight into the world of CERN, particle, and nuclear physics. During the event, 180 of the participants were given the opportunity to visit the Wigner Data Centre.

In November, we organised the **Wigner Open Days**, as part of the event Celebration of the Hungarian Sciences - Research Centres Open Gates organized by the Hungarian Academy of Sciences, during which 100 secondary school students visited our 12 laboratories and got a glimpse of the work being done.



Programs for Students. — In March as part of the XIII. Particle Physics Masterclass 50 secondary school students (aged 15-18) were introduced to the most cutting edge advances in modern physics, both theoretical and experimental – with an emphasis on particle physics.



Between May 22 and June 2 2017 as first among the 22 CERN Member States Hungary had the opportunity to send 22 students to Geneva for the 2-week HSSIP student research program. The Hungarian students worked in pairs under the supervision of Hungarian physicists, engineers, or computer science mentors abroad on current assignments. The preparation for the program was done in Budapest at the Nuclear- and Particle Physics Institute.



High school participants of the VI. Eötvös Natural Science Camp, who stand before their maturity exam, spent their final day at our research centre, gaining hands-on experience about the research at our institutes and the physicist profession.

Student Researchers' mentoring program. — We continued our mentorship program for talented high school students. Students learnt about detector physics at the High Energy Physics Department directly from experienced young physicists with first-hand knowledge on projects at CERN. Students were given the task to design and build basic measuring instruments, and carried out measurements, gaining close insights to the secrets of the micro world.

Teacher Program. — A tender dossier was assembled in order to organise the Teacher Program at CERN, where 21 high school teachers were given the opportunity to participate in a one-week vocational training at CERN.

Festivals. — Our colleagues from the Plasma Physics Department were present at the largest summer festivals in Hungary - the '*Sziget*' and '*Volt*' music festivals. They were able to answer the questions of visitors interested about our Research Centre, and its work.

Press. – Our researchers and their exciting fresh results are increasingly featured in the press and online media.

Our research centre is in contract with the „Palace of Wonders” to provide expert guidance consulting on the scientific content of their outreach programs. Researchers of our institutes participated in the lecture series entitled „Wigner Café – with physicists”, where their exciting new findings were discussed. We contribute a permanent exhibit at the “Palace of Wonders”, currently featuring Hungarian space research. We chose to showcase the '*Rosetta*', '*Cassini*' and '*Obstanovka*' mission supported by space research community at Wigner.

INTERNATIONAL SCIENTIFIC COOPERATION

Valéria Kozma-Blázsik, scientific secretary



Wigner Research Centre of the Hungarian Academy of Sciences, with its 2 institutes and more than 200 physicists is the largest physics research institution in Hungary. The 40 research groups at the twin Institutes of Particle and Nuclear Physics (RMI), and Solid-State Physics and Optics (SZFI), cover a wide range of sub disciplines within physics, and in recent years' interdisciplinary research has been gaining ground.

There are some differences in the scientific focus of the researchers at the two institutes, but the main shared goal is to conduct research at a high level by international standards. Another important common feature of both Wigner institutes is their active participation in a wide range of topics investigated in the framework of national and international cooperation both at the individual and institutional levels.

At Wigner all levels of scientific cooperation's are present, starting from bottom-up endeavours based on the ideas of individual researchers in the form of common articles, invited lectures delivered in international conferences all over the world, the exchange of visiting scientists, participation in editorial boards of scientific journals, and referee activities. 28 researchers represent Wigner on various editorial boards. 104 researchers are members of international scientific committees, five of them fulfil leadership roles.

Another example of the embeddedness in the international scientific community is that almost two thirds of all scientific publications are written with co-authors. In 2017, researchers at Wigner published 1040 international **publications** 787 from RMI and 221 from SZFI. However, in this field there is a difference between the two institutes. In the case of SZFI articles are written by less co-authors, while in the case of RMI a great number of the publication are written through large collaborations. This difference is a result of researchers representing Hungary in large scientific cooperations such as ALICE, NA61, CMS, TOTEM, AWAKE at CERN, or at EUROFUSION's ITER in France, Virgo in Italy, KSTAR with Korean or EAST with Chinese partners. To make the list more complete we must mention JET with the UK and GSI-FAIR, the Darmstadt cooperation, which got a green light recently in late 2016.

While the main profile of RMI is participation in large collaborations, in contrast at SZFI "table top" experimental research, carried out at in-house laboratories is the most common form of investigation. Compared to the research on large research infrastructures 'table-top' experiments are less investment intensive; thus high-level frontier research is achieved at the on-campus laboratories. Researchers at SZFI tailor generic equipment and components available on the market into specialized high-tech equipment with a high added value.

At SZFI another strength is their highly international research based on strong theoretical foundations, primarily in the fields of material science and quantum physics. In 2017, with the aid of the coordinating role of the Quantum Optics Department, an unprecedented national

grant was awarded (NKFIH HunQTech 2017-1.2.1-NKP-2017-0000) resulting in a good chance that SZFI will become the second significant quantum technology centre in pair with BME.

The in-house cooperation between the theoretical and experimental groups such as the Raman spectroscopy and infrared spectroscopy are strongly supported by the leadership as well as different collaborations in laser, plasma, and complex fluid physics. However, in a few areas research groups at the institute lack critical size, thus it is crucial that group members liaison with international partners.

Another indicator of international reputation is the number of researchers working abroad, currently about 100 scientists. A recent trend is that a number of foreign researchers choose to work in research groups mostly within the framework of European Union projects. The number of foreign PhD students is also on the rise, in 2017, their number reached 8, while another 7 foreign researchers are working in various research groups. Short-term visiting researchers are the most numerous, in 2017 98 spent shorter periods at our institutes.

Most of the international mobility connected to participation in international projects like EU, ESA, NIH, or bilateral mobility grants of the Hungarian Academy of Sciences and work done in research infrastructures, a couple of which we had already mentioned earlier.

The other form of international involvement is participation in **large-scale research infrastructures** (RIs). We have already mentioned CERN. In addition to this, there are a number of open laboratories, related to other significant big European Large-scale RIs, like ESS, ELI, or others.

At our research centre one of the most significant RI is the Budapest Neutron Centre hosting the 10 MW Budapest Research Reactor (BRR), a cold neutron facility that is one of the largest and most important research infrastructures in Hungary. While ESS will produce neutrons via spallation rather than a nuclear reaction, the BRR's beamline serves as a testing ground both to characterise the ESS moderator as well as to develop reactor-based applications of the novel moderator concept, mostly within the framework of European Union projects.

Wigner ADMIL fabricates and validates samples from non-commercialized technologies for growing unique doped, functionalized ceramic, semiconductor, or metallic nanostructures or thin layers. These structures have prospective applications as nanoscale biosensors (DNA research, neurology), quantum optics (single-photon emitters), cutting-edge energetics (nanocrystals for photovoltaic applications, ceramics for fourth-generation nuclear reactors), and nanomagnetism.

At Wigner-ADMI, not only are the most widespread methods of fabrication and validation tools available, those based on melting and vaporization, but others, such as mechanical grinding, colloidal or electrolytic chemical procedures, doping or decomposition by ion implantation, doping or crystalline relaxation by annealing, as well as methods based on gas discharge and CVD growth. Combinations of these techniques are also used. Wigner-ADMI is an open laboratory, its facilities and services may be used by third-party users and partners.

At the Applied and Nonlinear Optics Department there are several open laboratories: The Wigner Ultrafast Nanooptics Laboratory, which is registered as a Strategic Research Infrastructure and is also listed on the European MERIL register, and an associate member of Laserlab Europe. The others are the Femtosecond Lasers and the Laser applications and

measurement techniques, Nanostructures and applied spectroscopy and the hELlos laboratory.

Laser measurement technology and environmental laboratory provides laser based and environmental measurements for institutions and offers measurement services for customers. Most of the instruments and equipment of the laboratory developed in our institute or purchased in the frame of research projects and other grants.

They perform expedient measurements according to the requirements of our customers with the above instruments in the field of optical surface analysis, optical homogeneity and contamination analysis, measurement of optical properties and composition, and in the field of environmental and health protection. The laboratory has ISO9001 certification.

It is worth mentioning the following projects:

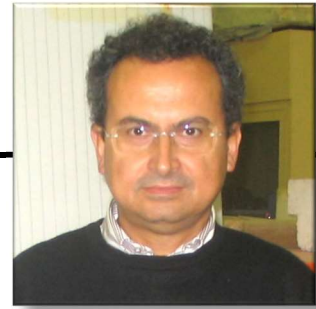
A utility patent filed in Japan, owned jointly by Wigner RCP and Tokyo University, for the “Muography Observation System” (MOS). This detector system installed in Japan at the Sakurajima volcano (on the southern island).

Long run space exploration projects are also present, notably including one of the longest interplanetary missions, the NASA-led Cassini-Huygens mission, which ended on 15th September 2017. Cassini-Huygens involved 17 countries. The mission launched in Cape Canaveral in 1997, and the missile reached the Saturn area in 2004.

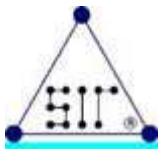
The organization of international conferences are another avenue that supports the formation of future long-term research ties. In 2017, our researchers participated in 128 local and 302 international conferences and workshops, and participated in the organizing committees of 53 conferences held in different countries.

Another excellent example for long-term scientific cooperation of which you can read more details in the following pages written by Dr Massimo Rogante, is the **2nd International Conference on Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage (NINMACH) 2017** was organized in Budapest Hungary, by the staff of the Budapest Neutron Centre. The event’s predecessor was a collaboration with the International Atomic Energy Agency (IAEA). [NINMACH 2013](#), organized in Garching, Germany, was the first event of this conference series that addressed both neutron scientists and archaeologists and conservators. At NINMACH archaeologists and conservators take part from museums and universities with the aim of understanding the potential of neutron methods in cultural heritage research.

ROGANTE ENGINEERING OFFICE AND THE BUDAPEST NEUTRON CENTRE — 20 YEARS OF COOPERATION



Dr. Eng. **Massimo Rogante**, Director of REO



The Rogante Engineering Office (REO, STUDIO D'INGEGNERIA ROGANTE) <http://www.roganteengineering.it> and the Budapest Neutron Centre (BNC) <http://www.bnc.hu> are now celebrating 20 years of cooperation.

REO, which is primarily a nuclear and mechanical engineering office, is a landmark in Italy for Industrial Applications of Neutron Techniques (Applicazioni Industriali delle Tecniche Neutroniche®), and it is qualified supplier of Institutions and Companies at international level.

Dr. Eng. Massimo Rogante, Director of REO, has been working in the neutron field for over 25 years. He has a Degree in Mechanical Engineering, PhD in Nuclear Engineering, he is also a Member of the International Scientific Advisory Committee of the BNC, as well as Member of various other International and National Scientific Institutions (e.g., the Scientific Selection Panel of the Centre of Accelerators & Nuclear Analytical Methods of the Nuclear Physics Institute of the Czech Academy of Sciences). In Italy, during the preparatory phase of the European Spallation Source (ESS) project, REO has been selected and committed to coordinate Italian industry, i.e. the Workgroup "Industry and Industrial Applications" in the frame of the ESS-Italia Project Committee. The said Committee has been formed by the Italian Research Council, the Italian Nuclear Physics Institute and the Trieste's Synchrotron (see the web page <http://www.roganteengineering.it/public/ESS-ITALIA-WG13.pdf>).



Several pioneering experiments have been carried out by the REO at the BNC related to different industrial fields (e.g. automotive, energy, medical, building, footwear, welding, as also presented in the BNC official web page <http://www.bnc.hu/?q=node/33>, in which the cooperation with REO is underlined), as well as in the Cultural Heritage sector.

Some works carried out by Dr. Rogante at the BNC have been selected by the

responsible of the NMI3 Project (Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy) in the frame of the EU 6th Framework Programme (FP6), as the first works:

- in the NMI3 report “Engineering, Archaeology, Earth Sciences and Environment”
- representing Engineering in the NMI3 Scientific Highlights Section.



In these 20 years, more than 50 publications have been produced by Dr. Rogante and BNC colleagues as co-authors, also in high impact factor journals. Researchers from both institutions presented the results of the mutually fruitful cooperation at many international conferences, e.g. the Int. Conf. on Mechanical Technologies and Structural Materials (co-organized by the REO in Split, Croatia), the Int. Conf. on Materials, Energy and Design 2006 (co-organized by the REO in Dublin, Ireland), the 20th Bratislava

International Conference on Macromolecules, Advanced Polymeric Materials 2006, June 11-15, 2006, or the International Conference on Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage (NINMACH) 2017.



In the year 2008, Dr. László Rosta of the BNC attended the 1st Italian Workshop for Industry "Industrial Applications of Neutron Techniques - AITN 2008", organized by the REO in Civitanova Marche, Italy, as a keynote speaker. This workshop involved the participants in a "full-immersion" in the world of neutron techniques for the investigation of materials and components of industrial interest.

The cooperation of the REO with the BNC has

also included:

- collaborations with related scientific and technical Institutions, i.e. Wigner Research Centre for Physics (WRC), KFKI Atomic Energy Research Institute (AEKI), MTA Research Institute for Solid State Physics and Optics, HAS Centre for Energy Research, ESS Hungary Non-profit Plc.
- collaboration in the frame of the Central European Training School on Neutron Scattering (CETS) in Budapest and other training courses.

Perspectives for the future are to enhance further this mutual cooperation and to exploit neutrons in many others of the forefront areas of science and technology: investigating various other materials and industrial components, as well as more archaeological artefacts; developing investigation projects related to different strategic industrial fields and beneficial for the industrial community at the international level.

OUTSTANDING RESEARCH GROUPS*

MTA's "Momentum" Research Teams



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

Wigner Research Groups

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

* **Abbreviations in the researcher lists of the scientific projects:**

#: PhD student

A: associate fellow

E: professor emeritus

R-C. Gravitational physics

Wigner research group

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



The Gravitational Physics Research Group of the Wigner RCP is carrying out research in theoretical physics related to gravitational phenomena. The members of the group have solid background in particle physics and general relativity. Moreover, they have experience in the development of optimal numerical algorithms and implementation of these algorithms into efficient computer procedures that can be run on grid and GPU clusters. Being a member of the Virgo Scientific Collaboration operating the VIRGO detector, the European gravitational wave observatory one of the main motivations of our research interest originates from gravitational wave (GW) physics. The scientific results of the last year are summarized below.

Gravitational waves. — 2017 represents a rich and exciting year in gravitational physics. The main objective of GW research has been achieved in 2015 with the first direct observation of gravitational waves from coalescing black holes with the Advanced LIGO detectors. Following an upgrade period of few years the European VIRGO detector started its operation with improved sensitivity in February 2017. As an important milestone, the first three detector observation was achieved in August, 2017, during the 1 month joint data taking period of the LIGO and VIRGO detectors. Only a few days later, an other very significant event, the collision of two neutron stars was recorded with gravitational waves and electromagnetic observations also. The original alert of the Fermi satellite initiated an observation campaign with the participation of nearly 70 observatories. Due to the improved sky localization of the source with three GW detectors scientists from all over the world could follow the GW and electromagnetic signal of the collision within a few weeks period. This parallel gravitational and electromagnetic observation of NS collision represents a breakthrough in multi-messenger astronomy. This remarkable observation was preceded by long years of developments and upgrade periods. The efforts of the gravitational community were awarded with the Nobel Prize in October 2017 for the direct detection of gravitational waves.

Joining to the international LIGO-Virgo collaboration our research projects aimed to analyze important and interesting compact binary sources of GWs and study the astrophysical and cosmological implications of the observations. For ground-based interferometric GW detectors compact binary systems of stellar mass black holes and neutron stars are important sources considering the present sensitivity of GW detectors. Specific waveform templates are ready for offline searches and parameter estimation studies for these kind of sources within the software package of the LIGO-Virgo Collaboration, e.g. the *PyCBC* and *GstLAL* packages. In data analysis processes matched template filtering is the most optimal method for the identification of theoretical waveforms and source parameter estimation. Matched filtering for compact binary sources is implemented in the *PyCBC* software package which is available on Institutional resources, i.e. the *Wigner Cloud*.

Continuous gravitational waves. — Continuous GWs are faint signals for gravitational wave detector produced by systems with almost constant and well-defined frequency, e.g. single

stars rotating about their axis with a large mountain or other irregularity on it. These sources are expected to produce weak gravitational waves since they evolve over longer periods of time and are usually less catastrophic than sources producing inspiral or burst GW. The collaboration with our colleague Michal Bejger aims the optimization of an all-sky data-analysis pipeline developed initially by the Polish POLGRAW group. The pipeline is an implementation of the targeted search for almost-monochromatic gravitational-wave signals from rotating, non-symmetric, isolated neutron stars. During the visit, the CUDA accelerated all-sky search application underwent a major rewrite with several motivating factors behind this effort. The GPU codebase was an evolutionary step going forward from the serial and OpenMP parallelized codes. As a result, it has accumulated many deprecated dependencies as many dead code paths. During the rewrite, the entire source base was analyzed and dead code paths were eliminated, as linking to unused libraries were dealt with. Moreover, the codebase originally targeted Linux systems, but it was our intent to bring the codebase over to Windows Systems, which would increase the potential user base, as well as enable Windows-only developer tools to be employed on the code base. To further widen the potential end systems and users that the program targets, we not only created a cross-platform version, but this code is also cross-vendor, having moved from naked CUDA, cuFFT and cuBLAS to naked OpenCL, clFFT and clBLAS. Thus AMD and Intel Phi architecture support opened up, as well as mitigating the need to maintain the OpenMP codebase, due to OpenCL being able to target multi-core CPUs. Furthermore the code refactoring enabled us to implement various features which are of interest to further analysis (parametrize on the types on various points of the pipeline), as well as applying global code cleaning (compiling the sources without compiler warnings, eliminating potential sources of hidden bugs) resulting in a more maintainable codebase. Having made these changes, the way is made clear to implement multi-device and cluster parallelism, which can now be implemented in a significantly less amount of time. Being the result of a major refactoring, the code requires testing to its functionality.

Mass and radius of neutron stars. — Neutron stars (NS) are important sources of gravitational waves. The most intense part of the observed GW signal is coming from the merger part of the coalescence carrying essential information about the NS characteristics and the merger itself. Advances ground-based interferometric GW detectors allow the observation of such sources at their present sensitivity. In August 2017, the LIGO-Virgo collaboration has detected the first binary neutron star inspiral (so-called GW170817), and 70 other observatories collaborated to detect its electromagnetic counterpart. In our work we have analyzed neutron star interiors with the assumption of spherical symmetry. In this case the metric tensor is time dependent and the equations characterizing the neutron star interior are decouple to the Tolman-Oppenheimer-Volkov (TOV) equation and a differential equation for the time evolution of the radius. For a two-component polytropic equation of state we have analyzed the Mass-Radius relation for neutron stars. The analysis was extended to other equation of states describing Newtonian and neo-Newtonian stars, and neutron star matter with hyperon content. The recent observation of GW170817 presents bounds on NS mass and limits the parameter range of possible equation of states.

Frequency and dissipation of gravitational waves in interstellar medium. — The propagation of locally plane, small-amplitude, monochromatic gravitational waves through cold compressible interstellar gas was studied in order to provide a more accurate picture of expected waveforms for direct detection. Gravitational waves were treated as linearized

perturbations on the background inner Schwarzschild spacetime. The perturbed quantities lead to the field equations governing the gas dynamics and describe the interaction of gravitational waves with matter. We have shown that the transport equation of these amplitudes provides numerical solutions for the frequency-alteration. The decrease in frequency is driven by the energy dissipating process of GW-matter interactions. The decrease is significantly smaller than the magnitude of the original frequency and too small to be detectable by present second- and planned third-generation detectors. The effect exhibits a power-law relationship between original and decreased frequencies. For sources in the 1–2 kHz frequency range, the influence of the interaction on the signal may increase significantly compared to that of the value on initial frequency of 100–200 Hz. Such high-frequency signals are expected to be emitted from the post-merger phase of low-mass neutron-star (NS) collisions such as the GW event GW170817 which originated from a BNS system. The frequency deviation was examined particularly for the first observed transient signal GW150914.

Black hole geometries and holographs. — In our recent work we combined two results of the quasilocal theory of black holes (BH). Near horizon geometries (NHG) of extremal BHs are exact solutions of the Einstein equations obtained by a naturally defined limit of neighborhoods of extremal (degenerate) Killing horizons. The second topic is the recent stationary black hole holograph (BHH) relying on the characteristic Cauchy problem for the electrovacuum Einstein’s equations. If two transversal null surfaces are nonexpanding, then they become components of a bifurcated Killing horizon. Based on the observation that NHGs also admit bifurcated Killing horizons NHGs can be referred as special cases of the BHHs. In our work we have determined conditions on the BHH data that are necessary and sufficient for the corresponding hologram spacetime to be a NHG. This result may be considered as the first step in using the BHH construction in a quest for an interesting generalization of the NHG idea. For simplicity, our work was restricted to 4D spacetimes and the vacuum Einstein’s equations.

The idea that inequalities arise from the geometrical attributes of different objects is not new. One of the best known example is the isoperimetric inequality which states that among closed planar curves with fixed length the circle has the smallest area. In general relativity similar reasoning yields relations between physical parameters through the coupled nature of geometry and physics. The most successful application of these kind of relations is putting constraints on black hole evolution. Black holes are relatively simple objects described by few parameters but their evolution can easily develop complex structures. Nevertheless the geometrical nature of black holes results in relations between its parameters which remain valid even in extremely complicated cases.

We studied the case of spherically symmetric spacetimes. In spherical symmetry there is a highly accepted notion for defining the amount of mass included within a domain, the Misner-Sharp mass. This notion makes possible to investigate such inequalities in more general spacetimes than before and domains that are not necessarily black holes but normal bodies instead.

Matra Gravitational and Geophysical Laboratory*. — The lower frequency bound of the Advanced GW observatories are around 20 Hz. For the planned European next generation GW

* This is an intergroup organization with P. Ván, R. Kovács, E. Fenyvesi, G.G. Barnaföldi from the Heavy Ion Physics

detector this value is 2 Hz. There are three fundamental limitations at low frequency of the sensitivity: seismic noise, the related gravitational gradient noise (so-called Newtonian noise) and the thermal noise of the mirrors. To circumvent these limitations the new infrastructure is planned as an underground site to reduce the effect of seismic and Newtonian noise with cryogenic facilities to cool down the mirrors to directly reduce the thermal vibration of the test masses. The Mátra Gravitational and Geophysical Laboratory was constructed 88 m deep below the surface in an unused mine near Gyöngyösoroszi in 2015. In a collaboration with several Institutes the aim of the Laboratory is to perform long-term seismic, infrasound and electromagnetic noise measurements, and monitor the variation of the cosmic muon flux. After the publication of the first data taking period, March and August, 2016, the second one has been started from August, 2016. In this period, the members of our group focused on the study of the seismic noises by improving and specifying the processing algorithm and by clarifying the derived quantities for the site selection of any 3rd generation GW underground facilities. By the end of 2017, more than 600 days of data have been collected and analyzed in order to study monthly and yearly change of seismic noises which is essential for a next generation GW detector. By the collected data from Mátra 400 m and the Jánossy-mine (located at the KFKI Campus) the reduction of seismic noises with depth could also be studied.

Outreach. — With the first direct detection of the collision of two neutron stars with gravitational and electromagnetic waves this year marks a significant breakthrough in multi-messenger astronomy. The announcement of the first detection of gravitational waves with three GW detectors and other black hole mergers was generated a very intense public interest and attention to this research field. It was further intensified that the Nobel Prize in Physics this year was awarded for the direct observation of gravitational waves. Similarly to the previous year's appearances our group members were actively participated in public outreach. We have given several successful scientific and public lectures, radio and TV interviews about the detection of gravitational waves and neutron star collisions.

Grants

OTKA¹ K-115434: Developing and applying new methods to solving the Cauchy problem in general relativity (I. Rácz, 2015-2019)

NKFI² K-124366: Geophysical noises in gravitational wave detection (P. Ván, 2017-2020)

International cooperation

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

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

Long-term visitors

Michal Bejger (M.F. Nagy-Egri, 2 weeks)

Philippe LeFloch (I. Rácz, 1 week)

Research Group (R-B) and Z. Zimborás form Field Theory Group (R-A).

¹ OTKA: National Scientific Research Fund

² NKFI: National Research, Development and Innovation Office

Ingemar Bengtsson (I. Rácz, 1 week)

Naresh Dadhich (I. Rácz, 1 week)

Philippe LeFloch (I. Rácz, 1 week)

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See also: R-B.2, R-B.26

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R-E. Theoretical neuroscience and complex systems

Wigner research group

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



We have published a new data analysis method, called skCSD, to reveal membrane currents on single neurons, based on extracellular multichannel electrode array measurements. The new method provides higher precision in membrane current source density reconstruction due to the inclusion of the morphology information into the calculation. We have applied the new method to the first available parallel extracellular and intracellular data and showed the spatial propagation of the currents during action potential generation on the dendritic branches of the cell. (Fig. 1) The scripts for the analysis, written in R, were tested and made publicly available as an open source program package.

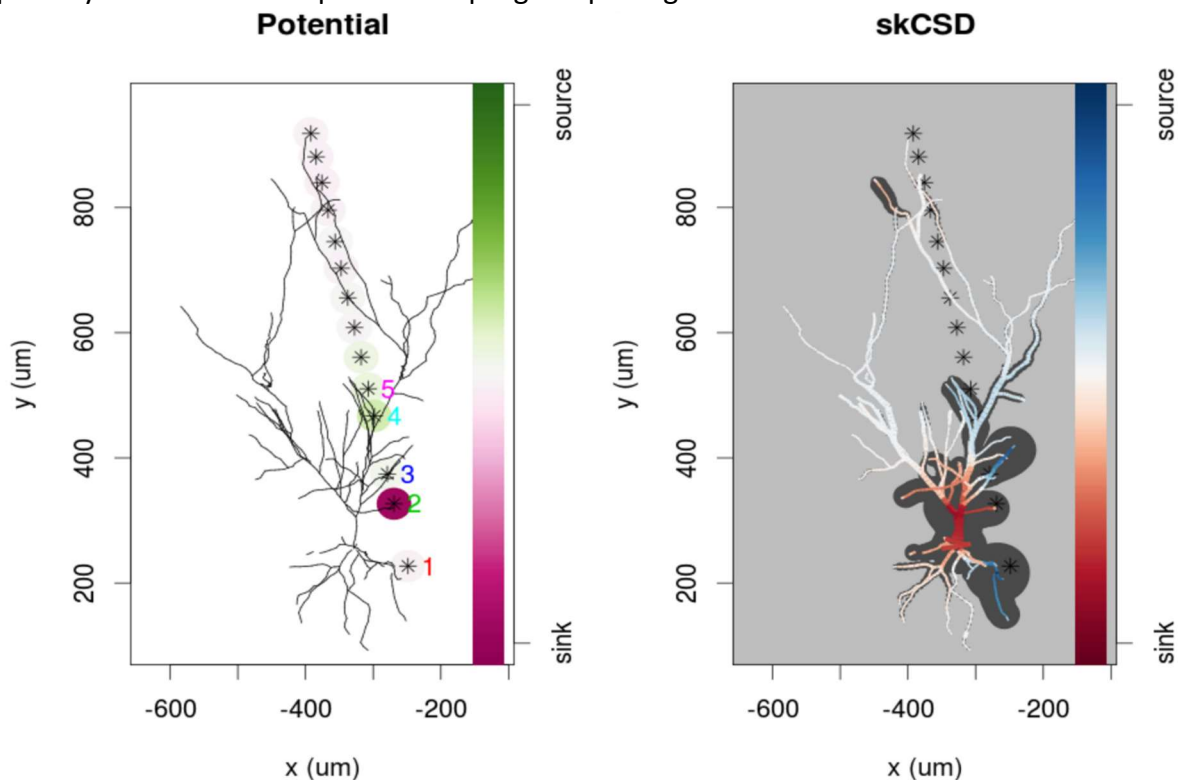


Figure 1: Left: Electrode positions (stras) and reconstructed morphology of the pyramid cell from the CA1 region of the rat hippocampus. The color coded circles on the electrodes show the measured momentary electric potential at the moment of the peak of an action potential generated by the neuron. Right: The reconstructed current source density distribution along the dendritic tree of the neuron. Warm colors mark inward positive currents to the neuron (sink) cold colors mark the outward currents from the neuron (sources).

We have published the first results on the analysis of the parallel recordings on intrinsic optical and local field potential by a transparent electrode array. The new method makes possible the fusion of the two methods, by exploiting the advantages of both, the excellent

spatial resolution of the optical imaging and the excellent temporal resolution of the electric signal.

We applied our coherence clustering method, to determine the cortical structures and areas from the measurements with the transparent cortical surface electrode grid, parallel to the intrinsic optical signal measurement. The methodology and the first results were published on a conference and in a proceedings journal.

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

We showed that in the somatosensory cortical circuitry, which is largely responsible for tactile perception, lateral interactions mostly depend on the intra-areal connections complemented by the neuronal feedback originating from areas with higher order functional representations. In contrast, feedforward connections from lower order areas exhibit spatially restricted lateral spread indicating higher functional specificity. Our results also suggest that the population activity is mostly determined by the target regions of the feedforward connections overlapping the strong local input within an area. The manuscript including these findings has been submitted for publication and is now under major revision.

To better understand somatosensory, and in general cortical communication, we studied the synaptic organization of the above mentioned connections in 3D by way of electron microscopy. Using state of the art data analyses techniques we found that the size of axon terminals is an important distinguishing morphological feature of the cortical synapses. We also found that the size of the mitochondria and postsynaptic densities (the active zone of the signal transmission) relative to the size of the axon terminals also exhibit important distinguishing characteristics and that their positive correlation can be explained by the energy need of synaptic transmission. The manuscript summarizing these findings is going to be submitted soon.

Our ongoing studies show that the robustness and synchronizability of the network of cortical areas is especially sensitive to targeted removal of the network edges on the basis of their convergence degree introduced previously by our group.

By including a Bayesian evaluation algorithm, the development of our new causality analysis method, now we call it dimensional causality method (DC), has been completed. The DC method has been tested on various simulated systems, such as coupled Lorentz systems, coupled logistic maps and coupled Hindmarsh-Rose models. These simulated dynamical systems pose different challenges towards the DC algorithm but we found, that all the DC method was able to infer all possible causal relations (unidirectional, circular, independent and hidden common cause) in all the three model cases. Preliminary applications were made on neurophysiological data from epileptic patients, during photostimulation experiment and during epileptic seizure.

Grants

OTKA K-113147, Micro-electric imaging: modeling, source reconstruction and causality analysis for multi-electrode arrays. (Z. Somogyvári, 2015-2018)

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

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

International cooperations

Nencki Institute of Experimental Biology, Warsaw, Poland (D. Wójcik – D. Cserpán, Z. Somogyvári)

VTT Technical Research Centre of Finland (Espoo, Finland), Regular structure in networks and graphs (H. Reittu – F. Bazsó)

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

Neuroscience Research Unit, Pfizer Global Research and Development, Cambridge, MA, USA. Tau-pathology in Alzheimer’s disease (L. Scott – T. Kiss)

Translational Neuropharmacology, Section of Comparative Medicine, Yale University School of Medicine, New Haven, CT 06520, USA. Tau-pathology in Alzheimer’s disease (M. Hajós – T. Kiss)

Universiteit van Amsterdam, Netherland. Investigating the canonical organization of neocortical circuits for sensory integration (C. Bosman and U. Olcese – L. Négyessy, Z. Somogyvári)

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

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

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Book, book chapter

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R-F. Holographic quantum field theory

“Momentum” research team

Zoltán Bajnok, János Balog, Tamás Gombor[#], Árpád Hegedűs, Márton Lájér[#], Gábor Puzstai, Gábor Zsolt Tóth, Ch. Wu



Correlation functions of the maximally symmetric 4D quantum gauge theory and finite volume form factors. — The AdS/CFT correspondence relates string theories on anti de Sitter (AdS) backgrounds to conformal gauge theories on the boundary of these spaces. The energies of string states correspond to the scaling dimensions of local gauge invariant operators which determine the space time dependence of the conformal 2- and 3-point functions completely. In order to build all higher point correlation functions of the CFT one needs to determine the 3-point couplings, which is in the focus of recent research.

String theories on many AdS backgrounds are integrable and this miraculous infinite symmetry is the one which enables us to solve the quantum string theory dual to the strongly coupled gauge theory. In the prototypical example the type IIB superstring theory on the $AdS_5 \times S^5$ background is dual to the maximally supersymmetric 4D gauge theory. Integrability shows up in the planar limit and interpolates between the weak and strong coupling sides. The spectrum of string theory, i.e. the scaling dimensions of local gauge-invariant operators are mapped to the finite volume spectrum of the integrable theory, which has been determined by adapting finite size techniques such as thermodynamic Bethe Ansatz (TBA).

Further important observables such as 3-point correlation functions or nonplanar corrections to the dilatation operator are related to string interactions. A generic approach to the string field theory (SFT) vertex was introduced in our previous work which can be understood as a sort of finite volume form factor of non-local operator insertions in the integrable worldsheet theory. There is actually one case when the 3-point function corresponds to a form factor of a local operator insertion. In the case of heavy-heavy-light operators the string worldsheet degenerates into a cylinder and the SFT vertex is nothing but a diagonal finite volume form factor, as we pointed out in our previous publications.

The string field theory vertex describes a process in which a big string splits into two smaller ones. In light-cone gauge fixed string sigma models on $AdS_5 \times S^5$ and some similar backgrounds, the string worldsheet theory is integrable and the conserved S^5 charge serves as the volume, so that the size of the incoming string exactly equals the sum of the sizes of the two outgoing strings.

Initial and final states are characterized as multiparticle states of the worldsheet theory on the respective cylinders and we are interested in the asymptotic time evolution amplitudes, which can be essentially described as finite volume form factors of a non-local operator insertion representing the emission of the third string. In order to be able to obtain functional equations for these quantities we suggested to analyze the decompactification limit, in which the incoming and one outgoing volume are sent to infinity, such that their difference is kept fixed. We called this quantity the decompactified string field theory (DSFT) vertex or decompactified Neumann coefficient. We formulated axioms for such form factors, which

depend explicitly on the size of the small string, and determined the relevant solutions in the free boson (plane-wave limit) theory. Taking a natural Ansatz for the two particle form factors we separated the kinematical and the dynamical part of the amplitude and determined the kinematical Neumann coefficient in the AdS/CFT case, too. These solutions automatically contain all wrapping corrections in the remaining finite size string, which makes it very difficult to calculate them explicitly in the interacting case, especially for more than two particles. It is then natural to send the remaining volume to infinity and calculate the so obtained octagon amplitudes. One can go even further and introduce another cut between the front and back sheets leading to two hexagons, which were introduced previously and has been explicitly calculated. Since we are eventually interested in the string field theory vertex, we have to understand how to glue back the cut pieces. Our recent paper was an attempt going into this direction. Clearly, gluing two hexagons together we should recover the octagon amplitude. Gluing two edges of the octagon we get the DSFT vertex, while gluing the remaining two edges we would obtain the finite volume SFT vertex, which would be the ultimate goal for the interacting theory. For the details see Fig. 1.

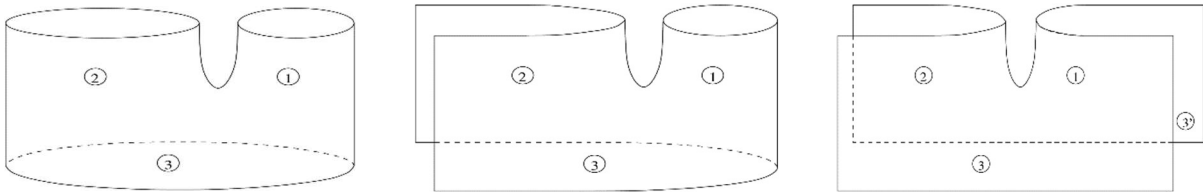


Figure 1. *The string field theory vertex describes the amplitude of the process in which a big string splits into two smaller ones. Initial and final states are characterized as finite volume multiparticle states and the asymptotic time evolution amplitudes can be understood as finite volume form factors of a non-local operator insertion (left figure). In calculating these quantities we go to the decompactification limit, in which two of the volumes are sent to infinity, leading to infinite volume form factors (middle figure). By sending the remaining volume to infinity we obtain the octagon amplitudes (right figure).*

The study of various observables in integrable quantum field theories in finite volume in a natural way can be decomposed into a number of stages. Firstly, the problem posed in infinite volume typically yields a set of axioms or functional equations for the observable in question which often can be solved explicitly. The key property of the infinite volume formulation is the existence of analyticity and crossing relations which allow typically for formulating functional equations. Secondly one considers the same problem in a large finite volume neglecting exponential corrections of order e^{-mL} . In this case the answers are mostly known like for the energy levels, generic form factors and diagonal form factors. However, some of these answers were still conjectural until we proved them in the last year. Thirdly, one should incorporate the exponential corrections of order e^{-mL} , which are often termed as wrapping corrections as they have the physical interpretation of a virtual particle wrapping around a noncontractible cycle. The key example here are the Lüscher corrections for the mass of a single particle and their multiparticle generalization what we obtained a few years ago. Once one wants to incorporate multiple wrapping corrections, the situation becomes much more complicated however in some cases this can be done.

In the case of the spectrum of the theory on a cylinder, fortunately one does not need to go through the latter computations as there exists a thermodynamic Bethe Ansatz formulation

which at once resums automatically all multiple wrapping corrections and provides an exact finite volume answer. Unfortunately for other observables like the string interaction vertex we do not have this technique at our disposal and we hoped that understanding the structure of multiple wrapping corrections shed some light on an ultimate TBA like formulation. This was another motivation for our work and in fact one of our new results is an integral representation for the exact pp-wave Neumann coefficient which involves a measure factor reminiscent of various TBA formulas.

We argued in our paper that the quantitative structure of the gluing procedure may be efficiently understood within the so-called cluster expansion (equivalently compactification in the mirror channel). There the main ingredient was the asymptotic large mirror volume expectation value for the observable in question which decomposed into a linear combination of measure factors and appropriate infinite volume quantities. This is a standard way to understand ground state energy and the LeClair-Mussardo formula for one point expectation values in relativistic integrable theories. In our paper we adopted this framework to the case of the octagon and the decompactified SFT vertex. We demonstrated that one can resum the multiple wrapping corrections for the octagon into the exact decompactified SFT vertex. This necessitates a nontrivial, but quite natural modification of the multiple wrapping measure. We then proceed to interpret this modification through the cluster expansion where it turns out to arise from certain diagonal terms. We then show that similarly one can resum the decompactified SFT vertex and recover the exact finite volume pp-wave Neumann coefficients.

Grants

OTKA K-109312: Holographic solutions of gauge theories (Á. Hegedűs 2013-2017)

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

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

International cooperations

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

Gatis+ Reseach Network

Long-term visitor

Haryanto Siahaan, 2017.11.01-2018.06.30

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R-G. Computational systems neuroscience

“Momentum” research team

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Information processing in the visual system. In order to understand how the brain handles visual information, we build mathematical models of the visual cortex, and compare predictions derived from them to experimental data. Assessing how variability is introduced to neuronal firing is a prerequisite to modelling responses. By comparing two competing models of spike generation, we demonstrated that near-deterministic firing is compatible with measured higher-order statistics, while Poissonian spiking is not. We published these results in an international journal and presented them at an international conference.

The hierarchical model of visual processing we developed predicts the dependence of neural response correlations on stimulus content. We tested this prediction using recorded neural responses from the V1 of macaques, using our experimental design at the Ernst Strüngmann Institute in Frankfurt. We developed novel control procedures to deal with confounding effects between measured signals. The results confirmed the prediction of our model and corroborated the earlier finding that the secondary visual cortex is involved in the representation of textures. The results are published on a preprint server, are being submitted for publication to an international journal and have been presented at two international conferences.

The way stimuli are encoded in neural activity can be determined by decoding stimulus properties from recorded neural responses. We investigated whether second-order statistics play a significant role in the decodability of natural image stimuli from spike trains recorded from V1, and determined their importance. We also examined how decodability evolves over the course of an experimental session, and what aspects of the neural activity are essential to decode task-related experimental variables. We presented these results at two international conferences, and we are preparing them for publication in an international journal.

Using semantic memory to compress episodic memories. Continual learning, constructing and continually updating a model of a complex environment based on experiences, arose in recent years as a major field of interest in machine learning, while also being a longstanding challenge for cognitive science since human learning takes place in the same regime. One of the chief challenges in continual learning is how previously obtained information can be efficiently represented, that is, what kind of memory should a continual learning agent have. Traditional approaches based on optimising point estimates in deep learning architectures suffer from ‘catastrophic forgetting’: updating the model compromises performance on already learned tasks. While a Bayesian approach does not suffer from this issue, resource constraints that result in information loss render learning the structure of the environment impossible. In preceding years we have proposed that a combination of semantic and episodic memories can mitigate this issue and enable continual learning of model structure.

Our previous work contained the simplifying assumption that episodes are remembered verbatim, which is empirically known to be unrealistic for human learning and is a presumably wasteful use of memory resources. To remedy this, we have proposed that semantic memory, a latent variable hierarchical generative model of the environment, can be used to compress the episodes. We have argued that this corresponds to a specific choice of distortion function in rate-distortion theory, where predictive ability is prioritized over reconstruction of experiences in data space. We have shown that this choice explains robust biases in human memory errors in a classic experimental setting that tests memory for sketch drawings. To do this, we have approximated semantic memory for human sketches by training a latent variable generative model on the recently published QuickDraw database and shown that our compression algorithm qualitatively reproduces the distortions found in the experiments. We have shown on a simple model of hierarchical mixture of gaussians that the hierarchy of latent variables can enable compression with variable level of detail and approximate the optimal rate distortion curve. In the following year, we will test whether semantic compression of episodes can explain a greater variety of memory distortion experiments, and whether the inference of model structure is possible when episodes are compressed.

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

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

The next step in our research is to identify the cornerstones of efficient learning in a dynamical environment. There are a number of competing modelling ideas that can equally account for observable data, however, they impose qualitatively different inductive biases. Ideally, a normative account of the learning problem would point at specific sets of inductive biases, which in turn could be contrasted with human behaviour.

Another key to connecting learning of different temporal domains is the capability of extracting meaningful segments from a stream. This is equivalent to identifying events, actions, subgoals in the theory of mind domain, words, word-elements in the language domain, basic elements of motion, collisions and other types of interactions in the intuitive physics domain. The adequate discretisation of the stream is essentially tied to the temporal structure present in any given domain. Inference of the segmentation as well as of the structure over the segments is required to be handled simultaneously.

Public outreach activities. In our vision it is central to inform the public, and provide access

to advances in the field of systems neuroscience and machine learning. We pursued three different paths to achieve these goals. In a number of media appearances, which included radio interviews, television shows, and written reports, we disseminated our research achievements. Traditional university lectures in a number of courses reached a large number of students with varying backgrounds arriving from a wide spectrum of universities. Finally, we have started a Junior Brain Computer Interface Lab for high school students. The goal of this lab is to provide access for a small team of high school students to the world of AI, machine learning, and systems neuroscience through designing computational tools that can be used to control devices, such as small robots or computer games, on line by signals recorded from a so-called e-cog device.

Grants

“Momentum” Program of the HAS (G. Orbán, 2012-2017)

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

International cooperation

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University of California, Los Angeles (Los Angeles, CA, USA) P. Golshani

Columbia University (New York, NY, USA), A. Losonczy

Central European University (Budapest), J. Fiser

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

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R-I. “Lendület” innovative gaseous detector development

“Momentum” research team

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The present year has concluded the “Momentum” grant support of the group from the HAS, which will continue as a permanent funding. The key focus of the group was the completion of the already existing commitments. This includes contributions to specific CERN experiments, such as the ALICE, NA61 and RD51. Detector physics projects and neutron detector development were financed by H2020 grants. Using detectors developed by the group, an active volcano imaging has been performed in collaboration with Tokyo University and the NEC company.

Contributions to CERN Collaborations. — The activities of the group in the Time Projection Chamber (TPC) Upgrade Collaboration has reached nearly half way, with about 200 large size gas electron multiplier (GEM) foils processed in Budapest. The Advanced Quality Assurance testing site which was established, is the second step of the TPC construction after production (at CERN), and the foils are forwarded to Germany and the USA. Within the framework of the NA61 Collaboration, three new TPC-s were built and installed to capture the forward particles.

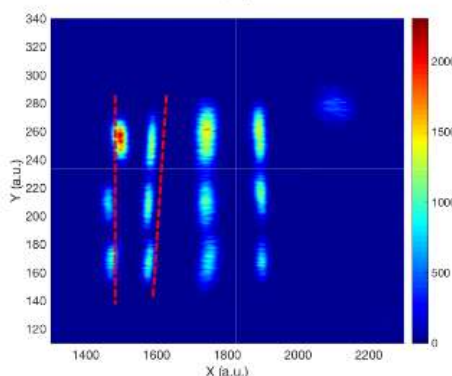
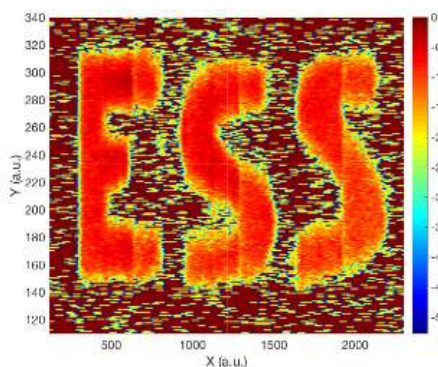
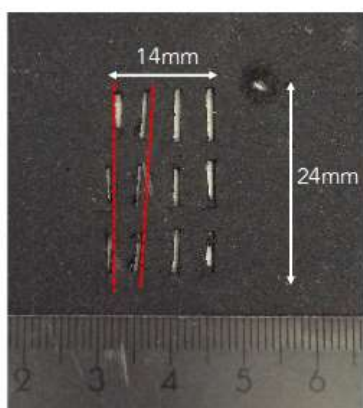
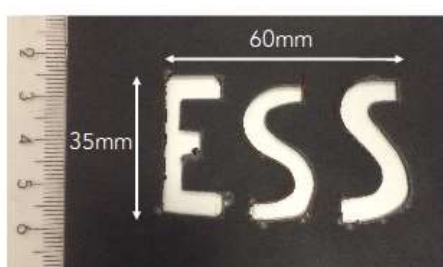


Figure 1. Images taken with the Multi-Blade detector, using neutrons at the Budapest Neutron Center. Precise and high contrast images have been recorded, consistently with the design goal for neutron reflectometry at ESS.

Multi-Blade detector demonstrator for ESS. — The high intensity, high position resolution neutron detector, called the Multi-Blade, has been tested with cold neutron beam at the Budapest Neutron Center. The results show that the position resolution, below 0.5mm in one direction, is indeed reached. Other testing has clarified the intensity tolerance of the design,

which, by the delicate interplay between geometry and detection mechanism, is higher than most other competing versions. Demonstration images are shown in Fig. 1.

Imaging with cosmic muons. — The application of cosmic muons for large scale imaging has been a research direction in the group in the previous years. An important application for cosmic muons detectors, developed in the last years by the group, is imaging the interior of volcanos. This direction was pursued by Japanese and various European groups. Gaseous tracking detectors, and in our case, a specific type of a multi-wire proportional chamber (MWPC) developed by our group, are highly competitive with the traditional scintillators in terms of cost, weight and power consumption. A utility patent has been filed in Japan, owned jointly by Wigner RCP and Tokyo University, for the so-called “Muography Observation System” (MOS). The detector system has been installed by the Sakurajima volcano in Japan (southern island), to demonstrate the true applicability and sufficiently low level of background, and to gain experience for the future developments. Presently 1.2 square meter sensitive area is installed, which will increase in the coming years. The Japanese NEC company, which has licensed the MOS for research purposes, has started a cooperation with the patent owners to understand the market needs for muography.

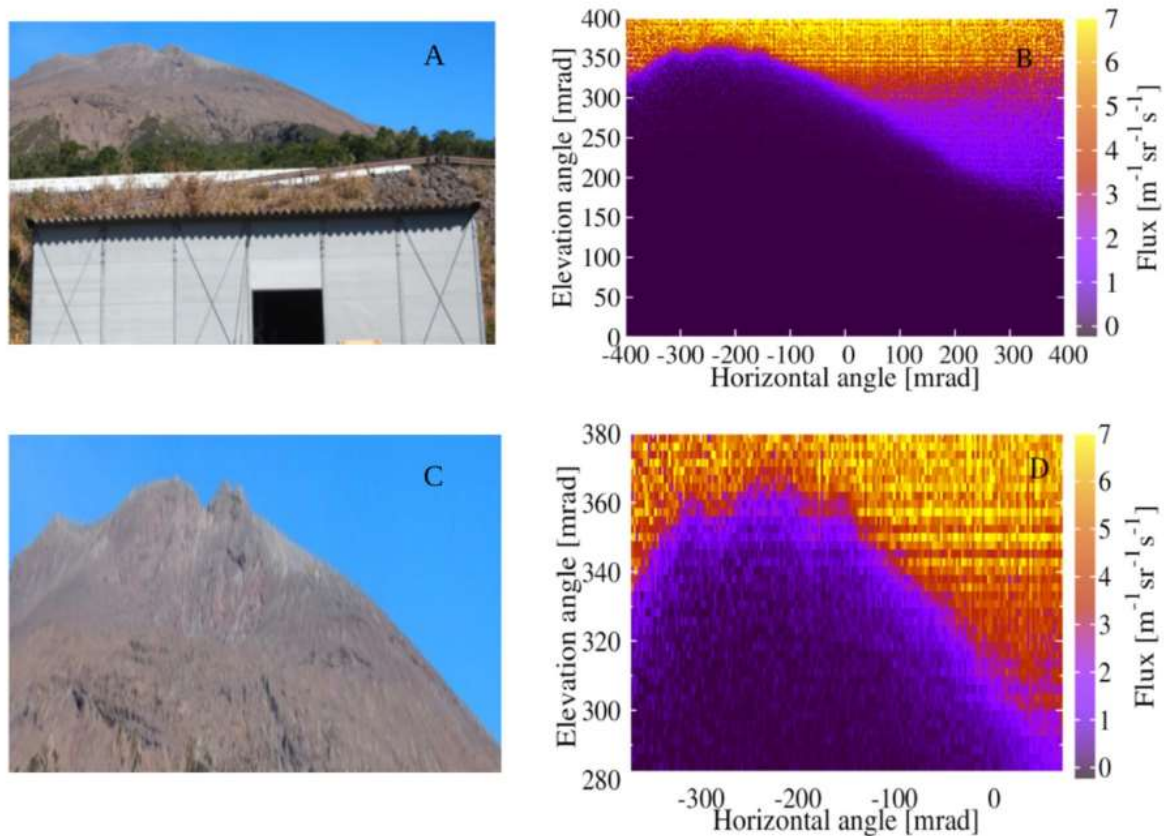


Figure 2. Visual (left) and muographic (right) images of the Sakurajima volcano in Kyushu (Japan), taken with the MOS. The detectors were developed at Wigner RCP, installed in a structure designed and constructed by Tokyo University.

Grants

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

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

BrightnESS (Research Infrastructure for ESS), H2020 support (D. Varga, 2015 - 2018)

NKFI FK 123959, (A. László, 2017-2020)

Japanese-Hungarian TÉT, Serbian-Hungarian TÉT, (2017-2019)

International cooperation

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

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

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

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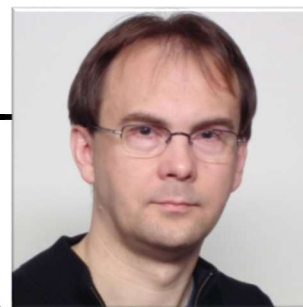
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See also: R-B.2, R-H. Aduszkiewicz A et .al, R-H. Bencédi G, R-H. Bencédi G, S-M.4

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

R-K. Femtosecond spectroscopy and X-ray spectroscopy



“Momentum” research team

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Hard X-ray spectroscopy is a powerful probe of the electronic and local atomic structure, combined with high penetration, element, orbital and spin selectivity. Here we report on experimental results and technical developments using X-ray probes in investigations of transformations of transition metal complexes. First, we demonstrate valence-to-core X-ray emission spectroscopy as a novel ultrafast probe with high chemical sensitivity. Second, we show that laboratory spectrometers can do more than has been expected, monitoring the concentration dependence of the Ni speciation in solution with X-ray absorption spectroscopy. Finally, we show the realization of total reciprocity violation in the phase for photon scattering.

Probing the dynamics of the valence electrons at a spin state in transition metal complexes.

— Pump-probe experiments are powerful structural dynamics tools, which apply an ultrashort laser excitation pulse, and study the time evolution of the system with a probe pulse at chosen time delays. Unveiling the details of the relaxation processes that follow the light excitation can lead to a complete understanding of the involved mechanisms, which, for instance, shall promote the design of more efficient functional molecules. Here we report on experimental results and technical developments using an X-ray probe in time-resolved investigation of a transition metal complex that is a model system for molecular switches; the experimental work is aided by quantum chemistry. We probed the dynamics of valence electrons in photoexcited $[\text{Fe}(\text{terpy})_2]^{2+}$ complex in aqueous solution to gain deeper insight into the electronic structure changes that lead to changes of the Fe-ligand bonds using hard X-ray emission spectroscopy (XES). A picosecond-time-resolved measurement of the complete 1s X-ray emission spectrum captures the transient photoinduced changes and includes the weak valence-to-core (vtc) emission lines that correspond to transitions from occupied valence orbitals to the nascent core-hole. As DFT-calculations predict (Fig. 1A), vtc-XES offers particular insight into the molecular orbitals directly involved in the light-driven dynamics. As the result of the excitation, antibonding orbitals are populated and the metal ligand orbital overlap becomes weaker, resulting in intensity reduction as well as energy shift in the experiment (Fig. 1C), in excellent agreement with our calculations (Fig. 1B). More subtle features at the highest energies reflect changes in the frontier orbital populations. The results are shown in Figure 1.

This result demonstrates the potential of vtc-XES as an ultrafast probe, which, combined with femtosecond time resolution in future experiments at X-ray free electron lasers, will shed more light on the intricate details of the elementary transition processes. (*The full article can be accessed at <http://dx.doi.org/10.1021/acs.jpcc.6b12940>.*)

Extending laboratory X-ray absorption spectroscopy for routine measurements in solution phase. — A novel laboratory von Hámos X-ray absorption spectrometer had been built and tested with solid samples the previous year by the group. This year the spectrometer was

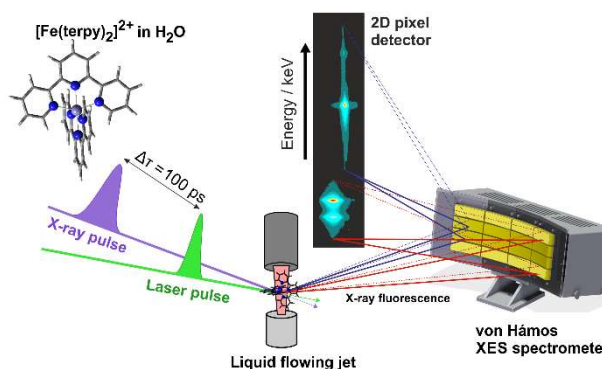
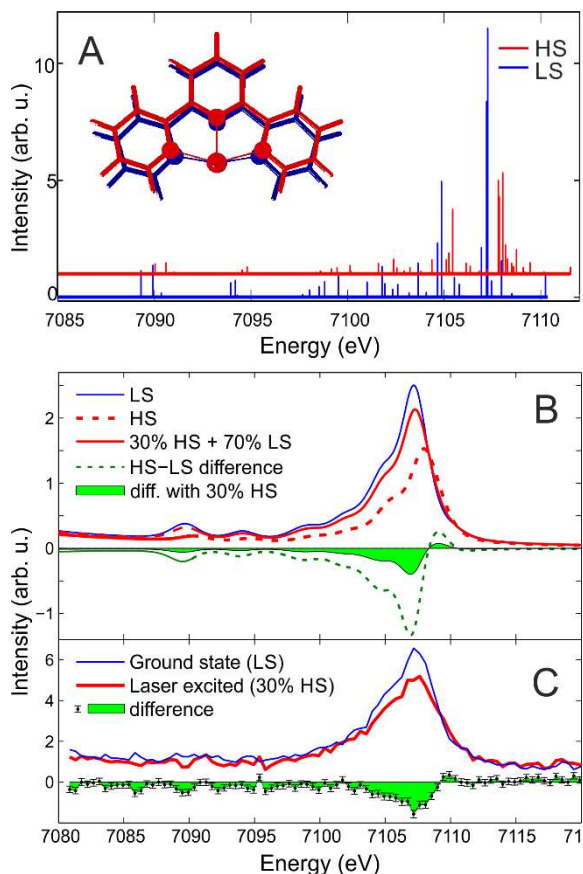


Figure 1 (top) The experimental setup showing the 16-crystal von Hámos spectrometer installed in a pump-probe geometry. Two different sets of 8 Si analyzer crystals were used to collect both $K\alpha$ and $K\beta$ plus vtc X-ray emission simultaneously. The detector image shown is a cropped actual frame from the pixel detector recorded during the experiment. On the left the molecular structure of the $[\text{Fe}(\text{terpy})_2]^{2+}$ complex is shown. **(A)** Stick diagram of the molecular orbital contributions to the vtc -XES spectra of LS and HS $[\text{Fe}(\text{terpy})_2]^{2+}$ (blue and red, respectively). The variation of the molecular structure is also shown on an iron with a single terpy ligand. Calculated **(B)** and measured **(C)** vtc -XES spectra of LS and HS $[\text{Fe}(\text{terpy})_2]^{2+}$.



applied to obtain structural data on liquid samples, thereby widening the range of laboratory measurements that previously could only have been performed at synchrotron sources. We successfully demonstrated on the $\text{Ni}^{2+} - \text{EDTA} - \text{CN}^-$ ternary system that a complete speciation study can be performed from laboratory XANES (*X-ray absorption near edge structure*) measurement series, including the determination of the formation constants of the corresponding complexes. Moreover, the technique permits us to determine the local atomic structure around the Ni ion, with particular sensitivity to variations in symmetry. *To best of our knowledge this is the first time that laboratory X-ray absorption spectroscopy was used for such a comprehensive study in solution.*

The $\text{Ni}^{\text{II}} - \text{EDTA} - \text{CN}^-$ (EDTA = ethylenediaminetetraacetic acid) ternary system, in spite of its fairly simple components and numerous investigations, can have several molecular combinations, all of them not being identified unambiguously beforehand. In order to achieve a detailed understanding of the reaction steps and chemical equilibria, methods are required in which the structural transitions in the different reaction steps can be followed via element-selective complex spectral feature sets. While standard optical spectroscopies failed to excel in this task, with the help of our recently developed von Hámos type high energy resolution laboratory X-ray absorption spectrometer, both the structural variations and stability constants of the forming complexes were determined from the same measurement series.

Figure 2 outlines the main results of the study. Fig. 2A shows the FEFF9 calculated XANES spectra for the $[\text{NiEDTA}]^{2-}$, $[\text{NiEDTA}(\text{CN})]^{3-}$, $[\text{Ni}(\text{CN})_4]^{2-}$, and $[\text{Ni}(\text{CN})_5]^{3-}$ complexes (the inset shows the preedge region for each complex calculated via TD-DFT/TDA), which were expected to appear in the studied concentration ranges of the different constituents. Panel B shows the experimentally recorded spectra for a series of Ni^{II} -EDTA-CN⁻ mixtures with different CN⁻ concentrations. In the inset a significant change of the preedge features with a peak around 8336 eV can be observed, representing the formation of four- and/or five-coordinated nickel(II) complexes. From the relative areas of these preedge peaks, the ratio of the tetra- as well as the pentacyanide Ni complexes could be deduced, which is compared to literature based calculated distributions. Based on this distribution, the calculated XANES spectra for the measured samples could be reconstructed (panel D), which agree remarkably well with the experimental ones in panel B.

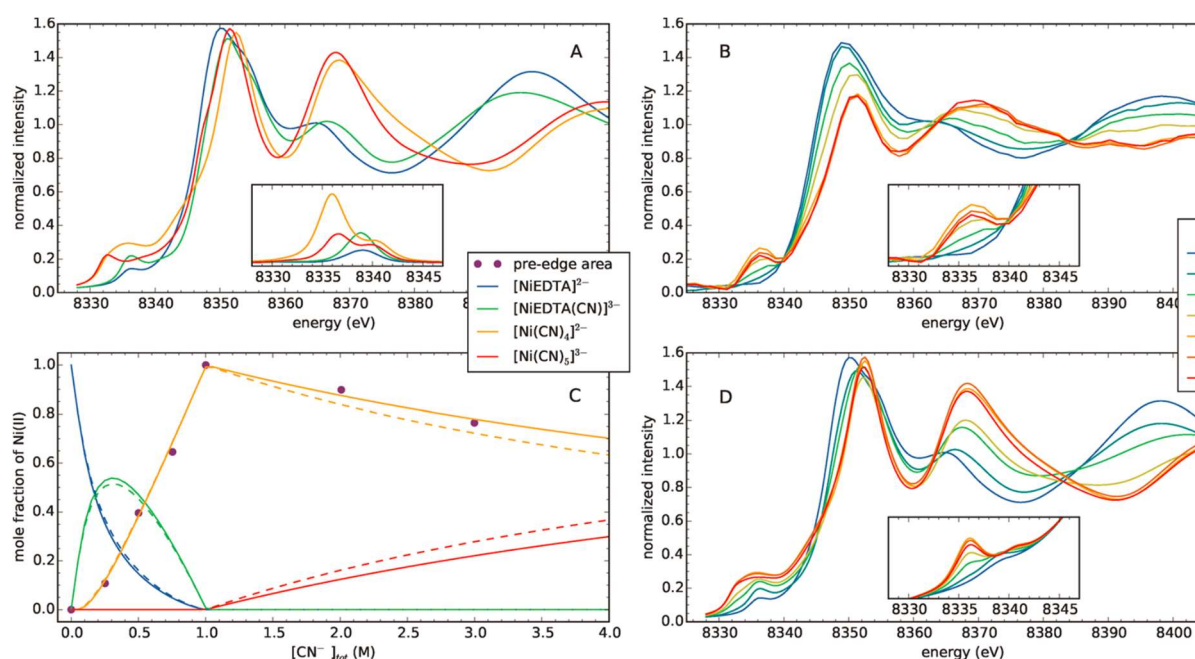


Figure 2. (A) Calculated XANES spectra of the four base complexes. (B) Laboratory XANES spectra of solutions containing constant 0.25 M NiCl_2 and 0.30 M EDTA, while the concentration of the added KCN was varied between 0 and 3 M. (C) Distribution diagram of the following species: $[\text{NiEDTA}]^{2-}$ (blue), $[\text{NiEDTA}(\text{CN})]^{3-}$ (green), $[\text{Ni}(\text{CN})_4]^{2-}$ (yellow), and $[\text{Ni}(\text{CN})_5]^{3-}$ (red). The dashed lines stand for the calculated-, the continuous ones for the XANES preedge fitted distributions. (D) Calculated XANES spectral series for the measured samples based on the determined nickel distribution shown in (C). (The full article can be accessed at <http://dx.doi.org/10.1021/acs.inorgchem.7b02311>.)

Realizing total reciprocity violation in the phase for photon scattering. — The reciprocity principle requires the scattering amplitude to be symmetric for the transposition of the detector and the source. While reciprocity involves the interchange of source and detector, it is fundamentally different from rotational invariance, and is a generalization of time reversal invariance, occurring in absorptive media as well. Reciprocity can be proved as a theorem in many situations and is found violated in other cases. For polarization dependent scatterings reciprocity is often violated, but violation in the phase of the scattering amplitude of X-ray photons oscillating in the attosecond range is much harder to experimentally observe than violation in magnitude.

Enabled by the advantageous properties of nuclear resonance scattering of synchrotron radiation (SR), a maximal - i.e., 180-degree - reciprocity violation in the phase was found. For accessing phase information a new version of stroboscopic detection of nuclear resonance scattering of SR was developed. The scattering setting was devised based on a generalized reciprocity theorem that opens the way to construct new types of reciprocity related devices. The experiment realizing the direct and reciprocal scattering processes was performed at the High Resolution Dynamics Beamline P01 of the PETRA-III synchrotron source of the Deutsches Elektronen Synchrotron (DESY). The beam was scattered on a pair of ^{57}Fe containing foils placed between a polarizer and an analyser, both having an extinction of 10^{-8} , and was subsequently detected by a Si avalanche photo diode. One of foils was a single-line stainless steel absorber mounted on a Mössbauer drive, and the other foil produced the polarization dependent scattering as a result of being magnetic. Each of the six high-frequency and narrow nuclear resonance signals in the magnetic foil gets superposed and produces beats with the corresponding nearby frequency resonance signal in the reference foil. These lower frequency beats are not only more easily detectable but, thanks to the heterodyne setup, also tuneable by the Doppler shift of energy caused by the v_D velocity of the Mössbauer drive. After a pulse, resonances decay as time passes, and one detects counts – essentially, intensity – as a function of time as well as of the drive velocity. This intensity gets multiplied, in the stroboscopic evaluation, by appropriate window functions and then integrated giving spectra shown in Fig. 3. The predicted 180° phase difference between direct and reciprocal data is apparent in Fig. 3d. (The full article can be accessed at <http://dx.doi.org/10.1038/srep43114>.)

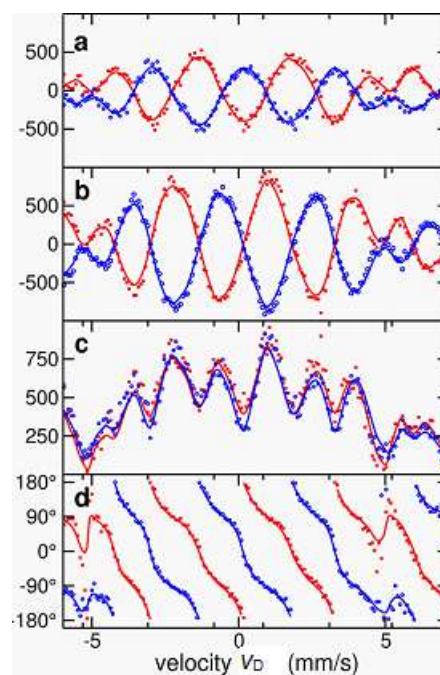


Figure 3. Real part (a), imaginary part (b), magnitude (c) and phase (d) of the complex scattering amplitude. The figure displays the range of the -1^{st} order stroboscopic resonances; dots are experimental signals and continuous lines are theoretical simulations. The agreement between direct (red) and reciprocal (blue) data visible in (c) demonstrates magnitude reciprocity, while (d) shows maximal reciprocity violation in the phase (red and blue curves running with a 180° phase difference).

Grants

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

VEKOP_232-16-2017-00015 Ultrafast molecular and nano-optical switches (G. Vankó, 2017 – 2021)

NKFIH FK124460 Understanding and Controlling the Interplay of Local and Remote Interactions in Transition Metal Compounds with High Potential in IT (Z. Németh, 2017 – 2021)

International cooperation

Main cooperations: Prof. C. Bressler, Dr. W. Gawelda (XFEL.EU, Hamburg), Prof. M. M. Nielsen, Dr. K. Haldrup (Copenhagen), Dr. Thomas Penfold (Newcastle), Drs. G. Doumy, A. M. March, S. H. Southworth, L. Young (Argonne), Dr. Jakub Szlachetko (Kraków), Dr. Chris Milne (SwissFEL, PSI), Prof. F. M. F. de Groot (Utrecht), Dr. Kelly Gaffney (SLAC), Dr. A. Juhin (Paris)

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R-L. Functional nanostructures

Wigner research group

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In situ study of electric field controlled ion transport in the Fe/BaTiO₃ interface.

— The development of more advanced devices which can reflect upon the challenges of our world requires the exploration of novel material properties. Special systems which combine magnetic and electronic properties into a multifunctional material are excellent subject of this demand.

In multiferroic materials (in short *multiferroics*) the coexistence and coupling of ferroelectric and magnetic order enables the fine control and modulation of electric polarization by magnetic field (*direct magnetoelectric effect, ME*) or the magnetic field by electric polarization (*converse magnetoelectric effect*). The electric field control of magnetic spin will lead to significantly lower energy consumption in actuators, information storage and spintronics devices, a key issue for sustainable development. Not only the reduction of energy consumption but also the production of energy from ambient sources such as vibrations, sound, radiofrequency waves, light, temperature gradients and also novel medical applications give new perspectives for multiferroic materials. The Fe/BTO system, as a great example of strong ME coupling, is an excellent system to investigate this phenomenon. Several works reported as well that an applied electric field can alter the properties of this system.

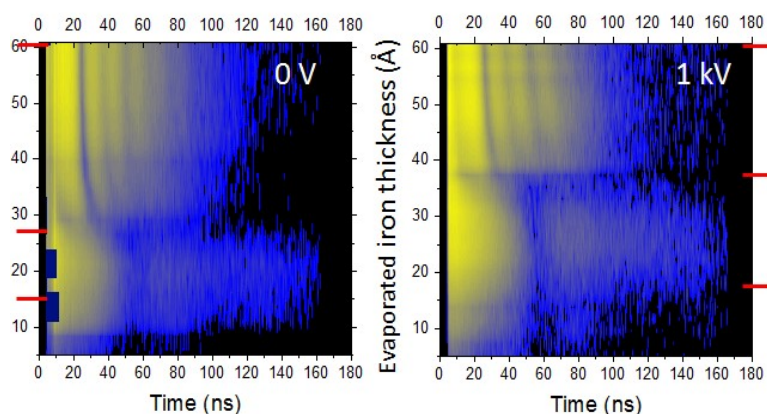


Figure 1. Nuclear forward scattering spectra as a function of deposited iron-57 on BaTiO₃ substrate in case of 0 V and 1 keV applied voltage.

Electric field controlled ion transport and interface formation of iron thin films on a BaTiO₃ substrate have been investigated by in situ nuclear resonance scattering and x-ray reflectometry techniques. At early stage of deposition, an iron-II oxide interface layer was observed. The hyperfine parameters of the interface layer were found insensitive to the evaporated layer thickness. When an electric field was applied during growth, a 10 Å increase of the nonmagnetic / magnetic thickness threshold and an extended magnetic transition region was measured compared to the case where no field was applied. The interface layer was found stable under this threshold when further evaporation occurred, contrary to the magnetic layer where the magnitude and orientation of the hyperfine magnetic field vary continuously. The obtained results of the growth

mechanism and of the electric field effect of the Fe/BTO system will allow the design of novel applications by creating custom oxide/metallic nanopatterns using laterally inhomogeneous electric fields during sample preparation (Fig.1).

Preparation of ^{57}Co ($\alpha\text{-Fe}$) Mössbauer sources of uniform lateral activity distribution. — The quality of Mössbauer source can influence the experimental results, which may lead to false scientific conclusions. Due to the self-absorption of the resonant radiation by the daughter nuclei, the effective half-life of a radioactive Mössbauer source can be significantly decreased in case of high specific activity. For a given initial activity and source area, the lifetime is the longest for the homogenous lateral activity distribution. Besides, for the precise absolute determination of resonant line intensities, the time-dependent effective Lamb–Mössbauer factor of the source needs to be exactly known, a condition which can only be fulfilled for a laterally perfectly homogenous source. This is especially important in Mössbauer polarimetry, a unique laboratory method for the determination of the alignment and direction of magnetisation in buried layers of thin films and multilayers. Due to special geometric and radiation protection conditions, the necessary ^{57}Co ($\alpha\text{-Fe}$) sources are not available commercially.

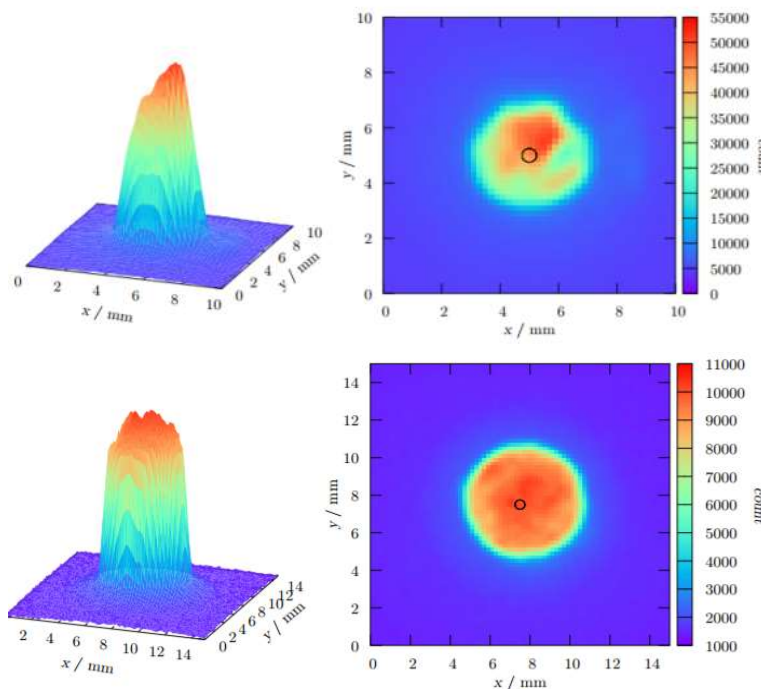


Figure 2. Activity distribution of ^{57}Co ($\alpha\text{-Fe}$) sources prepared without (top) and with (bottom) using the new preparation technology, respectively.

A new technology for preparing ^{57}Co ($\alpha\text{-Fe}$) Mössbauer sources of lateral activity homogeneity better than 10% was elaborated and an application for its patenting has been filed. The homogeneity of the lateral activity distribution was verified by a newly developed scanning setup of about 250 μm lateral resolution. In Fig. 2, the lateral scans of the activity distribution of ^{57}Co ($\alpha\text{-Fe}$) sources prepared without (top) and with (bottom) using the new preparation technology are shown, respectively. It can be seen, that a great improvement in the homogeneity could have been achieved, therefore this novel preparation technology of ^{57}Co ($\alpha\text{-Fe}$)

source is expected to be used widely in Mössbauer polarimetry applications.

International cooperation

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

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See also: R-K.2, S-L.22, S-L.23, S-L.25, S-M.4

R-T. Space technology

Wigner research group

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The long duration of space exploration projects is presented by one of the longest interplanetary missions, the NASA-led Cassini-Huygens mission which ended on 15th September, 2017. Cassini-Huygens involved 17 countries, including our team. The purpose of the mission was the exploration of Saturn and its Titan moon. The mission-carrying missile was launched in Cape Canaveral in 1997 and reached the Saturn area in 2004. Researchers of our institute and our team participated in the development of EGSE (Electronic Ground Support Equipment) for monitoring equipment and calibration systems, the on-board magnetometer (MAG) and the plasma spectrometer (CAPS).

We are involved in the tender of the Zero Magnetic Laboratory in Fertőboz. Our team was modeling ideas of physicists to select optimal implementation. Fig.1. shows the built model (1:6) of the Ruben-5 coil arrangement for external magnetic field attenuation.

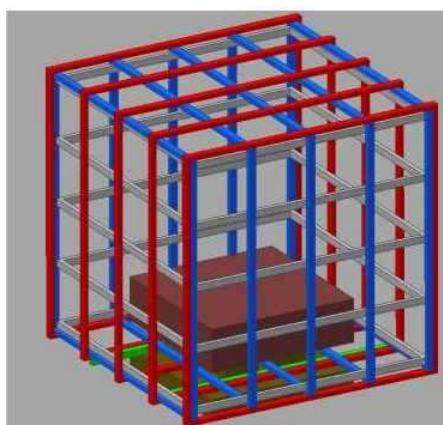


Figure 1. The model of Zero Magnetic Laboratory, and plan of coil system arrangement.

We are participating in the ESA Juice project, which will arrive at Jupiter in 2030, eight years after its start in 2022. It will take measurements for two years around Jupiter. We develop

high-reliability power supply units for this program. Juice has been redesigned several times over the past few years due to weight and performance problems, which also affected the power supply unit we developed. In 2017, the engineering models were produced and then delivered to the Swedish Institute of Space Physics in Kiruna (Fig.2).

Grants

ESA PRODEX- ? Juice (under construction, 2017-2019)

NFM IKF742/2017-NFM:SZERZ Chibis-Obsztanovka-2 (2017-2018)

NFM IKF/ 695 /2017-NFM_SZERZ STRANNIK (2017-2018)

ESA-EMITS -4000120190 Solar Orbiter (2017-2019)

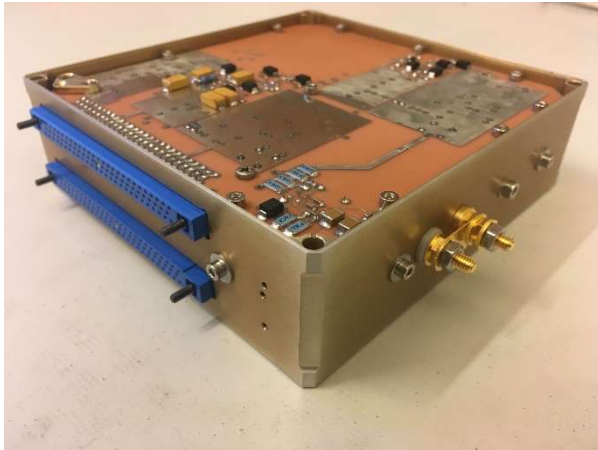


Figure 2. Engineering model of power supply unit supporting 2 DPUs and 3 sensors and individual power supply unit of JDC sensor (Jovian plasma Dynamics and Composition)

International cooperation

IRF (Swedish Institute of Space Physics, Kiruna); Imperial College, London, IKI Moskva; DLR Köln; ESOC, Darmstadt; MPS, Lindau; CNES, Toulouse; IRAP, Toulouse; IWF, Gratz; FMI, Helsinki.

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S-A. Strongly correlated systems

“Momentum” research team

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



Tensor factorization in high dimensional problems and applications to strongly correlated systems in condensed matter physics and quantum chemistry. — In this year we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG), *Matrix Product State* (MPS) and *Tree Tensor Network State* (TTNS) methods. In addition, we have further developed our scientific softwares (**Budapest QC-DMRG program package**), which have been used with great success in numerous research institutes and universities around the world for, e.g., simulating material properties of solid state systems or molecules, or for the quantum simulation of the information technology itself. Further algorithmic developments have also been carried out concerning the quantum chemistry DMRG and Coupled-Cluster (CC) algorithms, and we have carried out the most large-scale calculations available in the literature for tetramethylethane molecule. We have also implemented parallelization in several parts of the code, and worked on further MPI, open-MP and GPU based developments. In addition, during a two-week visit at PNNL (Prof. Karol Kowalski, PNNL, Richland, Washington State, USA) we started the migration of the DMRG algorithm into the NWChem (commercial) program package, which ensures the possibility of massive parallelization. In collaboration with guest researchers from the groups of Uni Ghent and Uni Marburg, we have been working on new algorithmic solutions on the tree-TNS algorithm. As will be presented below, among many others, we have examined strongly correlated electrons in magnetic materials in several quantum phases, exotic quantum phases in ultracold atomic systems, and we have determined multi-orbital correlation and entanglement patterns in molecules, playing important role in chemical compounds.

Interaction effects in a chaotic graphene quantum billiard. — We have investigated the local electronic structure of a Sinai-like, quadrilateral graphene quantum billiard with zigzag and armchair edges using scanning tunneling microscopy (STM) at room temperature in collaboration with the Research Institute for Materials Science, Centre for Energy Research, HAS. We have revealed that besides the $(\sqrt{3}\times\sqrt{3})R30^\circ$ superstructure, which is caused by the intervalley scattering, its overtones also appear in the STM measurements, which are attributed to the Umklapp processes. We have pointed out that these results can be well understood by taking into account the Coulomb interaction in the quantum billiard, accounting for both the measured density of state values and the experimentally observed topography patterns. The analysis of the level-spacing distribution substantiates the experimental findings as well. We have also revealed the magnetic properties of our system which should be relevant in future graphene based electronic and spintronic applications.

A magnetic phase-transition graphene transistor with tunable spin polarization. — Graphene nanoribbons have been proposed as potential building blocks for field effect transistor (FET) devices due to their quantum confinement bandgap. We have proposed a

novel graphene nanoribbon device concept, enabling the control of both charge and spin signals, integrated within the simplest three-terminal device configuration. In a conventional FET device, a gate electrode is employed to tune the Fermi level of the system in and out of a static bandgap. By contrast, in the switching mechanism we proposed, the applied gate voltage can dynamically open and close an interaction gap, with only a minor shift of the Fermi level. Furthermore, the strong interplay of the band structure and edge spin configuration in zigzag ribbons enables such transistors to carry spin polarized current without employing an external magnetic field or ferromagnetic contacts. Using an experimentally validated theoretical model, we have shown that such transistors can switch at low voltages and high speed, and the spin polarization of the current can be tuned from 0% to 50% by using the same back gate electrode. Furthermore, such devices are expected to be robust against edge irregularities and can operate at room temperature. Controlling both charge and spin signal within the simplest FET device configuration could open up new routes in data processing with graphene based devices.

Entanglement and magnetism in high-spin graphene nanodisks. — We have investigated the ground-state properties of triangular graphene nanoflakes with zigzag edge configurations. The description of zero-dimensional nanostructures requires accurate many-body techniques since the widely used density-functional theory with local density approximation or Hartree-Fock methods cannot handle the strong quantum fluctuations. Applying the unbiased density-matrix renormalization group algorithm, we have calculated the magnetization and entanglement patterns with high accuracy for different interaction strengths and compared them to the mean-field results. With the help of quantum information analysis and subsystem density matrices, we have revealed that the edges are strongly entangled with each other. We have also addressed the effect of electron and hole doping and demonstrated that the magnetic properties of triangular nanoflakes can be controlled by electric field, which reveals features of flat-band ferromagnetism. This may open up new avenues in graphene based spintronics.

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

Interplay between exotic superfluidity and magnetism in a chain of four-component ultracold atoms. — We have investigated the spin-polarized chain of ultracold alkaline-earth-metal atoms with spin-3/2 described by the fermionic Hubbard model with SU(4) symmetric attractive interaction. The competition of bound pairs, trions, quartets, and unbound atoms has been studied analytically and by DMRG. We have found several distinct states where bound particles coexist with the ferromagnetic state of unpaired fermions. In particular, an exotic inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-type superfluid of quartets in a magnetic background of uncorrelated atoms has been found for weaker interactions. We

have shown that the system can be driven from this quartet-FFLO state to a molecular state of localized quartets where spatial segregation between molecular crystals and ferromagnetic liquids emerges, and this transition is reflected in the static structure factor.

Role of the pair potential for the saturation of generalized Pauli constraints. — The dependence of the (quasi-)saturation of the generalized Pauli constraints on the pair potential is studied for ground states of few-fermion systems. For this, we have considered spinless fermions in one dimension which are harmonically confined and interact by pair potentials of the form $|x_i - x_j|^s$ with $-1 \leq s \leq 5$. Using the DMRG approach and large orbital basis sets ensures the convergence on more than ten digits of both the variational energy and the natural occupation numbers. Our results confirm that the conflict between energy minimization and fermionic exchange symmetry results in a quasi-saturation of the generalized Pauli constraints (quasipinning), implying structural simplifications of the fermionic ground state. However, a self-consistent perturbation theory reveals that most of that relevance has to be assigned to Pauli's original exclusion principle, except for the harmonic case, i.e., $s=2$. This emphasizes the unique nature of the strong, non-trivial quasipinning found recently for the Harmonium model.

An entropy production based method for determining the position diffusion's coefficient of a quantum Brownian motion. — Quantum Brownian motion of a harmonic oscillator in the Markovian approximation is described by the respective Caldeira-Leggett master equation. This master equation can be brought into Lindblad form by adding a position diffusion term to it. The coefficient of this term is either customarily taken to be the lower bound dictated by the Dekker inequality or determined by more detailed derivations on the linearly damped quantum harmonic oscillator. We have explored the theoretical possibilities of determining the position diffusion term's coefficient by analyzing the entropy production of the master equation. We have shown that the obtained value has a linear dependence on the temperature, which is in marked contrast to previous studies.

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

Correlation analysis of electron-deficit bonds. — We have extended the use of quantum information theory to classify chemical bonds based on multiorbital correlations within the molecule to electron deficient bonds, employing the adequate multireference method of DMRG. First, we have analyzed the bonding structure of the standard diborane(B_2) molecule

and the newly discovered prototype, diborane(4), and we have confirmed that this theory is capable of correct description of bonding in electron deficient bonds, like diborans. Subsequently, we have studied neutral zerovalent s-block beryllium complex, a substance first synthesized in 2016, whose surprising stability was attributed to a strong three-center two-electron π -bond stretching over the C-Be-C core. Our calculations have provided quantitatively adequate images of correlations within the beryllium complex and confirmed the theoretical suggestions on the molecule's stability.

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

Full configuration interaction quantum Monte Carlo benchmark and multireference coupled cluster studies of tetramethyleneethane diradical. — We have performed an FCI-quality benchmark calculation for the tetramethyleneethane molecule in cc-pVTZ basis set employing a subset of CASPT2(6,6) natural orbitals for the FCIQMC calculation. The results are in an excellent agreement with the previous large scale diffusion Monte Carlo calculations by Pozun et al. and available experimental results. Our computations have verified that there is a maximum on potential energy surface of the ground singlet state (1A) 45° torsional angle and the corresponding vertical singlet-triplet energy gap is 0.01 eV. We have employed this benchmark for the assessment of the accuracy of MkCCSDT and DMRG-tailored CCSD (TCCSD) methods. Multireference MkCCSDT with CAS(2,2) model space, though giving good values for the singlet-triplet energy gap, is not able to properly describe the shape of the multireference singlet potential energy surface. Similarly, DMRG(24,25) is not able to correctly capture the shape of the singlet surface, due to the missing dynamic correlation. On the other hand, the DMRG-tailored CCSD method describes the shape of the ground singlet state with an excellent accuracy, but for the correct ordering, computation of the zero-spin-projection component of the triplet state (3B_1) is required.

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Freie Universität (Berlin, Germany), Basis optimization using MPS based approach (C. Krumnow, R. Schneider, J. Eisert); Application of quantum information theory to molecular systems (E. Fertitta, C. Stemmler, B. Paulus)

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Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Poland, Application of quantum information theory to molecular systems (K. Boguslawski, P. Tecmer).

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S-C. Long-range order in condensed systems

Wigner research group

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Superconductivity in layered heterostructures. — During the previous years, a novel and unique computer code was developed which allows us to study the nature of the Andreev bound states related to the proximity effect in normal metal–superconductor heterostructures based on the first-principles Bogoliubov–deGennes (BdG) equations. For the first time, we succeeded in applying the SKKR method for solving the Kohn–Sham–Bogoliubov–deGennes (KSBDG) equation which allowed us to investigate the quasiparticle spectrum of superconducting heterostructures. This year, a fully relativistic generalization of the BdG equations within Multiple Scattering Theory has been derived. The method allows the solution of the first-principles Dirac–Bogoliubov–de Gennes equations combined with a semi-phenomenological parametrization of the exchange–correlation functional. The major difficulty during the development was to derive simple conditions for the case when the right-hand-side and left-hand-side solutions must be treated separately while setting up the corresponding Green function. As an application of the theory, we calculated the superconducting order parameter in Nb/Fe and Nb/Au/Fe systems. We found Fulde–Ferrell–Larkin–Ovchinnikov like oscillations in the iron layers, but more interestingly an oscillatory behaviour is observed in the gold layers as well.

Thin Film Magnetism. — Non-collinear magnetic structures have been investigated in ultrathin films by combining *ab initio* electronic structure calculations with numerical spin model simulations. The experimentally observed significant increase in the spin spiral period as a function of temperature of three-atomic-layer thick Fe films on Ir(111) has been explained. *Ab initio* calculations revealed how the addition of hydrogen to a two-atomic-layer thick Fe film on Ir(111) leads to the formation of magnetic skyrmions in place of the spin spiral ground state of the pristine system, in agreement with scanning tunneling microscopy measurements. Theoretical predictions have been made on the characterization of skyrmionic structures with various topological charges.

High Entropy Alloys. — Looking for high-strength and high-temperature-resistant high-entropy alloys (HEAs) new refractory HEA compositions have been predicted theoretically by combining a refractory CrMoW alloy with late transition metals (LTM = Ni, Co, Fe, and Mn). *Ab initio* calculations revealed that the LTM additions increase the ductility, but reduce the strength of these CrMoW based alloys with single-phase BCC structure.

The magnetization components of permeability spectra for annealed nanocrystalline (Finemet) core have been studied and four contributions have been revealed for the first time in the literature: i) eddy current; ii) Debye relaxation of magnetization rotation, iii) Debye relaxation of damped domain wall motion and iv) resonant type DW motion. Although the relative weight of these contributions changes with the frequency and exciting field amplitude, the role of eddy current cannot be neglected even for the smallest applied field. These components can be found in the powder cores of soft magnetic composites as well.

Observation of spin-quadrupolar excitations in $\text{Sr}_2\text{CoGe}_2\text{O}_7$ by high-field electron spin resonance. — When we think of a spin, usually we imagine an arrow pointing somewhere (representing the expectation values of the components of the spin operator), and with the arrow we associate a magnetic moment. Upon time reversal, the arrow reverses its direction. This is a reasonable picture for the spin $1/2$ of the electron, but for larger spins this does not exhaust all the possibilities. For example, the dimension of the Hilbert space is 3 for the spin 1, and we can construct spin states for which the expectation values of all the three spin operators vanish — the state does not point anywhere, it cannot be represented by an arrow. The simplest example is the 0 eigenstate of the S_2 operator. In fact, there are three linearly independent such states (the zero eigenstate of the S_x , S_y and S_z operators), spanning the Hilbert space. Though they cannot be represented by an arrow, they still break the rotational symmetry, since quadratic forms of spin operators differentiate among them. Instead of arrows, we can use directors (like in the case of liquid crystals), as the rotation by π around an axis perpendicular to the director returns the same state (up to a phase factor). These states are called spin-quadrupoles. Furthermore, these states do not break the time-reversal symmetry.

Similarly, the long-range-ordered states of interacting spins are usually time-reversal-breaking states, with a configuration of “arrows” that repeats itself on the lattice. However, under favorable conditions, interacting spins can produce ordered states where the order parameter is of spin-quadrupolar character which does not break the time reversal symmetry. Theoretically, such phases have been established in spin-one Heisenberg models extended with higher-order spin interactions. Even more interestingly, time-reversal invariant ordered states can also be realized in spin- $1/2$ systems, where the quadrupole-like order parameter is distributed between two spins on a bond, leading to a so-called nematic ordering.

These theoretical developments have inspired the quest to nematic and quadrupole phases in real materials. However, when relying on standard experimental methods, such phases usually remain hidden. Most of the experimental probes detect spin-dipolar ($\Delta S=1$) transitions, and they do not interact with the spin-quadrupoles, as their detection requires $\Delta S=2$ transitions.

In a collaboration with experimental researchers from Osaka University, we found an unambiguous experimental observation of spin-quadrupolar excitations in the layered $\text{Sr}_2\text{CoGe}_2\text{O}_7$ multiferroic compound. In this compound, the Co ions are in the centers of tetrahedra formed by the four surrounding O ions (Fig. 1). Since the inversion symmetry is absent, the relativistic spin-orbit coupling allows the coupling of the electric polarizations to the spin-quadrupolar operators. Due to this magnetoelectric coupling present in the $\text{Sr}_2\text{CoGe}_2\text{O}_7$, the non-magnetic, purely spin-quadrupolar excitation becomes electrically active and detectable by electromagnetic waves, like the electron spin resonance spectroscopy.

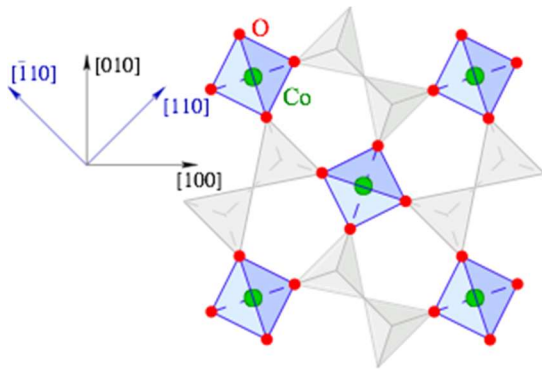


Figure 1. The schematic crystal structure of the $\text{Sr}_2\text{CoGe}_2\text{O}_7$ multiferroic compound projected onto the ab plane. The green spheres represent the magnetic Co^{2+} ions with $S = 3/2$ surrounded by four O^{2-} ions (red) in an alternating tetrahedral environment.

In the electron spin resonance spectra of $\text{Sr}_2\text{CoGe}_2\text{O}_7$ above the saturation field of 20T, a mode with twice the g-factor of the usual modes is observed (Fig. 2). This indicates the absorption of two magnons, just what is needed for the creation of a quadrupole wave. Indeed, we could explain the features of the experimental spectra taken in different geometries by a simple theoretical model of the spin-quadrupolar wave providing not only a qualitative description, but also a quantitative agreement.

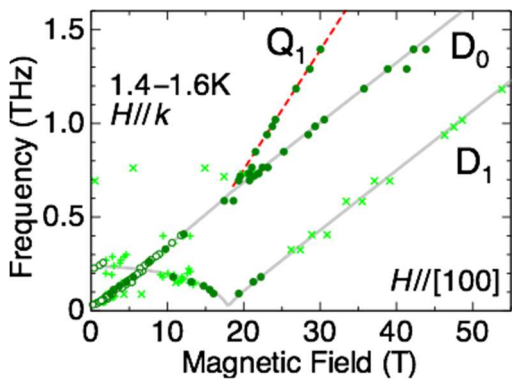


Figure 2. Frequency-field diagrams of the ESR resonance fields of $\text{Sr}_2\text{CoGe}_2\text{O}_7$ for magnetic fields parallel to the $[100]$ direction of the external magnetic field. The solid lines represent the dipolar resonance modes from the multiboson spin-wave theory. The red dashed line indicates a resonance mode with a slope twice larger than the others, corresponding to a two-magnon excitation — the quadrupolar mode.

The most significant point of our finding is the first observation of non-magnetic spin-quadrupolar excitation in an antiferromagnetic material (Fig. 3). Such quadrupolar degrees of freedom become inherent in systems with larger than $S=1/2$ magnetic moments, regardless of the presence of magneto-electric coupling. Upon condensing such multipolar excitations, magnetically disordered exotic quantum phases may arise. The experimental identification of quadrupole excitations with vanishing gap gives us a possibility to identify long-sought nematic phases, which stand without any usual magnetic fingerprint and are almost impossible to tell apart from other non-magnetic phases. Furthermore, our work will stimulate the application of the magnetoelectric effect as a spectroscopy tool.

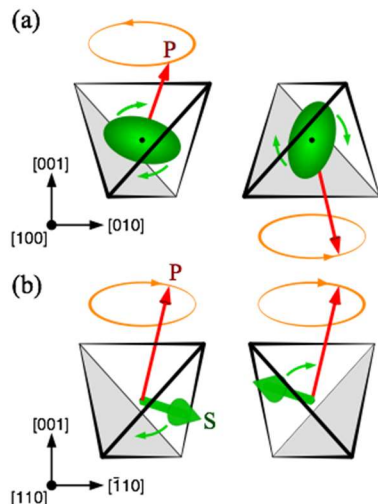


Figure 3. Schematic plot of (a) the Q_1 quadrupolar mode for $H//[100]$ and (b) the dipolar modes for $H//[110]$, as seen from the direction of the magnetic field. In both cases the oscillating component of the uniform electric polarization P (shown by orange ellipse) is perpendicular to the external magnetic field H , therefore they are active in the Faraday configuration. The green ellipse represents the rotating quadrupolar moments, while the green arrows the precessing dipolar spins on the two sublattices. The red arrows show the electric polarization vectors which are excited by the oscillating electric field.

Grants and international cooperation

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HAS NKM-44/2017: Optical magnetoelectric effect and spin dynamics in multiferroics (K. Penc, 2017-2019)

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S-D. Semiconductor nanostructures

“Momentum” research team

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Design and fabrication of semiconductor nanostructures for bioimaging, quantum computing and 3rd generation photovoltaics. — The research team is active in three main different fields: develop new type of i) biomarkers, ii) quantum bits for quantum computation, and iii) 3rd generation solar cells. Next, we summarize our important achievements.

Development of biomarker systems. — Biologists urgently need biomarker systems which trace, e.g., cancer cells in the blood stream or provide fluorescent signals depending on the activity of neurons in brain. Such systems have been developed so far, but most of them are either unstable or toxic, thus they are not suitable for therapy. Our Semiconductor Nanostructures Research Group is, however, seeking such solutions that can be applied *in vivo*. Molecular-sized colloidal SiC nanoparticles are very promising candidates to realize bioinert non-perturbative fluorescent nanoparticles for *in vivo* bioimaging. These SiC nanoparticles are prepared by wet chemical etching of large SiC particles. However, the mechanism behind the etching process was far from being understood. We developed a non-photon exciton generation chemistry (NPEGEC) theory based on the experiments on SiC polytypes as a model semiconductor (see Fig. 1). Our theory applies to materials with a finite band gap. Furthermore, we could demonstrate the control over the size of SiC nanoparticles that we produce from the cubic layers of bulk cubic silicon carbide that contains hexagonal inclusions.

Nitrogen vacancy center (NV). — 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. Diamond is a known host of solid state qubits and single photon emitters. NV center stands out among these qubits in terms of robustness of optical spin readout and initialization. The optical readout of electron spin is based on the intersystem crossing (ISC) between the optically active triplet states and the dark singlet states. However, the intricate details about the ISC processes were not fully understood. By combining the theory of dynamic Jahn-Teller system and first principles calculations, we could identify the ISC routes and their rates for the transition between the excited state triplet and a nearby singlet state (see Fig. 2).

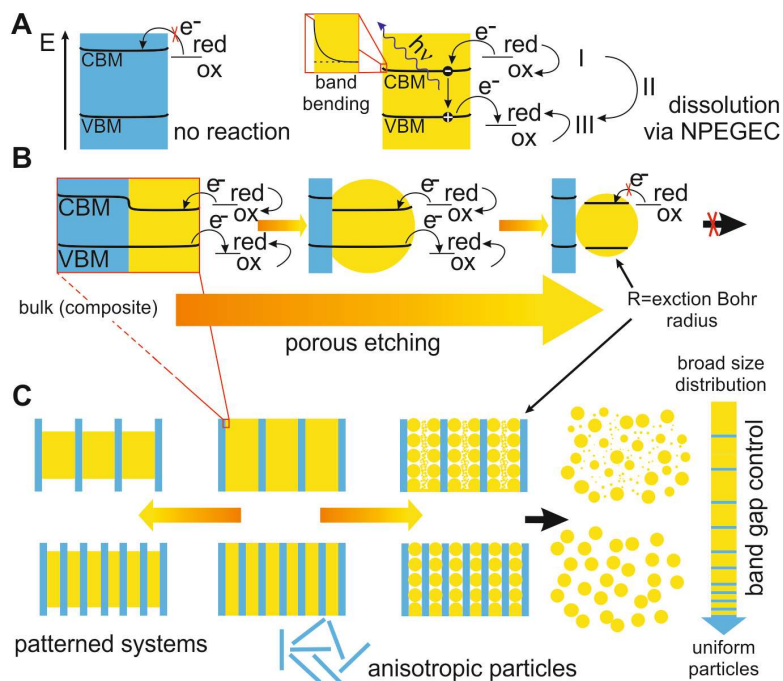


Figure 1. The mechanism “no-photon exciton generation chemistry” (NPEGEC) for stain etching of semiconductors. (A) The blue region depicts a semiconductor with a larger band gap that is resistive against etching while the yellow region represents a suitable material. A redox couple with redox potential higher (more negative) than the conduction band minimum (CBM) energy can inject electrons into the conduction band (I). The oxidized molecule itself, or the molecule formed after further transformation in the solution (II) can inject holes into the valence band (VB) with a maximum energy of VBM (III). The generated excitons can recombine with photon emission with energy $h\nu$ or can lead to material dissolution. (B) In a material with spatially varying band structure selective etching is possible. The exciton Bohr radius limits the radius (R) of the final nanoparticle. (C) Patterned band structure in a macroscopic material can serve as a template for various nanostructures including patterned nanowires, anisotropic or uniform particles.

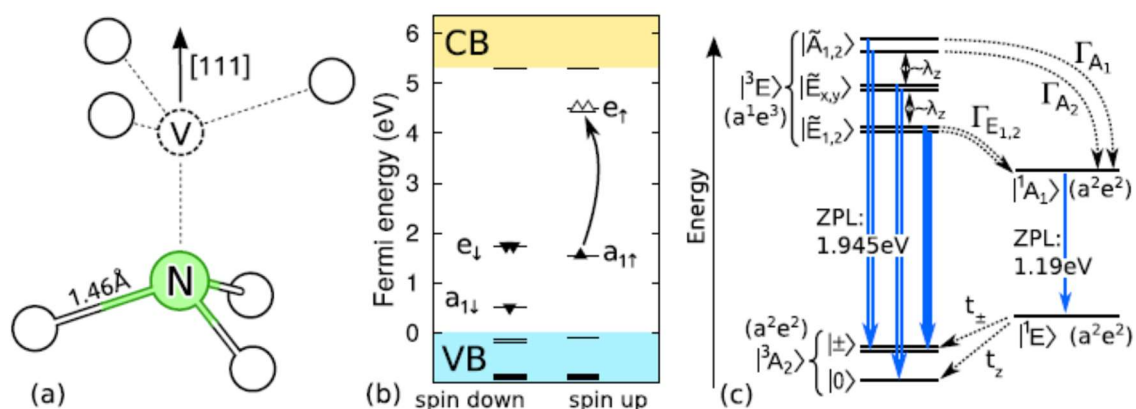


Figure 2. NV center in diamond. (a) Schematic diagram of the structure of the negatively charged defect with the optimized carbon-nitrogen bond length. The symmetry axis of the defect in the diamond lattice is shown. (b) The calculated defect levels in the gap are depicted in the ground state where the curved arrow symbolizes the Δ SCF procedure for creating the triplet excited state. The e states are double degenerate. VB and CB correspond to valence and

conduction bands, respectively. (c) The corresponding ground state and excited states are shown as well as the optical electron spin polarization cycle. The spin-orbit splitting λz is depicted that separates the sublevels in the triplet 3E excited state. The corresponding intersystem crossing rates between the 3E substates ($\sim A_{1,2}$, $\sim E_{1,2}$ double group representations) and the singlet 1A_1 are labeled by Γ_s . The tilde labels the vibronic nature of these states. The intersystem crossing (t_{\pm} and t_z) from the 1E to the triplet ground state is shown for the sake of completeness and closes the spin polarization cycle.

The diamond NV center can be used as a nanoscale sensor when engineered close to the diamond surface. However, the surface termination of diamond can affect the charge state and photo-stability of NV center that may compromise the sensitivity of NV center. We predict from first principles calculations that nitrogen-terminated (111) diamond would be ideal to maximize the sensitivity of near-surface NV centers (see Fig. 3). Furthermore, the array of $I=1$ nuclear spins of ^{14}N isotopes on the surface can be used to realize a quantum simulator of special spin systems.

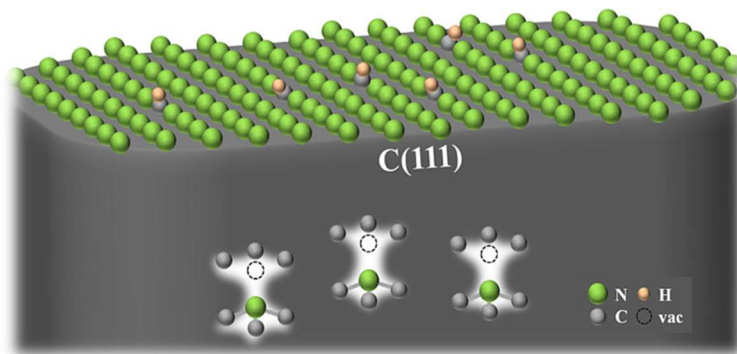


Figure 3. The (111) surface of diamond terminated with nitrogen atoms. Nitrogen vacancy centers below the terminated surface enjoy a near-bulk physical environment, e.g. long spin coherence time, which makes them useful for quantum bit and nanometrological applications.

Divacancy defect in SiC. — Another prominent solid state qubit candidate is the so-called divacancy defect in SiC which has a high-electron-spin ground state. Divacancy qubit can be formed in cubic and hexagonal polytypes, however, the key magneto-optical parameters and rates were not known for these qubits. In collaboration with the Awschalom group at Chicago University, we characterized thoroughly these qubits (see Fig. 4). We found that an efficient spin-to-photon interface can be realized by these divacancy qubits at cryogenic temperature and resonant optical excitation. Furthermore, we identified a room temperature qubit in hexagonal SiC as Si-vacancy at the so-called cubic site in hexagonal SiC by means of first principles calculations. This Si-vacancy qubit has a great potential in thermometry and magnetometry applications at the nanoscale.

Furthermore, we studied nanosystems that are promising in biomarker and solar cell applications. The silicon nanoparticles (Si NPs) are very promising in various emerging technologies and for fundamental quantum studies of semiconductor nanocrystals. Heavily boron and phosphorus codoped fluorescent Si NPs can be fabricated with diameters of a few nanometers. However, very little is understood about the structure and origin of the fluorescence of these NPs. We performed a systematic time-dependent density functional study of hundreds of codoped Si NPs representing millions of configurations. We identified the most stable dopant configurations and a correlation between these configurations and their optical gaps. We find that particular dopant configurations result in emission in the second biological window, which makes these nanoparticles viable for deep-tissue bioimaging applications. We also found that the radiative lifetime of Si NPs is intrinsically long, thus the

electron-hole pairs generated by illumination can principally be separated. This concludes that heavily doped Si NPs can be applied as an absorbant for Si based solar cells.

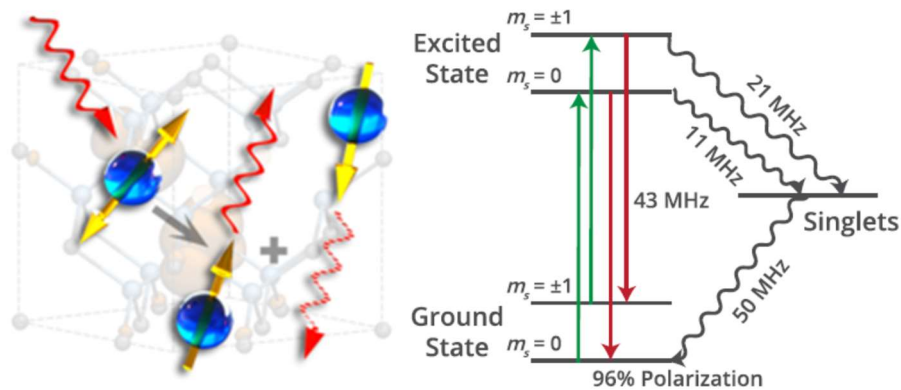


Figure 4. Dynamical model of the 3C-SiC divacancy. Left: An artistic view about the optical spin polarization of divacancy spins. Right: Diagram of the levels and major rates in the five-level rate-equation model. The transition rates and ground-state spin polarization are inferred from the combination of experimental data, group theory considerations and input from first principles calculations.

Grants

NKFI NN-118161: JST V4: Nanophotonics with metal – group-IV-semiconductor nanocomposites: From single nanoobjects to functional ensembles (NaMSeN, A. Gali, 2016-2018)

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International cooperation

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

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Materials Modeling and Development Laboratory, National University of Science and Technology "MISIS," (Russia), solid-state quantum bits (Igor A. Abrikosov)

Institute for Experimental Physics II, Universität Leipzig, solid-state quantum bits (Jan Meijer)

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S-J. Gas discharge physics

Wigner research group

Kinga Kutasi, Aranka Derzsi, Zoltán Donkó, Péter Hartmann, Péter Magyar[#], Pál Mezei[^]



Gas discharge physics. – We have addressed several aspects of charged particle kinetics and transport in low-temperature plasmas. Particular attention has been devoted to the non-linear effects, like the spontaneous pattern formation in electronegative discharge plasmas driven by radiofrequency (RF) voltage sources. In strongly electronegative gases, like carbon-tetrafluoride, a positive ion – negative ion plasma is formed with a strongly depleted electron density, due to the (dissociative) electron attachment to molecules, which in this way form negative ions. We have shown that a resonance between the excitation (radio) frequency and the eigenfrequency of the ion-ion plasma leads to an instability, which, in turn, creates prominent non-linear structures. The dependence of this pattern formation mechanism on the discharge conditions, such as the driving voltage amplitude and frequency, as well as the electrode separation and gas pressure, has been studied in detail.

By using our Particle-in-Cell/Monte-Carlo Collisions (PIC/MCC) simulation code, we have investigated the electron heating and ionization dynamics in capacitively coupled oxygen discharges driven by tailored voltage waveforms at different fundamental frequencies and at different pressures. We have found transitions of the discharge electron heating mode from the drift-ambipolar mode to the α -mode, induced by changing the number of consecutive harmonics included in the driving voltage waveform or by changing the gas pressure. We have found that changing the number of harmonics in the waveform has a strong effect on the electronegativity of the discharge, on the generation of the DC self-bias and on the control of ion properties at the electrodes. Furthermore, we have investigated the effect of the surface quenching rate of $O_2(a)$ metastable molecules on the spatio-temporal excitation patterns. We have obtained good agreement between the spatio-temporal distributions of the excitation rates obtained from the simulations and those derived from phase-resolved optical emission spectroscopy measurements. This benchmarking study was complemented with a sensitivity analysis of the results on the rates of selected plasma-chemical reaction processes.

We have developed a realistic model for the description of the electron-surface interaction in capacitively coupled plasmas and incorporated this model into our PIC/MCC simulation code. This realistic model considers the elastic reflection and the inelastic backscattering of electrons, as well as the emission of electron-induced secondary electrons taking into account the properties of the surface. By using this model, we have studied the influence of the electron-induced secondary electrons on the plasma parameters in argon gas at low pressures, for SiO_2 electrodes. Compared to the results obtained by using a simplified model for the electron-surface interaction, we have found that the electron-surface interactions strongly influence the electron power absorption and ionization dynamics (see Fig. 1).

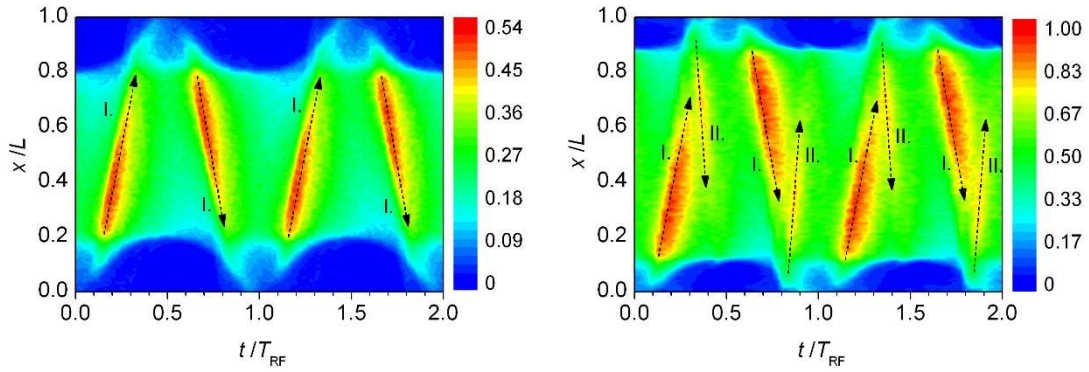


Figure 1. PIC/MCC simulation results on the spatio-temporal distributions of the ionization rate [$10^{21}m^{-3}s^{-1}$], based on a simplified model (left plot) and a realistic model (right plot) for the electron-surface interaction. Discharge conditions: argon, SiO₂ electrodes, 6.7 cm electrode gap, 0.5 Pa, 13.56 MHz, 1000 V. The horizontal axis corresponds to two RF periods. The vertical axis shows the normalized distance from the powered to the grounded electrode.

Strongly coupled plasmas. – In the field of strongly coupled plasmas (SCP), we have contributed by molecular dynamics simulations to the validation of the theoretical “method of moments” approach, which allows the determination of the characteristics of the collective modes (including their damping), based solely on static characteristics (i.e., the static structure factor, or the pair correlation function) of the plasma. We presented the first experimental measurement of the 3-point static structure factor, $S^{(3)}(k_1, k_2, k_0)$, of a 2-dimensional dusty plasma liquid. The higher-order structure factor was as well computed from molecular dynamics simulations and very good agreement was obtained between the two sets of data (see Fig. 2). Both the measurements and the simulations confirmed the existence of negative values of $S^{(3)}(k_1, k_2, k_0)$; this indicates the breakdown of the convolution approximation that gives $S^{(3)}(k_1, k_2, k_0)$ in a factorized form of $S^{(2)}$ (2-point) functions. According to the quadratic fluctuation-dissipation theorem, a changing sign of $S^{(3)}(k_1, k_2, k_0)$ implies a sign change of the quadratic part of the density response function of the system and an intriguing vanishing quadratic response at a certain wavenumber.

Dusty plasmas. – In the field of dusty plasma physics, we have developed a new, very simple and sensitive method to measure the sputtering rate of solid materials in stationary low-pressure gas discharges. The method is based on the balance of the centrifugal force and the confinement electric force acting on a single electrically charged dust particle in a rotating environment. We have demonstrated the use and sensitivity of this method in a capacitively coupled radio frequency argon discharge. We were able to detect a reduction of 10 nm in the diameter of a single dust particle and have measured the reduction rate of 6 nm/min of the particle radius.

A magnetic field was recently shown to enhance the field-parallel heat conduction in a strongly correlated plasma whereas cross-field conduction is reduced. With three-dimensional molecular dynamics simulations relevant to dusty plasmas, we have shown that in such plasmas, the magnetic field has the additional effect of inhibiting the isotropization process between field-parallel and cross-field temperature components, thus leading to the emergence of strong and long-lived temperature anisotropies when the plasma is locally perturbed. We have presented an extended heat equation, which is able to describe this process accurately.

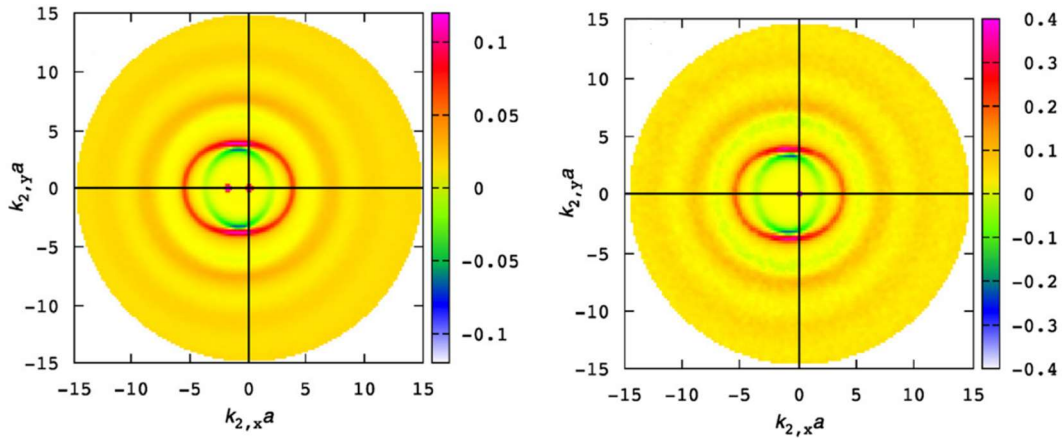


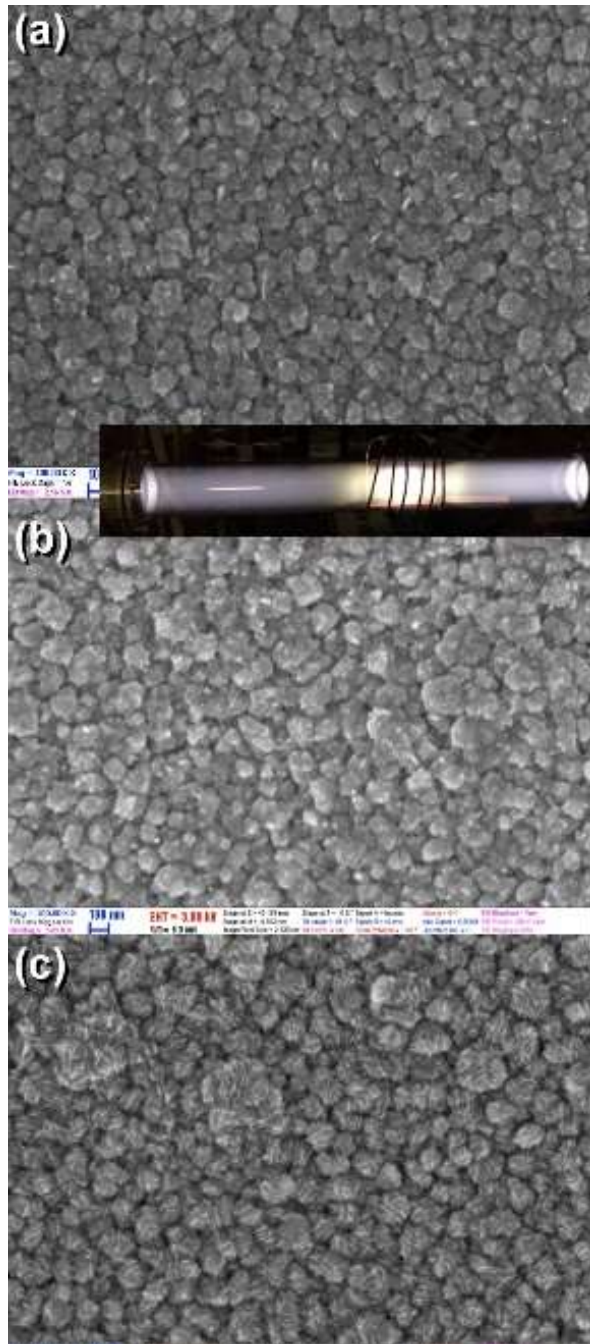
Figure 2. Maps of the full $S^{(3)}(k_1, k_2, k_0)$ 3-point static structure factor of strongly coupled Yukawa-liquids at a wave vector $k_1 a = (1.85, 0)$. Left: experimental data obtained on a 2-dimensional dusty plasma, right: results of molecular dynamics simulations at the same plasma parameters (a coupling coefficient of 95 and a screening coefficient of 0.7).

Technological application of high-frequency discharge systems. – Based on our experience gained during the biological decontamination studies on afterglow plasmas, we have joined another fast-developing field, namely plasma agriculture, which is aimed to develop new technology for agriculture. We used the afterglow of a surface-wave microwave discharge to investigate the effect of different afterglow plasmas on cereal crops. In our study, we treated non-infected and infected cereal crops, respectively, in the afterglow of Ar/N₂-O₂ surface-wave microwave discharges at 2-8 mbar pressure, using the following initial gas mixtures: (i) N₂-20%O₂, (ii) N₂-10%O₂, (iii) N₂-2%O₂, (iv) Ar-20%O₂, (v) Ar-40%O₂ and (vi) Ar-20%O₂ + N₂-2%O₂, which made possible to isolate different species and identify their role in the process. We have shown that the germination and vigour of non-infected seeds are not significantly effected when barley is treated max 120 s at 2 mbar and maize 240 s at 4 mbar. On the other hand, seeds can be disinfected from the germination inhibitors *F. graminearum* and *F. verticillioides*. The most efficient treatment, which also increases the germination of infected seeds above 80%, is the 3 min Ar-20%O₂ afterglow at 4 mbar for barley, while for maize the 4 min Ar-20%O₂+2 min N₂-2%O₂ afterglow at 8 mbar. The high NO-content mixtures and the heating of seed surface by the recombination of O and N-atoms inhibit barley germination.



Figure 3. The post-discharge system with the surface-wave microwave discharge operating in N₂-20%O₂ mixture during seed treatments.

We have studied the formation of oxide structures on copper plates in the discharge sheath and in the afterglow region of an inductively coupled rf discharge at different gas mixtures, input power and treatment time, as well as in the afterglow of a surface-wave microwave (mw) discharge, and compared the two systems. In the sheath of the rf discharge, regular shapes have been formed with incipient growth of nanowires as shown in Fig. 4 (a).



Higher power, which results in higher temperature, contributed to thicker layer formation, while lower powers to the structuring of the oxide layer. The oxidation in the afterglow was found to be much faster, in few minutes a thick layer was formed which detached after a threshold thickness. Depending on the oxygen content and gas temperature, different structures could be created. At lower O₂ content mixture (50 sccm Ar-10 sccm O₂), larger individual structures have been formed, with the attempt of wires to grow on them. At the same low flow rate, with further decrease of the input power, wall structures were found, and, similarly, also in the afterglow of the mw discharge at 500 sccm N₂ – 120 sccm O₂. Fig. 4 (b)-(c) show the restructuring of the copper-oxide layer created in RF afterglow with the N₂-O₂ mw afterglow, showing the wall shape structuring of the initial structures. In case of Ar-O₂ mw discharge, the oxidation rate is very low due to the lower temperature compared to the N₂-O₂. We have found that the wall structure, which is the basic element of the structures, can be created at lower oxidation rate, which is related to lower temperature and lower O-atom density. In case of a surface-wave microwave discharge system, this can be easily tuned with the gas flow rate and the position of the wave launcher along the discharge tube.

Figure 4. (a) Copper-oxide surfaces created in the discharge region of the 50 sccm O₂, 50 W rf discharge. (b) The copper-oxide surface created in the afterglow of the 10 sccm O₂, 20 W rf discharge. (c) The (b) surface restructured in the N₂-O₂ mw afterglow.

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OTKA K-104531 High and low-frequency discharges for biomedical applications and nanostructuring (K. Kutasi 2012-2017.08.31)

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NKFI K-119357 Non-equilibrium charged particle kinetics in ionized gases (Z. Donkó, 2016.11.01-2020.10.31.)

NKFI PD-121033 Reactive gas discharges excited by tailored voltage waveforms (A. Derzsi, 2016-2019)

NKFI K-115805 Complex plasmas in action (P. Hartmann, 2015-2019.08.31)

Bilateral HAS – Serbian Academy of Sciences Interaction of non-equilibrium atmospheric pressure plasmas with model surfaces (K. Kutasi, 2016-2018)

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International cooperation

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J.-P. Booth (Ecole Polytechnique, Paris)

Baylor University, Texas

Satoshi Hamaguchi (Osaka University)

Institute of Physics, Zagreb, Plasma agriculture (Slobodan Milosevic)

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

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

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

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S-K. Liquid structure

Wigner research group

Pál Jóvári, László Kőszegi^A, Ildikó Pethes, Szilvia Pothoczki, László Pusztai, Erzsébet Sváb^A, László Temleitner



Understanding disordered structures. — Our research group is involved in the investigation of short-range order of liquids, amorphous materials and disordered crystals. We combine experimental data such as X-ray and neutron diffraction structure factors 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 configurations (typically tens of thousands of atoms) are provided that are energetically reasonable and 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. The group is also responsible for the maintenance and operation of the MTEST neutron diffractometer installed at the 10 MW Budapest Research Reactor. Below, we provide some selected results from the year of 2017.

Metallic glasses. — The structure of glassy $\text{Cu}_{47.5}\text{Zr}_{47.5}\text{Ag}_5$ has been investigated by neutron diffraction with isotopic substitution, X-ray diffraction as well as with Cu and Ag K-edge extended X-ray absorption spectroscopy (EXAFS) measurements. Experimental datasets have been fitted simultaneously with the reverse Monte Carlo simulation technique. Nearest-neighbor distances and coordination numbers have been determined and compared with those of glassy $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{47.5}\text{Zr}_{47.5}\text{Al}_5$. It has been found that the Cu-Cu coordination number drops upon adding Al or Ag to $\text{Cu}_{50}\text{Zr}_{50}$. Both Ag and Al prefers Zr to Cu. The total coordination number of Ag is 13.9 ± 0.6 while that of Al is 10.2 ± 1.0 , suggesting that, in spite of their similar molar volumes, the effective size of Ag and Al in the Cu-Zr matrix is quite different. This is reflected both by the comparison of Zr-Al and Zr-Ag partial pair distribution functions and the Zr-X-Zr (X=Al, Ag) cosine distributions (see Fig. 1.)

Alcohol-water mixtures. — Our efforts concerning the structure of alcohol-water liquid mixtures have been extended to the study of the temperature dependence of the structure of aqueous solutions of methanol. The evolution of the structure of liquid water-methanol mixtures as a function of temperature has been studied by molecular dynamics simulations, with a focus on hydrogen bonding. The combination of the OPLS-AA (all atom) potential model of methanol and the widely used SPC/E water model has provided excellent agreement with measured X-ray diffraction data over the temperature range between 298 and 213 K, for mixtures with methanol molar fractions of 0.2, 0.3 and 0.4. Hydrogen bonds have been identified via a combined geometric/energetic, as well as via a purely geometric definition. The number of recognizable hydrogen bonded ring structures in some cases doubles while lowering the temperature from 298 to 213 K; the number of sixfold rings increases most significantly. An evolution towards the structure of hexagonal ice, that contains only sixfold hydrogen bonded rings, has thus been detected on cooling water-methanol mixtures. For a picture of typical hydrogen-bonded ring structures, see Figure 2.

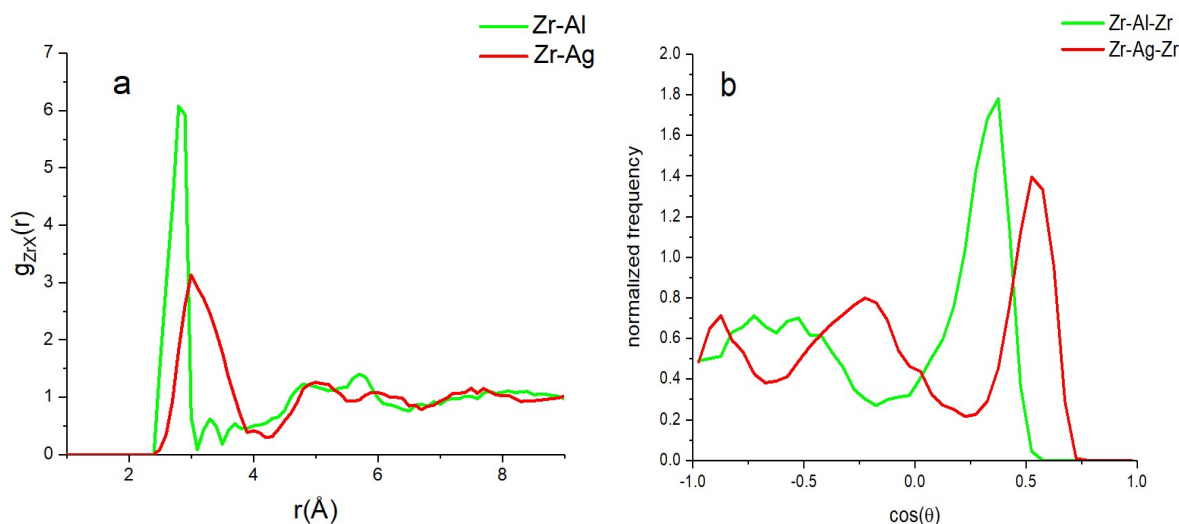


Figure 1. Effective size difference of Al and Ag atoms in the Cu-Zr host matrix as reflected by the position of the first peak of Zr-Al and Zr-Ag partial pair distribution functions (a) and by the Zr-Al-Zr and Zr-Ag-Zr cosine distributions (b)

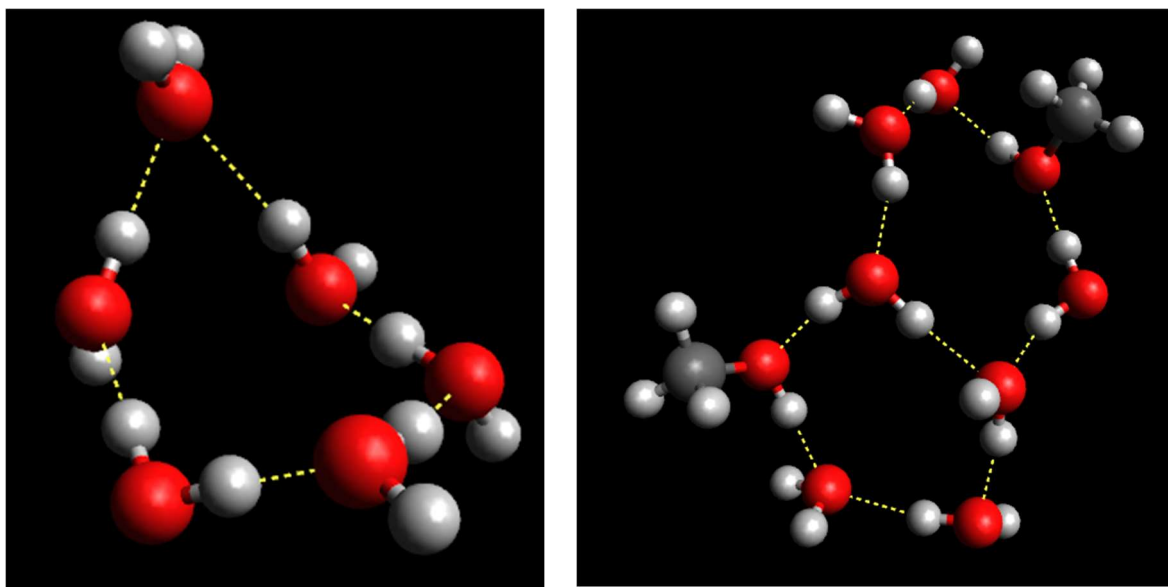


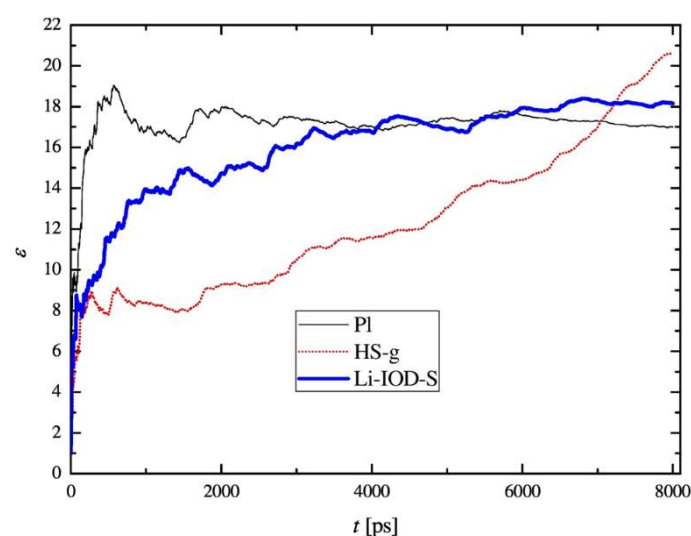
Figure 2. Hydrogen-bonded ring structures in methanol/water mixtures (Red: O atoms; light grey: H atoms; dark grey: C atoms. Dashed lines represent hydrogen bonds between molecules.)

Liquid chalcogenides. — The short-range order in the liquid state of GeTe, a prototypical phase-change material employed in data storage devices, has been investigated by X-ray and neutron diffraction in the temperature range from 1197 to 998 K. We have also measured the dynamic viscosity from 1273 to 953 K, which is 55 K below the solidification point, using an oscillating-cup viscometer. The measurements have been complemented with ab-initio molecular dynamics (AIMD) simulations based on density functional theory (DFT). Compatibility of the AIMD-DFT models with the diffraction data has been proven by simultaneous fitting of all datasets in the frame of the reverse Monte-Carlo simulation technique. It has been shown that octahedral order dominates in liquid GeTe, although tetrahedral structures are also present. The temperature dependences of the structural

parameters, dynamic viscosity and electronic properties extracted from the AIMD models have been analyzed and discussed. We have shown that GeTe keeps its semiconductor nature in the liquid and supercooled liquid state. Its viscosity obeys the Arrhenius law with a small activation energy of the order of 0.3 eV, which is indicative of a highly fragile liquid.

Aqueous salt solutions. — Aqueous lithium chloride solutions up to very high concentrations have been investigated in classical molecular dynamics simulations. Various force fields based on the 12-6 Lennard-Jones model parametrized for non-polarizable water solvent molecules (SPC/E, TIP4P, TIP4PEw) have been inspected. Twenty-nine combinations of ion-water interaction models have been examined at four different salt concentrations.

Densities, static dielectric constants and self-diffusion coefficients have been calculated (see, e.g., Figure 3).



Results derived from the different force fields scatter over a wide range of values. Neutron and X-ray weighted structure factors have also been calculated from the radial distribution functions and compared with experimental data. It has been found that the agreement between calculated and experimental curves is rather poor for several investigated potential models, even though some of them were previously applied in computer simulations.

Figure 3. Convergence of the static dielectric constant (ϵ) for three selected models (PI, HS-g and Li-IOD-S) at the concentration $m = 19.55$ mol/kg. The curve is converged for the PI model, still slightly evolving for the Li-IOD-S model, and definitely not converged even at 8 ns, for the HS-g model.

Grants

OTKA SNN-116198: Structure and thermodynamics of Hydrogen bonded liquids (L. Pusztai, 2016-2018)

HAS-LAS Hungarian-Latvian bilateral: X-ray Absorption Experiments for Disordered and Nanocrystalline systems: Interpreting Data via Reverse Monte Carlo Methods (L. Pusztai, 2016-2018)

NKFI K-124885: Investigation of electrolyte solutions by theoretical and experimental methods (I. Bakó, NSRC HAS; Wigner-responsible: L. Pusztai, 2017-2021)

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See also: S-L.12

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



“Momentum” research team

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

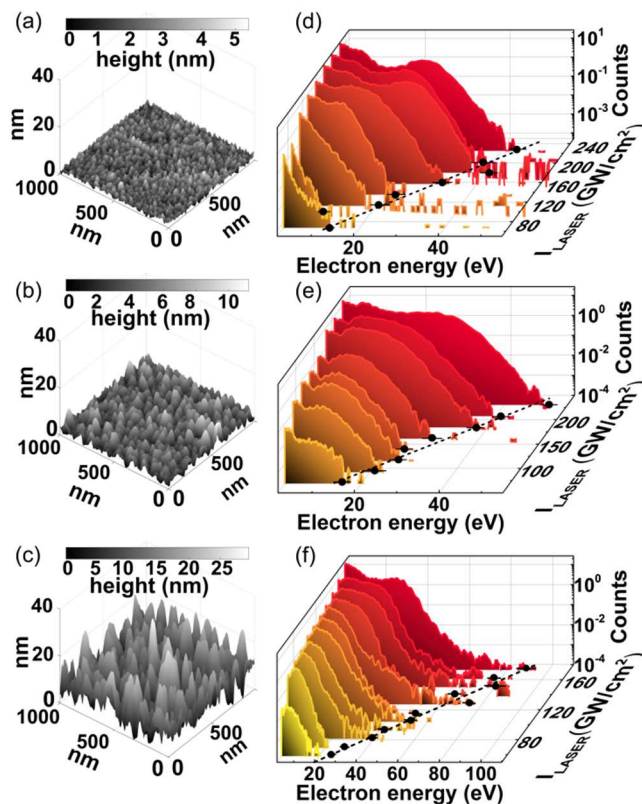


Figure 1. (a-c) Atomic force microscope scans of plasmonic surfaces with controlled, different rms roughnesses of 0.8 nm, 1.6 nm and 4.5 nm, after applying a tip shape deconvolution procedure. (d-f) Plasmonic photoelectron spectra (logarithmic scale) from the three surfaces by generating plasmons with a 38-fs laser pulse with different focused intensities. Black symbols correspond to electron spectral cutoffs. Cutoff error bars are determined according to fit uncertainty.

Surface plasmon experiments. — We studied electron emission induced by intense, femtosecond plasmon field on a periodically structured gold film. Results on previous, disordered samples agreed well qualitatively (see electron pairing at an intensity of around 80 GW/cm²), however, new phenomena were discovered as well. Most interestingly,

we found narrow resonances in time-of-flight electron spectra that can be interpreted as a quantum interference effect. Emission related to electron pairs produce different narrow resonances of this kind.

Femtosecond photonics. — Improving the laser-induced damage threshold of optical components is a basic endeavor in femtosecond technology. By testing more than 30 different femtosecond mirrors with 42 fs laser pulses at 1 kHz repetition rate, we found that a combination of high-bandgap dielectric materials and improved design and coating techniques enable femtosecond multilayer damage thresholds exceeding 2 J/cm² in some cases. We also studied damage threshold dependence as a function of the number of

interacting pulses and other relevant parameters. A significant x2.5 improvement in damage resistance can also be achieved for hybrid Ag-multilayer mirrors exhibiting more than 1 J/cm^2 threshold with a clear anticorrelation between damage resistance and peak field strength in the stack.

Theoretical research. — In studying the quantum phase properties of electromagnetic radiation fields, we have recently derived the regular-phase coherent states, which are in fact $SU(1,1)$ coherent states, introduced earlier in a more general context. In the one-mode representation, these states are generated by a perturbed electromagnetic oscillator Hamiltonian containing an intensity-dependent coupling term. By applying this abstract formalism for a completely different system, we have discussed a new physical realization of these regular-phase coherent states, which may be relevant in the non-perturbative theory of some strong-field processes. We have shown that the motion of a charged particle in a Coulomb field can naturally be described by using $SU(1,1)$ generators and a fictitious time parameter, the so-called eccentric anomaly. By analysing the interaction of a Rydberg atom with a strong microwave field at the main resonance, we have described squeezing and stretching in real space as a result of the generation of $SU(1,1)$ coherent states for the Coulomb problem. If the microwave field is linearly polarized along the z -direction, the Bargmann index of the sub-space of these states is $(|m|+1)/2$, where m is the (conserved) z -component of the angular momentum. In Figs. 2 and 3, we illustrate the resulting spatial distortions of the wave functions, for two initial set of parabolic quantum numbers.

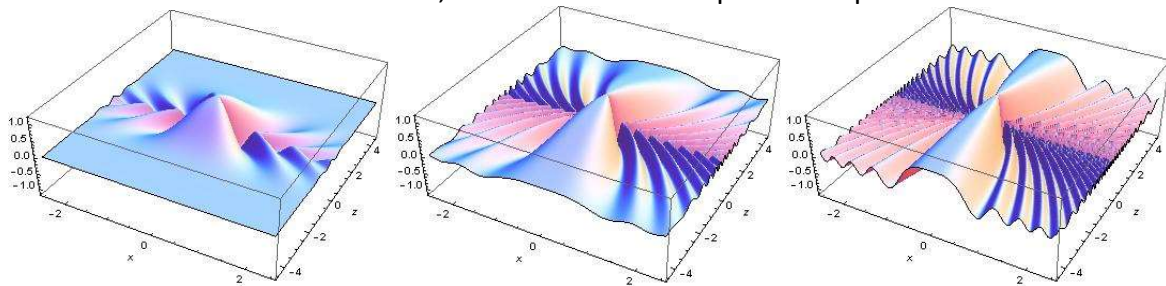


Figure 2. The left figure (a) shows the initial wave function (with parabolic quantum numbers: $m=0$, $n_1=0$, $n_2=60$) as a function of the x and z coordinates. The microwave field is assumed to be linearly polarized along the z -direction. The central (b) and the right (c) figures display the distorted wave functions (stretching along the polarization, after the microwave field has been switched on) at two instants: after one and two cycles of the scaled time parameter, respectively.

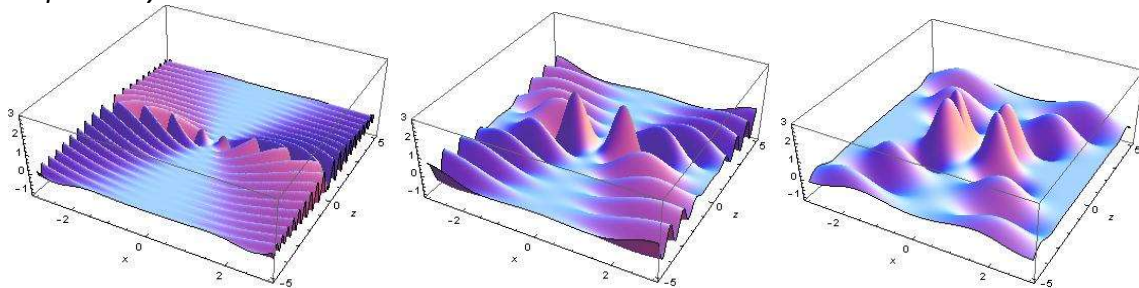


Figure 3. The same as in Figure 2, but now with different initial parabolic quantum numbers: $m=1$, $n_1=60$, $n_2=0$.

Grants

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

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

VEKOP Grant: Research on ultrahigh-speed molecular and nanooptical switches (P. Dombi, G. Vankó, 2017-2021)

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

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

International cooperations

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

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

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

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

University of Graz (Austria) with P. Dombi.

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S-S. Quantum optics

“Momentum” research team

Péter Domokos, Thomas W. Clark, András Dombi, Dávid Jakab[#], József Janszky^E, Gábor Kónya[#], Dávid Nagy, Gergely Szirmai, András Vukics



Cavity Quantum Electrodynamics, quantum critical phenomena. — Non-equilibrium phase transitions exist in damped-driven open quantum systems, when the continuous tuning of an external parameter leads to a transition between two robust steady states.

In second-order transitions, this change is abrupt at a critical point, whereas in first-order transitions, the two phases can co-exist in a critical hysteresis domain. In collaboration with the experimental group of the ETH Zürich, we found a first-order dissipative quantum phase transition in a driven-circuit quantum electrodynamics (QED) system. It takes place when the photon blockade of the driven cavity-atom system is broken by increasing the drive power. The observed experimental signature is a bimodal phase space distribution with varying weights controlled by the drive strength. The measurements showed an improved stabilization of the classical attractors up to the millisecond range when the size of the quantum system is increased from one to three artificial atoms. The theoretical work included the fitting of the experimental data as well as it contributed to prove the phase-transition character of the effect. Furthermore it was possible to prove theoretically that the photon-blockade-breakdown effect relies on a given range of the parameters of a three-level atomic system. We showed that the parameters of the actual experimental setup happen to correspond to this range.

Ultracold gases, Bose-Einstein condensates. — Modeling the coupling between a trapped Bose-Einstein condensate and a current carrying nanowire, we studied, in collaboration with an experimental group at Tübingen, the magneto-mechanical interaction by means of classical radio-frequency sources. We performed the spectral analysis and the local measurement of intensity correlations of microwave fields using ultracold quantum gases. The fluctuations of the electromagnetic field induce spin flips in a magnetically trapped quantum gas and generate a multimode atom laser. The output of the atom laser was measured with high temporal resolution on the single-atom level, from which the spectrum and intensity correlations of the generating microwave field have been reconstructed in accordance with our recently proposed scheme. We gave the theoretical description of the atom-laser output and its correlations in response to resonant microwave fields and verified the model with measurements on an atom chip. The measurement technique is applicable for the local analysis of classical and quantum noise of electromagnetic fields, for example, on chips, in the vicinity of quantum electronic circuits.

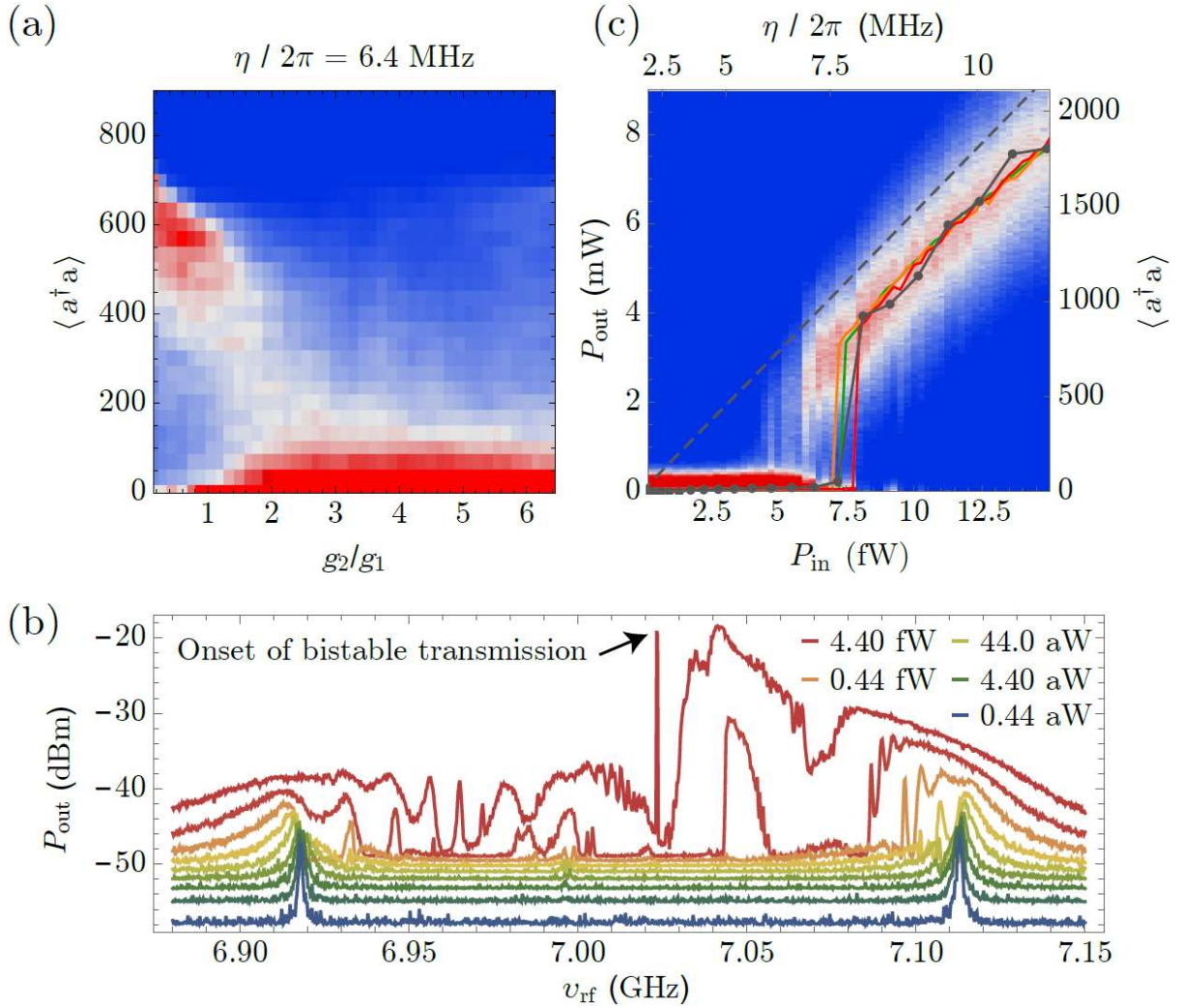


Figure 1. (a) Simulated histogram of the output intensity as a function of the coupling constant g_2 between the two excited atomic states $|e\rangle$ and $|f\rangle$ at a given driving amplitude η with red representing high probability and blue indicating zero probability. This plot shows that only a certain range of the ratio g_2/g_1 gives rise to bistability.

(b) Measured vacuum Rabi spectra for various input powers with all three atoms in resonance with the cavity. For better visibility the shown spectra are offset by 1.6 nW from each other. The sharp transmission peak shown in the inset appears stochastically. In this particular measurement (orange line at 4.4 fW input power), we observe only two frequency points with small but finite switching probability and we sample over multiple switching events resulting in a certain mean detected power. At lower drive power, no transmission is observed (no switching). At higher drive powers, the transmission peak approaches the cavity linewidth and scales linearly with input power (no switching again).

(c) Measured histogram of the detected power as a function of the cavity input power for a single transmon (density plot). The most likely photon numbers (line plots) are extracted from this measurement (red) and two similar measurements taken with 2 (orange) and 3 qubits (green) in resonance with the cavity mode. Simulation results for the single qubit case are shown with connected black symbols for comparison. The dashed line is for reference and represents the response of the empty cavity.

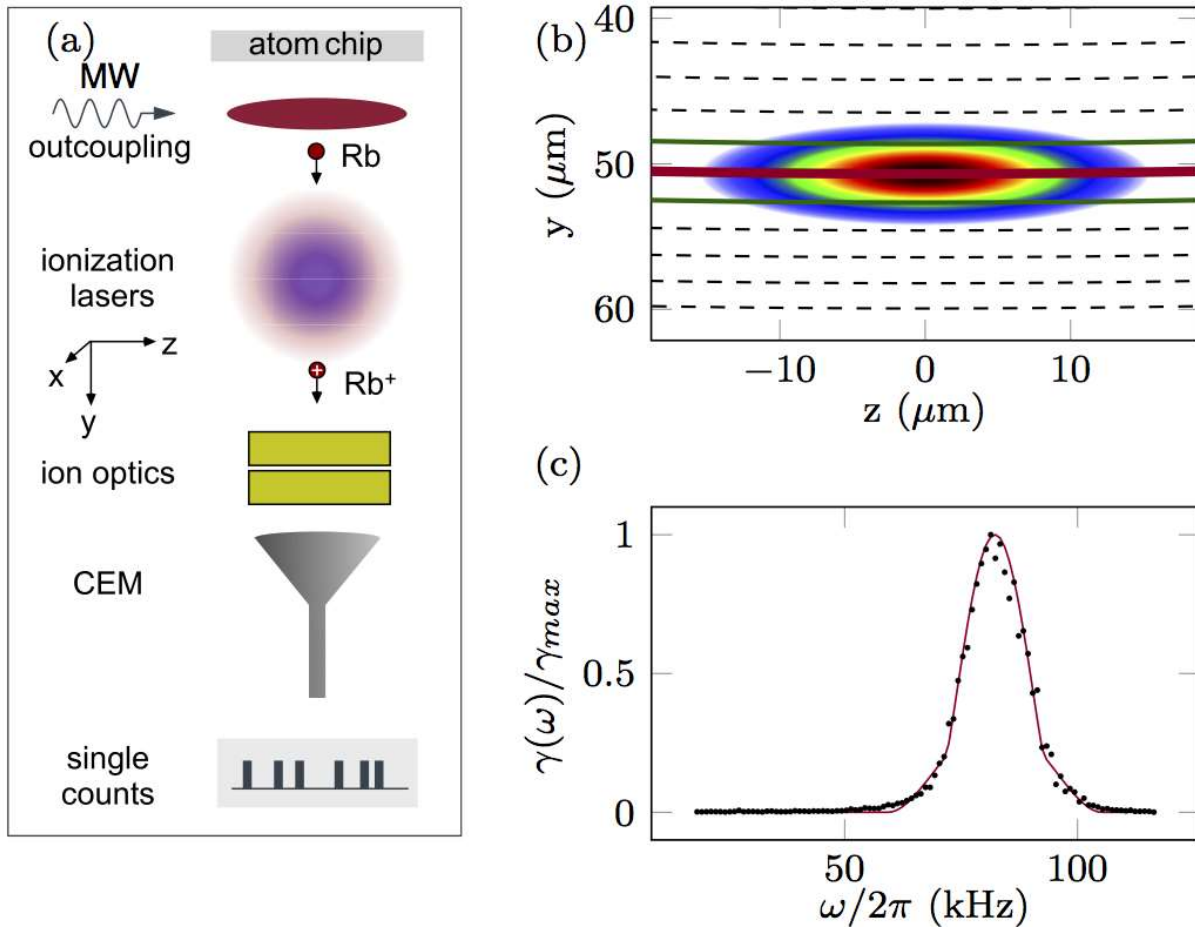


Figure 2. (a) Cold-atom spectrometer (not to scale) consisting of a magnetically trapped Bose-Einstein condensate and an ionization-based single-atom detector. (b) The microwave couples atoms at resonance surfaces given by equipotential surfaces of the atomic Zeeman potential, i.e., magnetic isofield lines (dashed lines). Due to gravity, the BEC is displaced from the magnetic trap center and the resonance surfaces become nearly plane. Without amplitude modulation, the microwave carrier couples atoms from a single resonance surface (red solid thick line) with a position given via ωc . Amplitude modulation at a single frequency generates sidebands to the carrier and outcoupling from two resonance surfaces (green solid thin lines). (c) Normalized spectral response $\gamma(\omega)/\gamma_{max}$ of a BEC to a single microwave frequency (black dots) and model function (red line).

Grants

“Momentum” Program of the HAS Quantum Measurement Theory in Hybrid Mesoscopic Couplers and Networks (P. Domokos, finalized in 2016)

National Excellence Program for Quantum Technology, HunQuTech Consortium: Preparation, distribution of quantum bits and development of quantum information networks (2017-1.2.1-NKP-2017-00001, 2017-2021)

OTKA K-115624: Open quantum system dynamics in the ultrastrong coupling regime (P. Domokos, 2015-2019)

International cooperation

Fortágh group, Physikalisches Institut, Eberhard-Karls-Universität Tübingen, D-72076 Tübingen, Germany

Johannes Fink, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria

Wallraff group, Department of Physics, ETH Zürich, CH-8093 Zürich, Switzerland

Publications

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See also: S-Q.3

S-T. Quantum information and foundations of quantum mechanics



Wigner research group

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Measurement-induced non-linear transformations. — We proposed a cavity quantum electrodynamical scenario for implementing a Schrödinger microscope capable of amplifying differences between non-orthogonal atomic quantum states. The scheme involves an ensemble of identically prepared two-level atoms interacting pairwise with a single mode of the radiation field as described by the Tavis-Cummings model (Fig. 1). We showed that by repeated measurements of the cavity field and of one atom within each pair, a measurement-induced non-linear quantum transformation of the relevant atomic states can be realized. The intricate dynamical properties of this non-linear quantum transformation, which exhibits measurement-induced chaos, allow approximate orthogonalization of atomic states by purification after a few iterations of the protocol and, thus, the application of the scheme for quantum state discrimination.

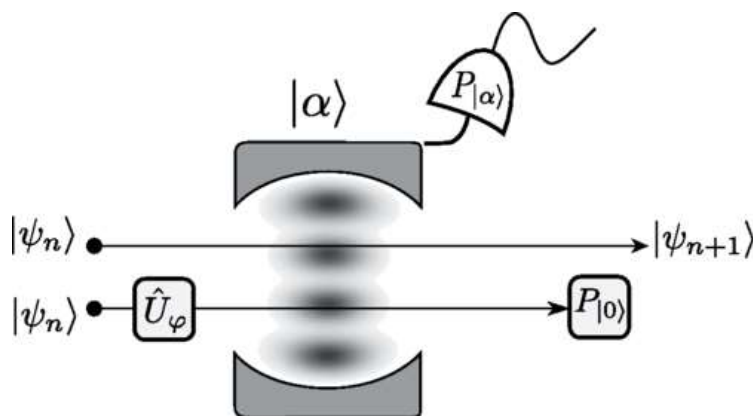


Figure 1. Illustration of the scheme. Two two-level atoms in the same state interact with the cavity field prepared in a coherent state. Before the interaction, a unitary gate is applied to one of the atoms, and after the interaction and the projection of the field onto the initial coherent state, this same atom is projected onto its ground state. Finally, the other atom is left in a non-linearly transformed state.

Topological phases. — We discovered topological features of the Hofstadter butterfly spectra of periodically driven systems. The butterfly is the fractal spectrum of energy eigenstates of a quantum lattice system in a magnetic field. It was discovered numerically (1976, predating the word "fractal"), analyzed analytically (contributing to the topological understanding of the quantum Hall effect), and it is about to be observed experimentally on laser-trapped cold atoms and in graphene. We found that in periodically driven systems, where the drive is very far from just a perturbation, the Hofstadter butterfly can "take flight", i.e., can "wind" in quasienergy (Fig. 2). This behaviour is closely related to a recently discovered topological invariant unique to such non-perturbatively driven systems, and gives us a way to numerically evaluate and perhaps experimentally observe this invariant in an efficient way.

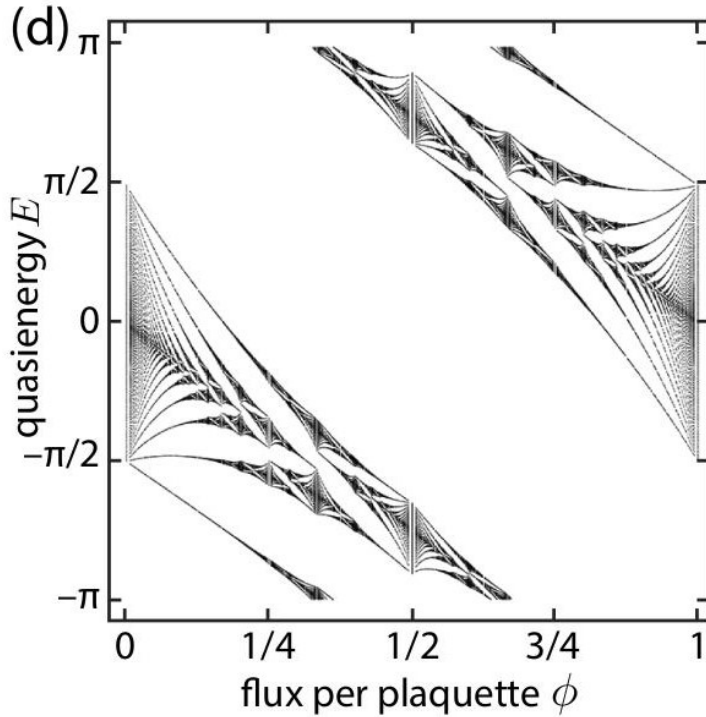


Figure 2. The spectrum of quasienergies of a periodically driven system (quantum walk) can wind as a function of applied magnetic field. The winding is quantized, and reveals a bulk topological invariant of the system.

Ro-vibrational quantum states in molecules. — Recently, a general expression for Eckart-frame Hamilton operators has been obtained by the gateway Hamiltonian method. The kinetic energy operator in this general Hamiltonian is nearly identical to that of the Eckart-Watson operator even when curvilinear vibrational coordinates are employed. Its

different realizations correspond to different methods of calculating Eckart displacements. There are at least two different methods for calculating such displacements: rotation and projection. In our work, the application of Eckart Hamiltonian operators constructed by rotation and projection was numerically demonstrated in calculating vibrational energy levels. The numerical examples confirm that there is no need for rotation to construct an Eckart ro-vibrational Hamiltonian. The application of the gateway method is advantageous even when rotation is used since it obviates the need for differentiation of the matrix rotating into the Eckart frame. Simple geometrical arguments explain that there are infinitely many different methods for calculating Eckart displacements. The geometrical picture also suggests that a unique Eckart displacement vector may be defined as the shortest (mass-weighted) Eckart displacement vector among Eckart displacement vectors corresponding to configurations related by rotation. Its length, as shown analytically and demonstrated by numerical examples, is equal to or less than that of the Eckart displacement vector one can obtain by rotation to the Eckart frame.

Nanophotonics. — We have worked out a true vectorial numerical method for the simulation of the non-linear second harmonic generation process by extending the finite difference frequency domain method (FDFD). Our non-linear method (NL-FDFD) operates directly on the electromagnetic fields, uses two meshes for the simulation (for ω and 2ω fields) and handles the non-linear coupling as an interaction between the two meshes. Final field distributions can be obtained by a small number of iteration steps. NL-FDFD can be applied in arbitrarily structured linear media with an arbitrarily structured $\chi(2)$ component both in the small-conversion-efficiency and the pump-depleted cases.

Grants

NKFI FK 124723J From topologically protected states to a topological quantum computer (J. Asbóth, 2017-2021)

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

NKFI K 124351 Dynamics and measurement of coherent and open quantumoptical networks (T. Kiss, 2017-2021)

National Excellence Program for Quantum Technology, HunQuTech Consortium: Preparation, distribution of quantum bits and development of quantum information networks (2017-1.2.1-NKP-2017-00001, 2017-2021)

International cooperation

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

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

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

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See also: S-Q.3

INSTITUTE FOR PARTICLE AND NUCLEAR PHYSICS*

* **Abbreviations in the researcher lists of the scientific projects:**

#: PhD student

A: associate fellow

E: professor emeritus

R-A. Field theory

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Quantum physics: universal gate sets and measurements. — For numerous applications of quantum theory it is desirable to be able to apply arbitrary unitary operations on a given quantum system. However, in particular situations only a subset of unitary operations is easily accessible. This raises the question of what additional unitary gates should be added to a given gate-set in order to attain physical universality, i.e., to be able to perform arbitrary unitary transformation on the relevant system. We studied this problem for three paradigmatic cases of naturally occurring restricted gate-sets: particle-number preserving bosonic linear optics, particle-number preserving fermionic linear optics, and general (not necessarily particle-number preserving) fermionic linear optics. Using tools from group theory, we were able to classify, in each of these scenarios, what sets of gates are generated, if an additional gate is added to the set of allowed transformations. This allowed us to solve the universality problem completely for arbitrary number of particles and for arbitrary dimensions of the single-particle Hilbert space. We also attacked the problem of describing quantum measurements, we constructed a two-step dynamical model for selective measurements in quantum mechanics. The first step is the non-selective measurement or decoherence described by a semigroup of completely positive maps, which is given by the linear, deterministic first order Lindblad differential equation. The second step is a process from the resulted decohered state to a pure state, which is described by an effective non-linear 'randomly chosen' toy model dynamics: the pure states arise as asymptotic fixed points, and their emergent probabilities are the relative volumes of their attractor regions.

Integrable systems and quantum groups. — We have derived new integrable many-body models of Ruijsenaars--Schneider--van Diejen type by applying Hamiltonian reduction to the Heisenberg double of the Poisson--Lie group $SU(2n)$, and clarified the global structure of the phase space for another model in the same family. We have also continued our study of describing algebraic structures that go beyond groups. In an earlier work, we have already studied a distinguished class of Hopf monads in monoidal bicategories. Hopf algebras and most of their known generalizations were shown to fit this class. Since then, however, some newer generalizations of Hopf algebras — so-called Hopf categories and Hopf polyads — appeared in the literature. In this year, we constructed a monoidal bicategory in which also these structures, as well as Turaev's Hopf group algebras, can be regarded as Hopf monads. In order to describe quantum we constructed a two-step dynamical model for selective measurements in quantum mechanics.

Gravitational theory: spinning binary black-hole systems. — The Lagrangian of the spinning binary system contains acceleration-dependent terms in some cases of spin supplementary condition (SSC). We constructed the nontrivial generalized Hamiltonian formalism with the high-order canonical moments proposed by Ostrogradsky and calculated the conserved

^A Associate fellow

quantities such as the energy and the magnitude of the orbital angular momentum for each SSC. Thus we computed the first integrals of the spinning dynamics and gave the perturbative radial and angle motion with the help of the generalized radial parameterization. Moreover, we defined the generalized Poisson brackets following the work of Yang and Hirschfelder and we have given the canonical structure of the spinning binary. Finally, we generalized the result of Kidder for the spinning waveform and for the dissipative part of relative motion during the gravitational radiation of each SSC (Fig. 1).

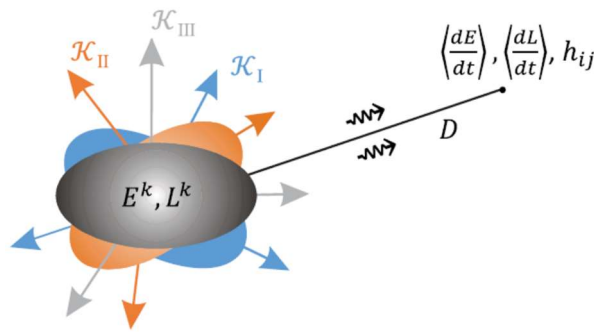


Figure 1. Dissipative quantities of the binary in the different spin supplementary conditions

Grants

OTKA K-108384, "Category Theoretical Investigations of Quantum symmetries", (G. Böhm, 2013-2017)

NKFI K-124138, "Crossed modules over Hopf monoids", (G. Böhm, 2017-2021)

OTKA K-111697, "Group-theoretic aspects of integrable systems and their dualities", (L. Fehér, 2014-2018)

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

International cooperations

Departamento de Álgebra and CITIC, Universidad de Granada, Spain

Department of Mathematics, Macquarie University, Sydney, Australia

Faculty of Mathematics, Higher School of Economics National Research University, Moscow, Russia

Paris Observatory, Meudon, France

Université de Tours, France

Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany

ICFO - Institute of Photonic Sciences, Barcelona Institute of Science and Technology, Spain

Institute of Theoretical Physics and Astrophysics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Poland

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See also: R-B. Dokshitzer Y

R-B. Heavy-ion physics



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High-energy heavy-ion physics is connected to a large variety of physics disciplines. Our research 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 Quantum Chromodynamics (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, MAP (China), UNAM (Mexico), and ERI (Japan). We highlight below some of our major published results in details.

New developments in the effective field theory of the strong interaction. — As a member of the CBM collaboration, we continued the planning of the details of the detector. We participated in the detector simulations concentrated on the phi meson and on the double strange hypernuclei. We studied the physics case as well.

We developed a linear sigma model extended with vector mesons, Polyakov loops and with quarks. We calculated the phase diagram. We found that there is a critical point at rather low temperature. By slightly changing the parameter set the critical point moves in the direction of the $T=0$ axes, and will disappear. In our model we also calculated the isentropic curves and compared them with lattice simulations. The agreement is remarkable.

The transport model developed here was extended to charmonium production in antiproton induced reactions. In the investigations the following picture arised: The antiprotons annihilate close to the surface of the heavy nuclei. The charmonium travels through the nuclei contribution to the dilepton spectra. Crossing again the thin surface the rest decay in vacuum. The higher lying charmonium states $\Psi(3686)$ and $\Psi(3770)$, expected to have a mass shift in dense matter in the range of about 100 MeV (see Fig. 1). We found that in the dilepton spectra the higher-lying charmonium states show up with two peaks. One of the peak is the contribution of the vacuum decay and the other one is developed from charmonium states decaying around ρ_0 density. The peaks are clearly separated and can be observed at the PANDA detector at FAIR/GSI.

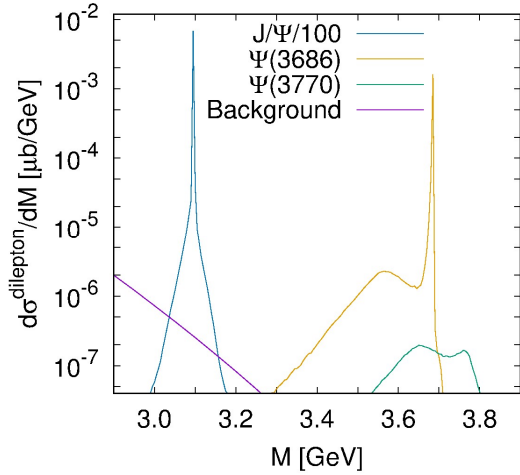


Figure 1. Charmonium contribution to the dilepton spectra in a \bar{p} Au collision at 6 GeV bombarding energies, where the in-medium modifications are accounted for.

Investigations of superdense matter and extra dimensions in compact stars. — Investigation of cold compact stars provides the opportunity to understand cold superdense matter and speculate on new states of matter. These theoretical developments are strongly connected to recent measurements of compact stars by multi-wavelength observations and

gravitational waves. Our projects are supported by theoretical networking EU COST actions: NewCompStar (MP1304) and PHAROS (CA162014).

In collaboration with A. Jakovác (ELTE) we constructed a framework using the functional renormalization group (FRG) technique for a one-fermion and one-boson theory with Yukawa-like coupling, where we calculated the equation of state (EoS) at finite chemical potential and zero temperature exactly – including quantum corrections. We investigated the effect of the quantum fluctuations on the nuclear equation of state and compact star observables. We demonstrated, that correction to the mean field model can result in 30% difference in the EoS, which modifies the neutron star mass and radius by 5%. The mathematical technique and the physical consequences of these results were presented on the Quark Matter 2017 conference and on several other conferences as invited talks.

In a joint work with E. Forgács-Dajka (ELTE⁴) the existence of stable compact stars in a simple extra dimensional, Kaluza–Klein space-time were modeled. The mass-radius, $M(R)$ -relation of a degenerated, non-interacting fermion star in extra dimensional space-time were presented in the cases of large- and small-sized extra dimension with several degrees of freedom (many-flavor model). As a result, we found both the observable maximal mass and the radius of a compact object may vary in a wide range as changing the size or the number of the extra dimensions.

Results from the non-extensive statistical approach. — High-energy heavy-ion collisions are good testbeds for the non-ideal, non-equilibrium, finite systems. The non-extensive statistical approach, developed by our group, can describe such a matter by enwidening the framework of classical thermodynamics and statistical physics towards non-equilibrium and complex system phenomena. This pioneering, novel approach to Rényi, Tsallis and further non-Boltzmannian entropy formulae have been applied by us in various physical phenomena like heavy-ion collisions, cosmology or network science.

We investigated the hadronization in high-energy pp and pPb collisions using the non-extensive statistical approach. We identified the mass and c.m. energy scaling of the Tsallis–Pareto parameters and compared our theoretical approach to the experimental data and other models. These results were published in a comprehensive study in the Entropy journal and presented on the JETC 2017 and QCD@LHC international conferences. We also compared

⁴ ELTE: Eötvös Loránd University, Budapest

different non-extensive models for transverse momentum spectra measured in heavy-ion collisions. In collaboration with K. Shen (CCNU Wuhan, China) we assumed to fix the relative variance of the temperature fluctuating event-by-event or alternatively a fixed mean multiplicity in a negative binomial distribution (NBD). We found linear relations between the temperature parameter, T and the Tsallis parameter, $q-1$. We revisited the “Soft+Hard” model by a T -independent average p_T^2 assumption.

Our description of the hadronization relies on the non-extensive approach may originated from the microscopical entropy driven (balanced) processes. Together with Z. Neda (Babes-Bolyai University), various models were tested: (i) the connection between transverse momenta and multiplicity distributions in a statistical framework. We connect the Tsallis parameters, T and q , to physical properties like average energy per particle and the second scaled factorial moment, measured in multiplicity distributions. (ii) applying a master equation, we developing a QCD-like branching model. (iii) A further unidirectional random growth branching with resetting were also presented, which can be applied to various networks, scientific citations and Facebook popularity, hadronic yields in high energy particle reactions, income and wealth distributions, biodiversity and settlement size distribution.

Phenomenology, transport, and hydrodynamics for heavy-ion collisions. — We investigated the emergence of the Chiral Magnetic Effect (CME) and the related anomalous current using the real time Dirac-Heisenberg-Wigner formalism. This method is widely used for describing strong field physics and QED vacuum tunneling phenomena as well as pair production in heavy-ion collisions. We extend earlier investigations of the CME in constant flux tube configuration by considering time dependent fields. In this model we can follow the formation of axial charge separation, formation of axial current and then the emergence of the anomalous electric current. Qualitative results have been calculated for special field configurations that help to interpret the predictions of CME related effects in heavy-ion collisions at different collision energies.

The Boltzmann transport model was also investigated together with D. Molnár (Purdue University, USA) and M.F. Nagy-Egri (Project R-C). We constructed parametrizations of nonlinear $2 \rightarrow 2$ transport model results in $0+1D$ Bjorken geometry, in order to better understand dissipative phase space corrections in kinetic theory and test simplified models/guesses for those commonly used in the literature. It was deemed most immediately suitable for GPGPU calculations because it mainly involves integration in two dimensions only.

In this year we have made three big steps in our ongoing fundamental research for constructing constitutive and evolution equations of internal variables with the second law of thermodynamics. First a new development of the methodology resulted in the Cahn-Hilliard equation for extensive internal variables. In our efforts for the validation of the developed theories we have analysed the low temperature NaF experiments, where the second sound and ballistic effects were detected together. Here we have shown that non-equilibrium thermodynamics with internal variables is capable to reproduce the available experimental observations better than other theories. An other important step of the validation was the discovery of non-Fourier heat conduction in several artificial and natural materials in macroscopic heterogeneous samples at room temperature. The experiments are analysed and the deviation from the Fourier theory is inevitable also considering the cooling of the samples.

An other interesting result of our thermodynamic research is related to Schwarzschild black holes. Here we have proved that introducing the volume as a new thermodynamic variable together with a new interpretation of the Bekenstein-Hawking entropy eliminates the negative heat capacity of the original theory.

Development for heavy-ion computer simulations. — In collaboration with the University of Berkeley (USA) and IoPP CCNU (Wuhan, China), we developed the HIJING++ heavy-ion Monte Carlo Generator with G. Papp (ELTE), G.Y. Ma (IoPP CCNU), and X.N. Wang (IoPP CCNU, LBNL). We transplanted the original, 20 years old code from FORTRAN to C++ programming languages, including new, parallel-computing features, resulting faster simulations as presented on Fig 2.

The development of the future Monte Carlo generator for the heavy-ion collisions, HIJING++ were reached the stage where we could present first preliminary physics results on pp and pPb collisions, however the new Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) -evolved, QCD-scale dependent nuclear shadowing is still under development. The first results were presented on Quark Matter 2017, FCC 2017, and QCD@LHC conferences and our predictions for pPb collisions at 8.16 TeV cm energy were accepted for publication.

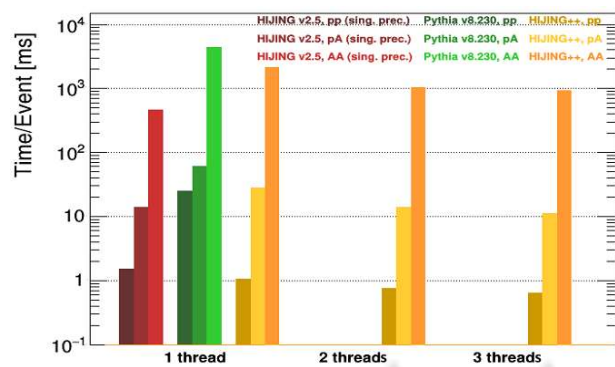


Figure 2. Speedup of the new version of the HIJING++ in comparison to other Monte Carlo simulators.

Identified hadron spectra with ALICE. — We participated in the actual data taking and analysis. We took ALICE shifts and provided on call experts for the ALICE HMPID (High Momentum Particle Identification Detector) and ALICE IF

(Interface) detectors.

The measurement of light flavor charged hadrons have been performed in pp collisions at 13 TeV around midrapidity with the ALICE detector. The p_T -differential production yields and ratio of yields with respect to produced pions have been measured. Results are preliminary ALICE Collaboration data. Recent results on small collision systems (pp) were also presented in the EPSHEP 2017 Conference in Venice on behalf of the ALICE Collaboration, which will be published in Proceedings of Science (PoS). Two-particle angular correlation measurements at ALICE on the PbPb and pp data collected in 2010 and 2011 were analyzed. We have found that the jet-peak broadens towards central events at low transverse momentum in PbPb collisions and that it becomes asymmetric. We have also found that an unexpected depletion develops around the center of the peak. By analyzing data from AMPT (A Multi-Phase Transport) Monte Carlo simulations, we concluded that both phenomena are accompanied by large radial flow, suggesting that the broadening and the depletion is caused by an interplay of jets and the flowing medium. Results were presented at the Rencontres de Moriond QCD and High Energy Interactions in 2017, which was followed by a proceedings, and on the 12. WPCF, and at the Zimányi School 2016.

Heavy-flavour (beauty and charm) quarks are produced almost exclusively in initial hard processes, and their yields remain largely unchanged throughout a heavy-ion reaction.

Nevertheless, they interact with the nuclear matter in all the stages of its evolution. Thus, heavy quarks serve as ideal self-generated penetrating probes of the strongly interacting Quark-Gluon Plasma (QGP). We started to determine the yield and nuclear modification of beauty jets in pPb collisions at 2.76 TeV recorded by ALICE during Run1 and Run2. We focused on developing b-jet identification techniques as well as the unfolding of the b-jet spectrum to correct for detector and background effects. We were appointed on DIS 2017, Zimanyi School 2016, Balaton Workshop 2017 QCD@LHC 2017 and Debrecen University Symposium 2017.

The Hungarian ALICE Group signed 56 SCI-referred collaboration papers, and several conference proceedings, and we presented several posters and talks on all these analysis results.

Coordination of the ALICE time projection chamber (TPC) upgrades. — We coordinate the Hungarian contribution to CERN's largest heavy-ion experiment ALICE. This activity is two-folded: In addition to data analysis, our group plays key role in the construction of the world largest, 90 m³-volume, gas electron multiplier (GEM) -based TPC for the ALICE. The ALICE TPC upgrade is a joint project with the Wigner's Innovative Particle Detector Development "Momentum" Group (D. Varga), the University of Helsinki (Finland), the GSI Darmstadt and TU Munich (Germany), the Oak Ridge National Laboratory (USA), and CERN. The Budapest Quality Assurance (QA) Center was built up to making the classification of GEM foils will be used in the ALICE TPC Upgrade project. The installation of necessary equipments in the Wigner's clean room were finished at late Autumn. The QA procedure is three-folded: high-definition optical scanning; long-term (5-20 hours) high-voltage leakage current tests, in N gas, with 500 V potential, monitoring the sparks and the leakage currents of the sectors of the GEMs; gain scanning (only in Budapest!) which is an operational test of the GEMs, measuring the gain features of the GEMs in realistic conditions with Fe-55, with similar spatial resolution as the optical scanning.

For these methods we use several equipments as the 3D High-Definition Scanner Robot with the ISEG controller, HD camera and optics, and led lighting with light controller (developed in Wigner RC); HV box for the long-term HV tests with picoAmper meter; and the gain scanner detector developed in Wigner RC. The main goal of gain scanning to study the correlation between the optical features (e.g. inhomogenities in ring diameter distribution) and the operational gain features of GEMs, and thus taking predictions for the operation phase. For the data taking and analysis we have developed a QA GUI application, which can process and classify the foils, displaying and evaluating both the leakage current and HD optical data. The code is open-source, and available on github.

There is also a middle step in the QA process to extract data from the images by a dedicated GPU based program running a neural-network-based image recognition routine. When the full QA procedure chain was installed and tested we organized a dedicated QA meeting in Budapest. We participated on the ALICE TPC UG TEST BEAM at CERN PS T10 experimental area, where the IROC GEM based test chamber were tested with 1-5 GeV PS beam.

The Budapest QA-center normal operation (for IROC and OROC2 GEMs) started in 2017 February. Between February and August 8 batch of GEMs (GEM Transport System, GTS) was classified in Budapest QA-Center: 1 GTS with 6 preproduction OROC2 GEMs + 7 GTS with 42 production IROC GEMs + 42 production OROC2 GEMs, which were totally: 90 GEMs. In details 90 GEMs went trough the optical scanning, 86 GEMs went trough the long-term HV test, 21

GEMs went through the gain scanning. After QA procedures we sent 7 shipments (GTS) with 68 GEMs to framing centers Bonn (OROC2 - 4 shipments), WSU-Detroit (IROC - 2 shipments), and 10 failed GEMs back to CERN (1 shipment).

Coordination of the ALICE CRU upgrades. — The R&D of the ALICE Data Acquisition system, ALICE O2 project, Common Readout Unit (CRU) FPGA Firmware Development continues to be an ongoing effort. We introduced a schedule of quarterly firmware releases, and indeed created the 1st, 2nd, and 3rd CRU firmware releases, each implementing more and more of the functionality required by the Run3 UG.

Currently implemented features include: receiving LHC Clock and trigger via PON from the Central Trigger Processor / Local Trigger Unit (CTP / LTU) units, or running without them in standalone mode using a local trigger emulator; playing back detector specific control sequences to signal reset / calibration / physics trigger / etc events to the front end electronics modules; support for multiple GBT links (up to 24); acquiring data in raw datalink recorder mode, GBT packet based communication mode, and user logic mode; flow control features of Run3 (Heartbeat Frames, Time Frames, HB Accept/Reject scheme); packet aware multichannel DMA engine, delivering the recorded data to buffers in memory, or to raw binary files on disk.

Detector groups started using the firmware, some to read out front end card under development (ITS), some to add their own detector specific extensions (TPC, TRD), and others for system integration tests (O2). Results of the FW development was presented on the TWEPP 2017 conference. Other experiments (sPHENIX, MPD NICA DUBNA, CBM/PANDA GSI/FAIR) expressed their interest in reusing the CRU hardware and firmware in their ongoing upgrade projects, the CRU project will be presented to them. Since 2015, several MSc students has been participated continuously from ELTE and BME our university-level laboratory course.

Operation and management of the ALICE GRID Tier-2 Center. — We extended our storage capacity: currently 3 storage servers are working. The newest, with 180TB capacity was configured and switched online in June 2017 with the full capacity of 500TB.

Coordination of the MGGL. — Our group, together with the Gravitational Wigner Research group of the Theory department, coordinated and organized the establishment of the Mátra Gravitational and Geophysical Laboratory of Wigner RCP. This is situated in the Gyöngyösorszi mine and performs various preparational underground measurements for future, third generation gravitational wave detectors. In 2017, we published the first data in a joint paper in Classical and Quantum Gravity and in the Geofizika journals. These data were presented for the LIGO/VIRGO collaborations and for various conferences and workshops.

Education, PR and future. — Connected to our group we had 3 BSc and 3 MSc students. Our young colleagues participated in young researcher's projects and a TDK thesis for competition: András Leitereg (special price OTDK, D. Berényi) and Ádám Takács (G.G. Barnaföldi) were awarded the "New National Excellence Program of the Ministry of Human Capacities (2017-18), the "30 Under 30 2017" by Forbes Hungary 2017, and the 2nd place at "Sci-ndicator National Scientific Communication Competition 2017".

In this year G.G. Barnaföldi received the “Physics Price of the H.A.S.”, PhDs student Róbert Kovács (P. Ván) László Oláh (GG Barnaföldi & D. Varga) defended their PhD at BME and ELTE doctoral schools, respectively. So far we have 7 young PhD fellow in the research group. Senior colleagues are members of the ELTE, BME, PTE doctoral programmes.

Group members participated in PR activities such as the Colorful Physics Bus of the Wigner Institute, Simonyi Day (Wigner RCP), Science Day (H.A.S.), the “50 Years of Pulsars” (H.A.S.), and CERN & Wigner Open Days. We receive regularly invitation by High Schools from Hungary and abroad for PR talks. Besides these activities, we established a good media connection: we participated in several appearances of news, in radio programs, outreach films and on television.

Grants

NKFI K-123815: Intelligent particle physics: the birth of hadrons (T.S. Biró, 2017-2020)

NKFI K-124366: Geophysical origin noises in gravitational wave detection (consortium leader: P. Ván, 2017-2020)

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

OTKA K-104260: Particles and intense fields (consortium leader: T.S. Biró, 2012-2017)

OTKA K-116197: Heat transport in extreme media and systems, consortium leader, (P. Ván, 2015-2019)

OTKA K-109462: Theoretical investigations of the strongly interacting matter produced at FAIR (CBM, PANDA) and NICA (Dubna) (Gy. Wolf, 2014-2018)

International cooperation

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

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

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

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

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

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

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

PHAROS EU COST CA16214 action (Hungarian Representatives: G.G. Barnaföldi – WG Task leader, M. Vasúth, 2017-2021)

Long-term visitors

Dénes Molnár, (G.G. Barnaföldi, 3 months), Michal Bejger (G.G. Barnaföldi, M. Vasúth 1 month), Yaxian Mao (G.G. Barnaföldi, 1 week), Antonio Ortiz Velasquez (G.G. Barnaföldi, 1 week), Constantino Tsallis (T.S. Biró, 2 weeks), Lilin Zhu (P. Lévai 2 weeks)

Publications

Articles

1. Barnaföldi GG, Jakovác A, Pósfay P: Harmonic expansion of the effective potential in a functional renormalization group at finite chemical potential. **PHYS REV D** **95**:(2) 025004/1-11 (2017)
2. Barnaföldi GG et al. incl. Dávid E, Hamar G, Huba G, Kovács R, Lévai P, Oláh L, Pázmándi P, Somlai L, Varga D, Vasúth M, Ván P [31 authors]: First report of long-term measurements of the MGGL laboratory in the Matra mountain range. **CLASSICAL QUANT GRAV** **34**:(11) 114001/1-22 (2017)
3. Barnaföldi GG, Biró G, Gyulassy M, Harangozó SM, Lévai P, Ma GY, Papp G, Wang XN, Zhang BW: First results with HIJING++ in high-energy heavy-ion collisions. **NUCL PART PHYS P** **289**: 373-376 (2017) (8th International Conference on Hard and Electromagnetic Probes of High Energy Nuclear Collisions. Wuhan, China, 23-27 September 2016)
4. Barnaföldi GG, Jakovác A, Pósfay P: An application of functional renormalization group method for superdense nuclear matter. **J PHYS CONF SER** **779**:(1) 012048/1-4 (2017) (SQM2016 - 16th International Conference on Strangeness in Quark Matter, Berkeley, USA, 27 June - 1 July 2016)
5. Bencédi G, Barnaföldi GG, Molnár L: Identified two-particle correlations and quantum number conservations in p-p and Pb-Pb collisions at LHC energies. **J PHYS CONF SER** **805**:(1) 012014/1-10 (2017) (10th International Workshop on High-p_T Physics in the RHIC/LHC Era, 9-12 September 2014, SUBATECH Nantes, France)
6. Biró G, Barnaföldi GG, Biró TS, Ürmösy K, Takács Á: Systematic analysis of the non-extensive statistical approach in high energy particle collisions-experiment vs. theory. **ENTROPY** **19**:(3) 88/1-21 (2017)
7. Biró G, Barnaföldi GG, Biró TS, Ürmösy K: Application of the non-extensive statistical approach to high energy particle collisions. **AIP CONFERENCE PROCEEDINGS** **1853**: 080001/1-7 (2017) (MaxEnt 2016 - 36th International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering, Ghent, Belgium: 10-15 July 2016)
8. Biró TS, Néda Z: Equilibrium distributions in entropy driven balanced processes. **PHYSICA A** **474**: 355-362 (2017)
9. Biró TS, Barnaföldi GG, Biró G, Shen KM: Near and far from equilibrium power-law statistics. **J PHYS-CONF SER** **779**:(1) 012081/1-4 (2017) (SQM2016 - 16th International Conference on Strangeness in Quark Matter, Berkeley, USA, 27 June - 1 July 2016)
10. Biró TS, Jakovác A, Schram Z: Nuclear and quark matter at high temperature. **EUR PHYS J A** **53**:(3) 52/1-29 (2017)
11. Biró TS, Néda Z: Dynamical stationarity as a result of sustained random growth. **PHYS REV E** **95**:(3) 032130/1-8 (2017)
12. Karsai S, Barnaföldi GG, Forgács-Dajka E, Pósfay P: Correspondence of many-flavor limit and Kaluza-Klein degrees of freedom in the description of compact stars. **ACTA**

- PHYS POL B Proceedings Supplement 10**:(3) 827-832 (2017) (Critical Point and Onset of Deconfinement 2016 and Working Group Meeting of COST Action MP1304, Wrocław, Poland, 30 May – 4 June 2016)
13. Kovács P, Wolf Gy: Phase diagram and isentropic curves from the vector meson extended Polyakov quark meson model. **ACTA PHYS POL B Proceedings Supplement 10**:(4) 1107-1112. (2017) (International Meeting Excited QCD 2017, Sintra, Portugal, 7-13 May 2017)
 14. Néda Z, Varga L, Biró TS: Science and Facebook: The same popularity law! **PLOS ONE 12**:(7) e0179656/1-11 (2017)
 15. Speranza E, Zétényi M, Friman B: Polarization and dilepton anisotropy in pion–nucleon collisions. **PHYS LETT B 764**: 282-288 (2017)
 16. Ürmössi K, Barnaföldi GG, Harangozó Sz, Biró TS, Xu Z: A 'soft + hard' model for heavy-ion collisions. **J PHYS-CONF SER 805**:(1) 012010/1-6 (2017) (10th International Workshop on High- p_T Physics in the RHIC/LHC Era, 9-12 September 2014, SUBATECH Nantes, France)
 17. Ván P: Galilean relativistic fluid mechanics. **CONTINUUM MECH THERM 29**:(2) 585-610 (2017)
 18. Ván P, Pavelka M, Grmela M: Extra mass flux in fluid mechanics. **J NON-EQUIL THERMODY 42**:(2) 133-151 (2017)
 19. Ván P, Berezovski A, Fülöp T, Gróf Gy, Kovács R, Lovas Á, Verhás J: Guyer-Krumhansl-type heat conduction at room temperature. **EUROPHYS LETT 118**:(5) 50005/1-4 (2017)
 20. Wolf Gy, Kovács P: The phase diagram in the vector meson extended linear sigma model. **ACTA PHYS POL B Proceedings Supplement 10**:(3) 759-763 (2017) (Critical Point and Onset of Deconfinement 2016 and Working Group Meeting of COST Action MP1304, Wrocław, Poland, 30 May – 4 June 2016)
 21. Wolf Gy, Balassa G, Kovács P, Zétényi M, Lee SH: Charmonium spectral functions in pA collision. **ACTA PHYS POL B Proceedings Supplement 10**:(4) pp. 1177-1182. (2017) (International Meeting Excited QCD 2017, Sintra, Portugal, 7-13 May 2017)
 22. Biró TS: Túl az exponenciális faktoron (Over the exponential factor, in Hungarian). **FIZIKAI SZEMLE 67**:(12) 407-411 (2017)
 23. Pósfay P, Barnaföldi GG, Jakovác A: Neutroncsillagok extrém anyagának vizsgálata új térelméleti módszerekkel (Study of the extreme matter of neutron stars by field theory methods, in Hungarian). **FIZIKAI SZEMLE 67**:(9) pp. 307-313. (2017)

Books, book chapters

24. Dokshitzer Y, Lévai P, Nyíri J (Eds.): *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Singapore: World Scientific Publishing, 2017 536p
25. Berezovski A, Ván P: *Internal variables in thermoelasticity*. Springer International Publishing, (Solid Mechanics and Its Applications; 243.) 2017 220p
26. Gogokhia V, Shurgaia A, Vasúth M: The temperature-dependent Yang-Mills trace anomaly as a function of the mass gap. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 240-252

27. Gogokhia V, Barnaföldi GG: General exact solutions for the full gluon propagator in QCD with the mass gap. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 253-270
28. Karsai Sz, Pósfay P, Barnaföldi GG, Lukács B: Testing a possible way of geometrization of the strong interaction by a Kaluza - Klein star. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 309-318
29. Ürmössy K, Rak J: Fragmentation in the ϕ^3 theory and the LPHD hypothesis. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 509-515

Others

30. Bencze Gy: Kvantumszobrászat (Quantum sculpting, in Hungarian). **TERMÉSZET VILÁGA 148**:(1) 40-41 (2017)
31. Bencze Gy: Szólásabadság és/vagy tudomány (Freedom of speech and/or science, in Hungarian). **TERMÉSZET VILÁGA 148**:(2) 92 (2017)

ALICE Collaboration

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

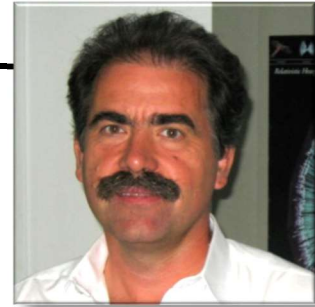
1. Acharya S et al. incl. Benedi G, Berenyi D, Biro G, Boldizsár L, Hamar G, Kiss G, Kofarago M, Lévai P, Olah L, Pochybova S, Vértési R [1027 authors]: Production of muons from heavy-flavour hadron decays in p–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV **PHYS LETT B 770**: 459-472 (2017)
2. Acharya S et al. incl. Benedi G, Berenyi D, Biro G, Boldizsár L, Hamar G, Kiss G, Kofarago M, Lévai P, Olah L, Pochybova S, Vértési R [1029 authors]: Production of π^0 and η mesons up to high transverse momentum in pp collisions at 2.76 TeV. **EUR PHYS J C 77**:(5) 339/1-25 (2017)
3. Acharya S et al. incl. Benedi G, Berenyi D, Biro G, Boldizsár L, Hamar G, Kiss G, Kofarago M, Lévai P, Olah L, Pochybova S, Vértési R [1026 authors]: Energy dependence of forward-rapidity J / ψ and $\psi(2S)$ production in pp collisions at the LHC **EUR PHYS J C 77**:(6) 392/1-21 (2017)
4. Acharya S et al. incl. Benedi G, Berenyi D, Biro G, Boldizsár L, Hamar G, Kiss G, Kofarago M, Lévai P, Olah L, Pochybova S, Vértési R [1042 authors]: Linear and non-linear flow mode in Pb–Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. **PHYS LETT B 773**: 68-80 (2017)
5. Acharya S et al. incl. Benedi G, Berenyi D, Biro G, Boldizsár L, Hamar G, Kiss G, Kofarago M, Lévai P, Olah L, Pochybova S, Vértési R [1026 authors]: Measurement of D-meson production at mid-rapidity in pp collisions at $\sqrt{s}=7$ TeV. **EUR PHYS J C 77**:(8) 550/1-21 (2017)

6. Acharya S et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1042 authors]: Searches for transverse momentum dependent flow vector fluctuations in Pb-Pb and p-Pb collisions at the LHC. *J HIGH ENERGY PHYS* **2017**:(9) 032/1-33 (2017)
7. Acharya S et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1041 authors]: Measurement of deuteron spectra and elliptic flow in Pb–Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV at the LHC. *EUR PHYS J C* **77**:(10) 658/1-20 (2017)
8. Acharya S et al. incl. [Benedi G](#), [Berenyi D](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1042 authors]: Measuring KS $0K_{\pm}$ interactions using Pb–Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. *PHYS LETT B* **774**: 64-77 (2017)
9. , Acharya S et al. incl. [Barnaföldi GG](#), [Benedi G](#) [1040 authors]: Charged-particle multiplicity distributions over a wide pseudorapidity range in proton-proton collisions at $\sqrt{s} = 0.9, 7,$ and 8 TeV. *EUR PHYS J C* **77**:(12) 852/1-23 (2017)
10. Acharya S et al. incl. [Barnaföldi GG](#), [Benedi G](#), [Lévai P](#), [Pochybova S](#) [1014 authors]: J/ψ Elliptic Flow in Pb-Pb Collisions at $\sqrt{s_{NN}} = 5.02$ TeV. *PHYS REV LETT* **119**:(24) 242301/1-13 (2017)
11. Adam J et al. incl. [Barnaföldi GG](#), [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#) [1009 authors]: J/ψ suppression at forward rapidity in Pb–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. *PHYS LETT B* **766**: 212-224 (2017)
12. Adam J et al. incl. [Barnaföldi GG](#), [Benedi G](#), [Berenyi D](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#) [985 authors]: Charged-particle multiplicities in proton–proton collisions at $\sqrt{s} = 0.9$ to 8 TeV. *EUR PHYS J C* **77**:(1) 33/1-39 (2017)
13. Adam J et al. incl. [Barnaföldi GG](#), [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1009 authors]: W and Z boson production in p-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. *J HIGH ENERGY PHYS* **2017**:(2) Paper 77. 27 p. (2017)
14. Adam J et al. incl. [Barnaföldi GG](#), [Benedi G](#), [Berenyi D](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#) [990 authors]: φ-Meson production at forward rapidity in p–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV and in pp collisions at $\sqrt{s} = 2.76$ TeV. *PHYS LETT B* **768**: 203-217 (2017)
15. Adam J et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#) [1003 authors]: Measurement of azimuthal correlations of D mesons with charged particles in pp collisions at $\sqrt{s} = 7$ TeV and p–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. *EUR PHYS J C* **77**:(4) 245/1-24 (2017)
16. Adam J et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1018 authors]: Flow Dominance and Factorization of Transverse Momentum Correlations in Pb-Pb Collisions at the LHC. *PHYS REV LETT* **118**:(16) 162302/1-12 (2017)
17. Adam J et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1007 authors]: Measurement of the production of high-pT electrons from heavy-flavour hadron decays in Pb–Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. *PHYS LETT B* **771**: 467-481 (2017)
18. Adam J et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1009 authors]: Measurement of electrons

- from beauty-hadron decays in p-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV and Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. *J HIGH ENERGY PHYS* **2017**:(7) 052/1-40 (2017)
19. Adam J et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsár L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Lévai P](#), [Olah L](#), [Pochybova S](#), [Vértési R](#) [1005 authors]: Anomalous Evolution of the Near-Side Jet Peak Shape in Pb-Pb Collisions at $\sqrt{s_{NN}} = 2.76$ TeV. *PHYS REV LETT* **119**:(10) 102301/1-13 (2017)
 20. Adamova D et al. incl. [Benedi G](#), [Berenyi D](#), [Biro G](#), [Boldizsar L](#), [Hamar G](#), [Kiss G](#), [Kofarago M](#), [Levai P](#), [Olah L](#), [Pochybova S](#), [Vertesi R](#) [1028 authors]: Azimuthally Differential Pion Femtoscopy in Pb-Pb Collisions at $\sqrt{s_{NN}} = 2.76$ TeV. *PHYS REV LETT* **118**:(22) 222301/1-12 (2017)

R-D. Femtoscopy

Tamás Csörgő, Gábor Kasza, Dániel Kincses[#], Dávid Lucsányi[#], Frigyes Nemes, András Ster



The Femtoscopy Research Group is actively participating in theoretical research and in experimental research in the PHENIX experiment at the RHIC accelerator, Brookhaven National Laboratory and in the TOTEM experiment at Large Hadron Collider (LHC) at CERN. We have achieved important breakthroughs in each research direction during 2017:

In our **theoretical femtoscopy related research**, we have discovered

- new families of exact solutions of 1+3 dimensional, rotating, multi-component, non-relativistic fireball hydrodynamics;
- new families of exact solutions of accelerating 1+1 dimensional, relativistic perfect fluid hydrodynamics with realistic equations of state;
- new families of perturbative solutions of accelerating, viscous 1+1 dimensional relativistic viscous hydrodynamics.

During the academic year we have organized and participated in an extremely large number of conferences where most of these new results were presented, and we started to write-up these results in conference proceedings and manuscripts submitted for a publication. We expect that most of the new solutions will be published subsequently during 2018.

In our **TOTEM related femtoscopy research**, we have discovered

- new structures in the excitation function of the total cross section, the rho and the B parameter of elastic proton-proton scattering. This result is interpreted as the discovery of the Odderon (or vector glueball, a 3-gluon bound state).

In our **PHENIX related femtoscopy research**, we have discovered

- that d+Au collisions and 3He+Au collisions feature perfect fluid properties down to as low nucleon-nucleon center of mass energies as 19.6 GeV. T. Csörgő acted as the Chairman of the Internal Review Committee on this publication.
- in 0-30% Au+Au collision at 200 GeV, the shape of the Bose-Einstein correlation function is significantly different from the usual Gaussian shape. The Levy form however describes the data, opening a new series of papers. The manuscript was submitted for a publication and several Levy related Bose-Einstein correlation measurements were presented by members of the Hungarian PHENIX group at conferences during 2017, with publications to appear in 2018.

Grants

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

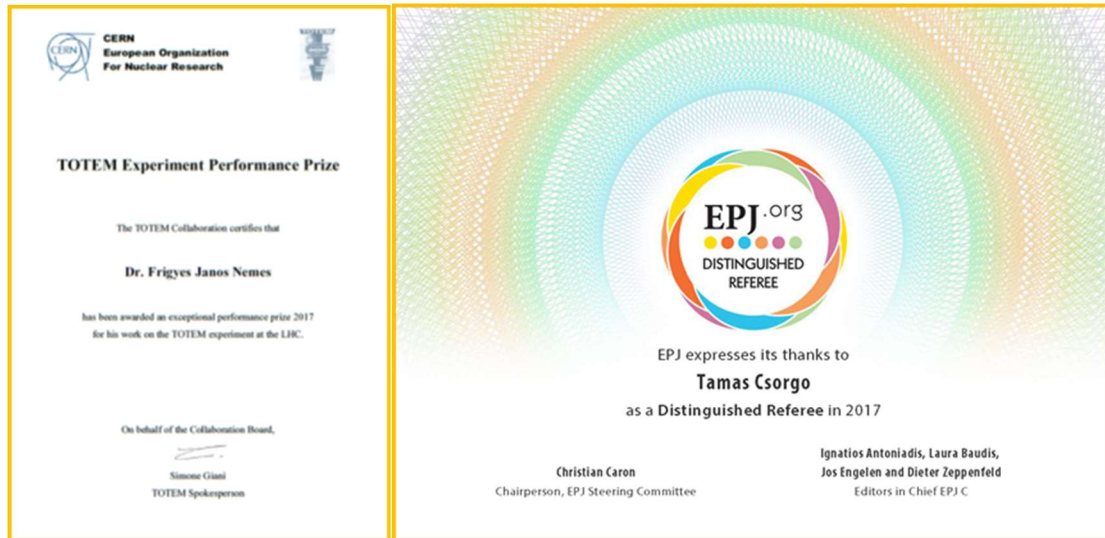


Figure 1. Two of four awards received in 2017. Left: TOTEM Experiment Performance Prize awarded to Dr. F. Nemes, on behalf of the TOTEM Collaboration Board by Prof. S. Giani, Spokesperson of the TOTEM experiment at CERN LHC. Right: EPJ Distinguished Referee Award by the Chairman of the Steering Committee and the Editors in Chief of European Physics Journal (EPJ) C, to T. Csörgő, MAE.

Hungarian Academy of Sciences - Ukrainian Academy of Science bilateral grant NKM-092/2017

Hungarian Academy of Sciences – Grant for the Organization of the BGL 2017 conference Participation, NKTIH FK 123842 and FK 123959 grants (PI: M. Csanád, ELTE & A. László, Wigner) Participation in EFOP EFOP 3.6.1-16-2016-00001 grant (PI: Papp József, EKE)

International cooperations:

PHENIX Collaboration (BNL, Upton, NY, USA)

TOTEM Collaboration (CERN LHC, Svájc)

Bogoliubov Institute for Theoretical Physics (Kiev, Ukraine)

Lund University (Lund, Sweden)

State University of New York at Stony Brook (Stony Brook, NY, USA)

Publications

Article

1. Csanád M, Csörgő T, Jiang ZF, Yang CB: Initial energy density of $\sqrt{s} = 7$ and 8 TeV p-p collisions at the LHC. **UNIVERSE 3**:(1) 9/1-15 (2017)

Book chapters

2. Nagy MI, Csörgő T: An analytic hydrodynamical model of rotating 3D expansion in heavy-ion collisions. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN*

Gribov (Budapest, Hungary, 17-20 June 2015).Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 109-119

See also: R-B.28

Phenix collaboration

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R-H. Hadron physics

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The aim of our research group is to better understand the strong interaction through collisions of nucleons and nuclei by performing basic and advanced measurements (cross sections, particle spectra and correlations), and by testing various theoretical ideas (quark-gluon plasma, gluon saturation, critical endpoint of the phase diagram). We participate in several complementary experiments (mainly ALICE and CMS), both in data-taking and physics analysis.

With the help of ultra-relativistic heavy-ion collisions, the properties of strongly-interacting hadronic matter can be studied under extreme conditions of temperature and energy density. Characteristics of this phase of matter are important for a better understanding of the strong interaction as well as to address cosmological questions of the early Universe. Recently the study of particle production in high-multiplicity events in small collision systems at the LHC has revealed unexpected new collective-like phenomena. In particular, for high-multiplicity pp and p-Pb collisions, radial flow signals, long-range angular correlations, and strangeness enhancement have been reported. Our activities this year focused on the above-listed topics.

Spectra of identified hadrons. — We have measured the transverse momentum spectra of identified charged hadrons (pions, kaons, and protons) in proton-proton collisions at $\sqrt{s} = 13$ TeV. The p_T spectra and integrated yields are compared to lower center-of-mass energy pp results and to Monte Carlo simulations. The average p_T increases with particle mass and the charged-particle multiplicity of the event (Fig. 1, left). A comparison with lower energy data shows only a moderate dependence of the average p_T on the center-of-mass energy. The PYTHIA8 CUETP8M1 event generator reproduces most features of the measured distributions, but EPOS LHC also gives a satisfactory description of several aspects. Particle production is strongly correlated with event multiplicity in all collision types, rather than with the center-of-mass energy or collision system. The data supports the assumption that the characteristics of particle production are constrained by the amount of initial parton energy that is available in any given collision.

Sources of radial flow patterns. — We have proposed a tool to reveal the origin of the collective-like phenomena observed in proton-proton collisions. We exploit the fundamental difference between the underlying mechanisms, color reconnection, and hydrodynamics, which produce radial flow patterns in PYTHIA8 and EPOS3 Monte Carlo event generators, respectively. The strength of the coupling between the soft and hard components, by construction, is larger in PYTHIA8 than in EPOS3. We studied the transverse momentum (p_T) distributions of charged pions, kaons and (anti) protons in inelastic pp collisions at $\sqrt{s} = 7$ TeV produced at mid-rapidity. Specific selections are made on an event-by-event basis as a function of the charged particle multiplicity and the transverse momentum of the leading jet reconstructed using the FastJet algorithm at mid-pseudorapidity. From our studies,

quantitative and qualitative differences between PYTHIA8 and EPOS3 are found in the p_T spectra when (for a given multiplicity class) the leading jet p_T is increased. In addition, we showed that for low-multiplicity events the presence of jets can produce radial flow-like behavior, shown in Fig. 1 (right). The observed differences between the two event classes (low and high multiplicities) similar to those seen in the hadrochemistry measured in the jet and bulk regions in pp and Pb-Pb collisions by the ALICE collaboration. Motivated by our findings, we proposed to perform a similar analysis using experimental data from RHIC and the LHC.

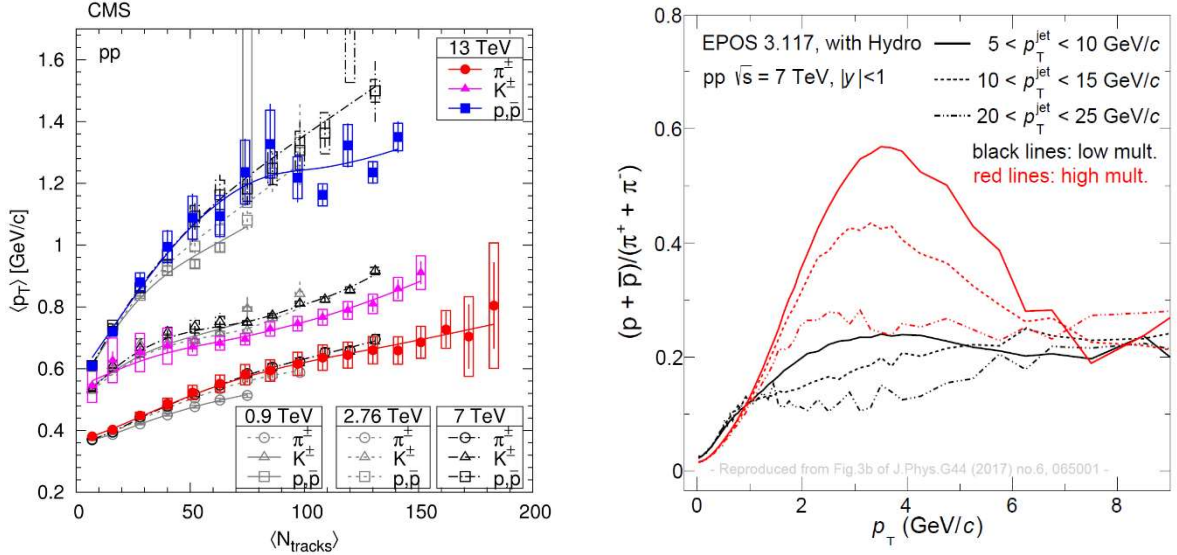


Figure 1. Left: Average transverse momentum of identified charged hadrons (pions, kaons, and protons) at mid-rapidity as a function of the corrected track multiplicity in the range $|\eta| < 2.4$, for pp collisions at $\sqrt{s} = 13$ TeV (filled symbols) and at lower energies (open symbols). Lines are drawn to guide the eye. Right: Proton-to-pion particle ratio as a function of p_T for low (black lines) and high (red lines) multiplicity event classes, and for different leading jet p_T intervals simulated by the Epos3 Monte Carlo event generator.

Angular correlations. — Previous studies have shown that several mechanisms can play a role in producing collective-like behavior. It has been demonstrated that multi-parton interactions and color reconnection as implemented in PYTHIA MC event generator produce radial flow patterns via boosted color strings. Also, azimuthal correlations have been studied in A Multi-Phase Transport model (AMPT), where the ridge structure can be generated assuming incoherent elastic scattering of partons and the string melting mechanism. Besides, phenomenological studies (as described above) show that it is possible to find a subclass of low-multiplicity events where radial flow patterns arise, despite the fact that at very low multiplicity hydrodynamics cannot be applied and color reconnection effects are small.

We have measured the two-particle angular correlations of charged particles in Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. The azimuthal angle ($\Delta\phi$) and pseudorapidity ($\Delta\eta$) difference of a trigger particle with high p_T and an associated particle with lower p_T are evaluated. In the distribution of these angles, jets manifest themselves as a peak around $(\Delta\phi, \Delta\eta) = (0, 0)$ and as an elongated structure in $(\Delta\eta)$ at $\Delta\phi = \pi$. Studying the centrality and p_T dependence of the shape of the jet peak and comparing it to the shape in proton-proton collisions can provide insight on the interaction of jets with the quark-gluon plasma (QGP). The jet peak is found to broaden at low p_T in Pb-Pb collisions towards central collisions (Fig. 2, left). It is also found to become asymmetric (broader in $\Delta\eta$ than in $\Delta\phi$). An unexpected depletion around $(\Delta\phi, \Delta\eta) = (0, 0)$ also develops at low p_T . The comparison of the modification of the jet peak with the AMPT model shows that both effects are accompanied by large radial and longitudinal flow, suggesting that they arise as a consequence of the interaction of the jets with the flowing QGP.

Quantum correlations. — We have measured short-range two-particle correlation functions of identified hadrons in pp, p-Pb, and peripheral Pb-Pb collisions. The extracted radii of the particle emitting source (via Bose-Einstein correlations) are in the range 1-5 fm, reaching highest values for very high multiplicity p-Pb and Pb-Pb collisions. The pp and p-Pb source is elongated in the beam direction, while in the peripheral Pb-Pb case the source is symmetric. The dependence of the radii on the multiplicity and k_T factorizes and appears to be less sensitive to the type of the collision system and center-of-mass energy (Fig. 2, right). The observed similarities may point to a common critical hadron density reached in the collisions.

Heavy flavour production. — Heavy-flavour (beauty and charm) quarks are produced almost

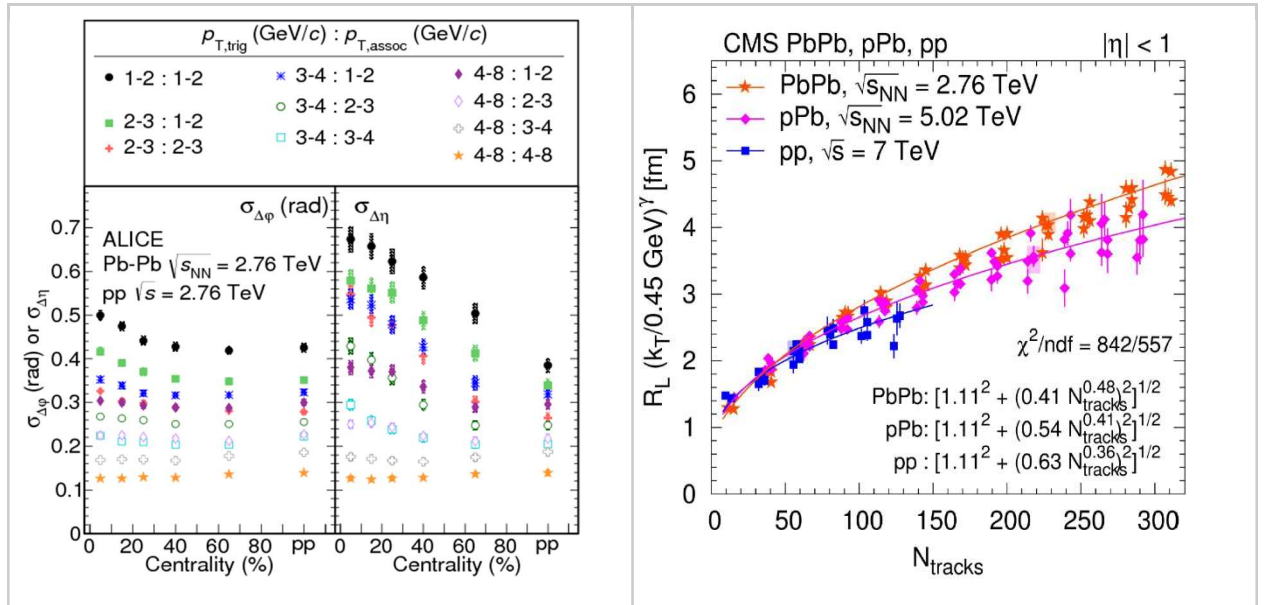


Figure 2. Left: Width of the jet peak in the $\Delta\phi$ and $\Delta\eta$ directions from Pb-Pb and pp (rightmost points) collisions at $\sqrt{s_{NN}} = 2.76$ TeV. Right: Cauchy-type radius parameters for pions from Bose-Einstein correlation analyses of various collision systems and center-of-mass energies as a function of the corrected track multiplicity in the range $|\eta| < 2.4$, scaled to $k_T = 0.45$ GeV/c with help of a specific parametrization.

exclusively in initial hard processes, and their yields remain largely unchanged throughout a heavy-ion reaction. Nevertheless, they interact with the nuclear matter in all the stages of its

evolution. Thus, heavy quarks serve as ideal self-generated penetrating probes of the strongly interacting QGP. Jets containing heavy flavour hadrons are also sensitive to flavour-dependent fragmentation and gluon splitting. Recent heavy-flavour jet measurements by the ALICE experiment, with contributions from our group, provide strong constraints on theoretical models of heavy-flavour production and fragmentation.

Jet structure. — Non-trivial behavior of high multiplicity events in small systems have also been observed in the heavy-flavour sector. Recent analyses of pp and p-Pb collisions show a universal enhancement of heavy-flavour particles that is usually attributed to multiple parton interactions and higher gluon radiation associated with short distance production processes. We have carried out extensive studies using MC event generators. We have given predictions for multiplicity-dependent jet structures, and proposed a way to validate the presence and extent of effects such as multiple-parton interactions or color reconnection, based on the detection of non-trivial jet shape modification in high multiplicity events. We proposed a way to use the multiplicity-dependent jet structures to experimentally differentiate between equally well-performing simulation tunes. We have also introduced a definition of a characteristic jet size measure that is independent of multiplicity. These studies can serve as a baseline for jet structure analyses in heavy-ion collisions as well as flavour-dependent studies.

New method for tracking of charged particles at high multiplicities. — We have developed a novel combination of established data analysis techniques for reconstructing charged particles in very high multiplicity collisions. It uses all information available while keeping competing choices open as long as possible. Suitable track candidates are selected by transforming measured hits to a track parameter space with help of templates. The highly connected network of track candidates and their corresponding hits is cut into very many subgraphs by removing a few of its vulnerable components, edges, and nodes. Finally, the hits distributed among the candidates by exploring a deterministic decision tree. A depth-limited search is performed maximizing the number of hits on tracks, and also the sum of track-fit quality measures.

Grants

NKFI K 109703: Consortial main: Hungary in the CMS experiment of the Large Hadron Collider (F. Siklér, 2013-2017)

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

International cooperation

ALICE, CMS, FOPI, NA49, and NA61 (CERN), PHENIX and STAR (RHIC)

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See also: R-I.1

CMS Collaboration

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

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NA61/SHINE Collaboration

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Nucleus-Nucleus Collisions (Quark Matter). Chicago, USA, 05. February 2017 – 11. February 2017)

STAR Collaboration

1. Vértési R and STAR Collaboration: Latest results on Y production in heavy-ion collisions from the STAR experiment. *J PHYS Pokol CONF SER 832*: 012025-1-4 (2017) (7th Workshop on Young Scientists on the Physics of Ultra-Relativistic Nucleus-Nucleus Collisions (Hot Quarks). Southbridge, USA, 12 September 2016 – 17 September 2016)

R-J. Standard model and new physics

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



Physics analyses and theoretical work. — Our group has measured cross-section limits on supersymmetric processes leading to strongly boosted top quark decays in the data recorded by the CMS detector at the LHC prior to the 2017 installation of the new pixel detector. We have also doubled the recorded collision data using the new pixel detector during 2017. We provided a member for the Publication Committee of the CMS Experiment at CERN and played an important role in publishing CMS results of low-x QCD studies.

The group participated in the ASACUSA experiment at the Antimatter Factory of CERN, which provides a test of the CPT invariance, the theorem stating the equivalence of matter and antimatter, via measuring the transition energies of antiprotons trapped helium atoms using laser spectroscopy. The method leading to the precise determination of the agreement between the proton and antiproton masses earlier was extended to superfluid helium; the data are still in analysis. The first steps were made to use two-photon laser spectroscopy on antiprotonic helium atoms cooled down below 1.7 K in cryogenic low-pressure helium gas.

We wrote and published the first Hungarian textbook of quantum information theory. We proposed the Principle of Least Decoherence and, based on it, improved the widely used theory of semi-classical gravity, which will henceforth not violate the linearity of quantum mechanics.

Work on instrumentation. — The group has successfully commissioned the new pixel detector installed at the CMS experiment in 2017, the control and read-out electronics of which device was developed and manufactured by our group. We have prepared the 3D detector model and the software for the reconstruction of the new data, organized the spatial and temporal alignment of the new detector, and completed the calibration of the reconstruction algorithms. We also verified that the detector performance meets its design requirements.

The stable operation of the T2_HU_Budapest grid site continued in 2017. Our site is used extensively by the entire CMS collaboration including our group for reconstructing collision data in physics analyses. The disk capacity committed to CMS has increased to 900 TB.

We have successfully tested two superconducting shield prototypes for the *Superconducting Shield Septum* project: a high-temperature superconductor and MgB₂. The performance of the MgB₂ prototype was satisfactory for its application. We have designed and constructed a device called “SPS Diffuser”, which will be installed in the CERN SPS accelerator to decrease the radiation load on the electrostatic septum.

Outreach. — Two education programs were organized by Wigner RCP at CERN with the leadership of our group: the High-School Student Internship Programme (22 May - 2 June 2017) with the participation of 22 students and the Hungarian Teachers Programme (15-21

August 2016) for 21 physics teachers. For the teachers we organized a meeting on November 25 at Wigner RCP in the presence of representatives of the Hungarian Physical Society, the Hungarian CERN Committee and the main sponsor, the Pallas Sthene Domus Innovationis Foundation. We also participated in the organization of the annual Hands-on Particle Physics Master-classes on two occasions with 22 high-school students attending each session. In addition to conference talks and university teaching, many popular lectures were given by our group.

Grants

OTKA K-109703: Consortial main: Hungary in the CMS experiment of the Large Hadron Collider (V. Veszprémi, Cs. Hajdu, D. Horváth, T. Vámi, 2013-2017)

NKFI K-124850 Consortial assoc.: The Standard Model and beyond: Searching for New Physics with the CERN LHC CMS experiment (V. Veszprémi, Cs. Hajdu, D. Horváth, T. Vámi, 2017-2021)

NKFI K-124945 Research and development of novel technologies for particle accelerators (D. Barna, 2017-2021);

OTKA K-103917 Antimatter studies at the Antiproton Decelerator of CERN (D. Barna, L. Diósi, D. Horváth, 2012-2017)

International cooperation

CMS Collaboration (200 institutes)

University of Tokyo, Japan

RIKEN, Wako, Japan

Max-Planck-Institut für Quantenoptik, Germany

Università di Brescia & Istituto Nazionale di Fisica Nucleare, Italy

Publications

Articles

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11. Horváth D: Antianyag-vizsgálatok a CERN-ben (Antimatter studies at CERN, in Hungarian). FIZIKAI SZEMLE 67:(4) pp. 115-121. (2017)
12. Horváth D: A részecskefizika sérült szimmetriái vajon megoldják-e a problémáit? (May the broken symmetries of particle physics solve its problems? In Hungarian) **TERMÉSZET VILÁGA** 148:(11) pp. 495-499. (2017)

Book chapter

13. Horváth D: Ultra-fast neutrinos: What can we learn from a false discovery?. In: *Gribov-85 Memorial Volume: Exploring Quantum Field Theory: Proceedings of the Memorial Workshop Devoted to the 85th Birthday of VN Gribov (Budapest, Hungary, 17-20 June 2015)*. Eds.: Dokshitzer Y, Lévai P, Nyíri J, Singapore: World Scientific Publishing, 2017 pp. 364-376

See also; R-H.1, R-H.2, R-I.1,

ATLAS collaboration

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

1. Aaboud M et al. incl. Toth J [2873 authors]: Search for the Dimuon Decay of the Higgs Boson in pp Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector. **PHYS REV LETT** 119:(5) 051802/1-49 (2017)
2. Aaboud M et al. incl. Toth J [2879 authors]: Search for Dark Matter Produced in Association with a Higgs Boson Decaying to $b\bar{b}$ Using 36 fb⁻¹ of pp Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector. **PHYS REV LETT** 119:(18) 181804/1-21 (2017)
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4. Aaboud M et al. incl. Toth J [2853 authors]: Measurement of the ZZ production cross section in pp collisions at $\sqrt{s} = 8$ TeV using the $ZZ \rightarrow \ell\text{-}\ell+\ell'\text{-}\ell'+$ and $ZZ \rightarrow \ell\text{-}\ell+\nu\nu$ channels with the ATLAS detector. **J HIGH ENERGY PHYS** 2017: 099/1-53 (2017)
5. Aaboud M et al. incl. Toth J [2851 authors]: Measurements of top quark spin observables in $t\bar{t}$ events using dilepton final states in $\sqrt{s} = 8$ TeV pp collisions with the ATLAS detector. **J HIGH ENERGY PHYS** 2017:(3) 113/1-50 (2017)
6. Aaboud M et al. incl. Toth J [2860 authors]: Measurements of $\psi(2S)$ and $X(3872) \rightarrow J/\psi\pi + \pi -$ production in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector. **J HIGH ENERGY PHYS** 2017:(1) 117/1-43 (2017)

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11. Aaboud M et al. incl. [Toth J](#) [2852 authors]: Probing the W tb vertex structure in t-channel single-top-quark production and decay in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector. *J HIGH ENERGY PHYS* 2017:(4) 124/1-50 (2017)
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See also: R-H NA49 Collaboration

R-M. Ion beam physics

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

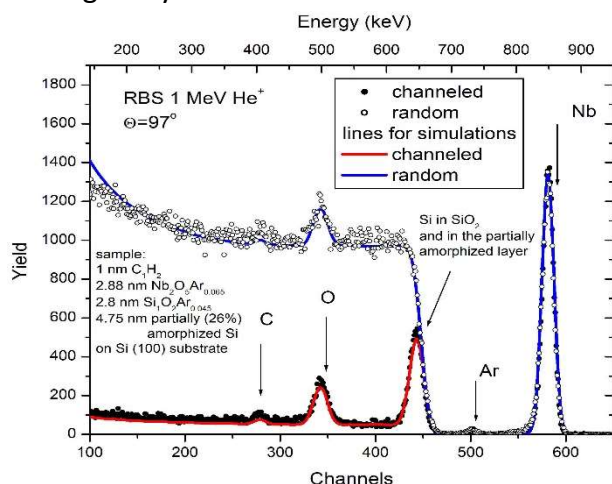


Various effects of ion implantation—Corrosion resistance of silicon carbide (SiC)-rich nanolayers produced by implantation and damage caused by radiofrequency sputtering of niobium oxide have been studied in collaboration with Institute of Technical Physics and Materials Science, Centre for Energy Research.

To produce SiC protective coatings C/Si/C/Si/C multilayer structures with different thicknesses on silicon substrates were irradiated by Ar⁺ and Xe⁺ ions at room temperature and at a fluence range of 0.5–3x10¹⁶ ion/cm². The C, Si and SiC distributions formed by the effect of ion beam mixing were determined by Auger electron spectroscopy. In corrosion point of view the best SiC-rich layer was produced from multilayer with thicknesses of 10 nm C and 20 nm Si by implanting with 120 keV Xe with a fluence of 3x10¹⁶ Xe/cm². As a result of the potentiodynamic experiments, the measured chemical corrosion resistance for this sample was orders of magnitude better than that of pure silicon.

To investigate the damage caused by radiofrequency sputtering, Nb₂O₅ layers were deposited to c-Si substrates in a gas mixture of O₂ and Ar at a pressure of 0.3 Pa, at an oxygen flow of 6 ml/min and at various DC sputtering voltage selected from the range of 1.0–2.0 kV. During the rf-sputtering the energetic O⁺, Ar⁺ ions and neutral atoms may penetrate into the c-Si substrate to a depth of several nm causing displacement of host silicon atoms and consequently producing damaged regions.

In cross-sectional transmission electron microscopy image of a Nb₂O₅ sample with a deposition time of 100 s at 2.0-kV (not shown) a 2.9 nm thick amorphous Nb-oxide film, a 4.5 nm thick amorphous layer, which can be either amorphous SiO₂ and/or amorphous Si, as well as single crystalline substrate can be observed. The partially damaged silicon layer was



identified on the substrate both by Rutherford backscattering spectrometry combined with channelling (as shown in Figure 1) and by multiple angle of incidence spectroscopic ellipsometry.

Figure 1. Channelled and random spectra taken on Nb₂O₅ film deposited by rf sputtering on single crystalline silicon substrate with a deposition time of 100 s at 2.0-kV.

Advanced cultural heritage research. —

External milli beam PIXE was applied to determine the composition of mineral pigments from ceramics objects excavated by Romanian archaeologists from archaeological sites of

important commercial settlements on Danube at the border between Ottoman Empire (Dobroudja) and Romanian Principalities – Piuia Petrii and Dinogetia-Garvan.. The mineral pigments used for Turkish Miletus (late XVth-XVIth centuries) and Iznik (XVIth-XVIIth centuries) ceramics are very important for the understanding of commercial routes of late Mediaeval period. The elemental composition of glaze, green, yellow, brown and especially blue pigments was determined. The most interesting case is the one of the Co-based blue pigments (as shown in Figure 2). The origin of the raw material for these pigments in the XVIIth Century could be the mining district of Schneeberg in Germany, characterized by the presence of smaltite and erythrite minerals and this study revealed a possible trade route connection between Saxony and Ottoman Empire during those times. Arsenic is of a special importance in the case of Co blue pigments, since it was observed to appear mostly in samples dated after the year 1520.

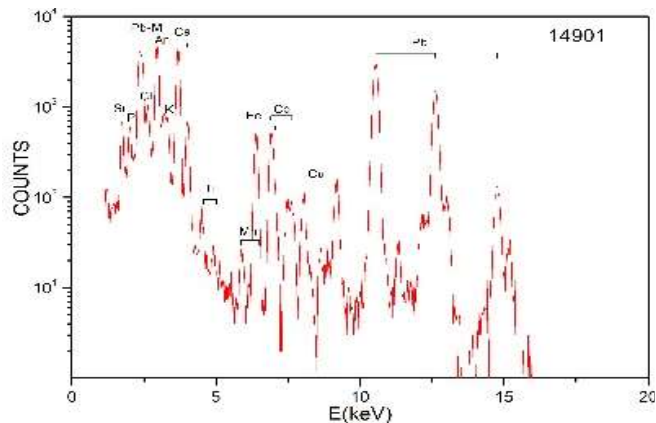


Figure 2. PIXE analysis of a dark blue area on Iznik glazed ceramics sherd (sample: CER 9)

Grants

OTKA K-115852: Development and optical monitoring of nanostructures for sensing (Principal investigator: P. Petrik, H.A.S. Centre for Energy Research, 2015-2018)

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

European Research Infrastructure for Heritage Science Preparatory Phase, Grant No. 739503 (E-RIHS PP, 2017-2019)

MTA Infrastructure Development: Running costs of some infrastructures of the department of Materials Science by Nuclear methods. (E. Szilágyi 2017)

International cooperation

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

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

Publications

Articles

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3. Nagy GUL, Lavrentiev V, Bányász I, Szilasi SZ, Havranek V, Vosecek V, Huszánk R, Rajta I: Compaction of polydimethylsiloxane due to nitrogen ion irradiation and its application for creating microlens arrays. THIN SOLID FILMS 636: pp. 634-638. (2017)
4. Rácz A S, Kerner Z, Németh A, Panjan P, Péter L, Sulyok A, Vértesy G, Zolnai Z, Menyhárd M: Corrosion resistance of nanosized silicon carbide-rich composite coatings produced by noble gas ion mixing. **ACS APPL MATER INTER 9**:(51) 44892-44899 (2017)
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6. Szirmai P, Náfrádi B, Arakcheeva A, Szilágyi E, Gaál R, Nemes NM, Berdat X, Spina M, Bernard L, Jaćimović J, Magrez A, Forró L, Horváth E: Cyan titania nanowires: Spectroscopic study of the origin of the self-doping enhanced photocatalytic activity. CATALYSIS TODAY 284: pp. 52-58. (2017)
7. Bányász I: Tökéletlen holográfia: A rögzítőanyag nemlinearitásának és véges feloldóképességének hatása a rekonstruált holografikus képre. **FIZIKAI SZEMLE 67**:(7-8) pp. 255-259. (2017)
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9. Bányász I, Nagy GUL, Havranek V, Vosecek V, Agocs E, Fried M, Rakovics V, Pelli S: Recent progress in ion beam fabrication of integrated optical elements. In: *ICTON 2017 - 19th International Conference on Transparent Optical Networks (Girona, Spain, 02-06 July 2017)* Eds.: Jaworski M, Marciniak M, Washington: IEEE Computer Society, 2017. Paper 8024871. 4 p.
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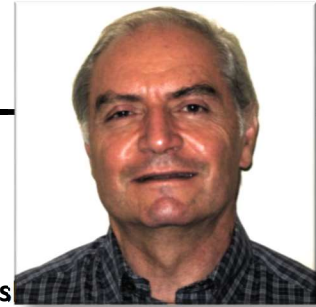
Other

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See also: S-L.22, S-L.23

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

Gagik P. Dzsotjan, Lószef Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós Kedves, Béla Ráczkevi, Zsuzsanna Sörlei^A



Time-resolved diagnostics of rubidium plasma generated by ultra-s

This research is closely related and correlated with the AWAKE (advanced wake field acceleration) experiment at CERN and is continuation of our research conducted in 2016. The main goal of the AWAKE experiment is construction of a novel plasma-based particle accelerator that will utilize the proton bunch available at Large Hadron Collider (LHC) to accelerate electrons (positrons) to TeV energies in a single acceleration stage. An extended volume of extremely homogeneous plasma is an indispensable part of the acceleration scheme. This plasma will be used for splitting the LHC proton bunch into micro-bunches using self-modulation instability in the plasma to provide coherent wake-field acceleration of electrons by the proton bunch. Our experimental setup may be considered as a tabletop analogy of the laser plasma source for the AWAKE experiment. In 2017 the experiments were conducted in our newly renovated “clean room” lab with a new Ti:Sa laser system Hydra of Coherent Co. with pulse energy about 25-30 mJ and pulse duration of 30-40 fs (see Fig.1) .

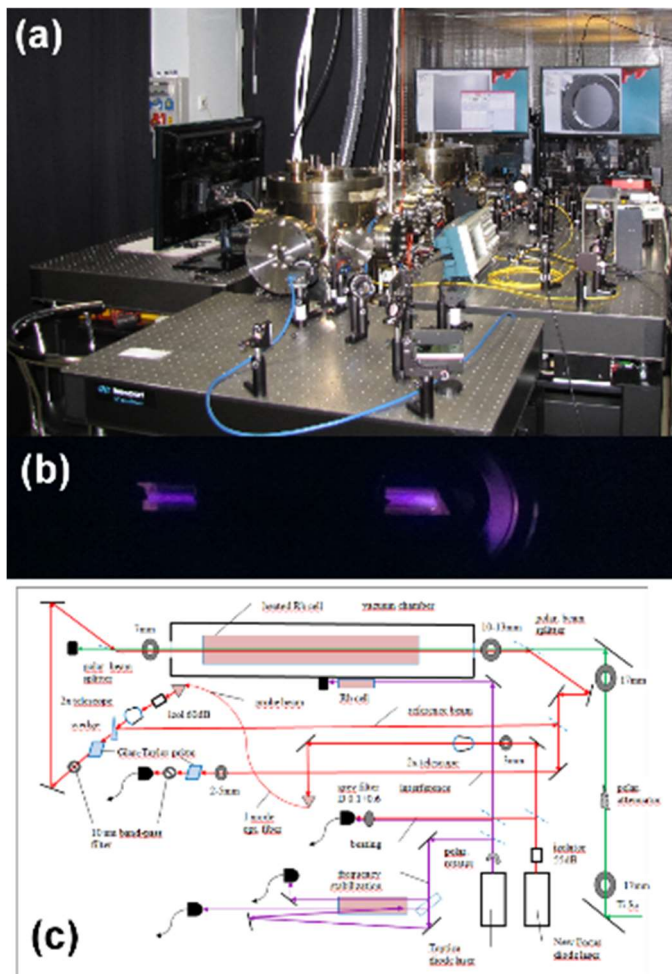


Figure1. The experimental setup (a) with the generated plasma (b) and the scheme of the real-time interferometric diagnostics (c).

We applied our interferometric diagnostics scheme to determine parameters of the created Rb plasma at different values of temperature (density) of the Rb vapor and different values of intensity of the ionizing laser pulses. The diagnostics of the generated plasma is performed using a Mach-Zehnder-type interferometry, Fig.1. The measurements were provided by a CW diode laser with frequency close to D2 line of Rb. Accordingly, the probe diode laser beam propagates in direction opposite to the ionizing laser pulse through a glass cell filled with Rb vapor located in a one arm of the interferometer. This probe beam creates a fringe pattern with a reference beam from the same laser propagating in the air in the other arm of the interferometer. Time variation of the interferometric signals is measured by fast detectors in

a real-time regime. Our fitting technique allows us to measure the plasma density-length product and its variation in time, along with the recombination time constants. An example of the interferometry signal is shown in Fig.2 with the cosine fitting function applied. Results of our studies allow us to understand the physical mechanisms of generation of *extended* laser plasma, as well as to characterize the induced plasma instabilities. These results will be used to create optimal conditions for generation of highly homogeneous plasma for application in the AWAKE project at CERN.

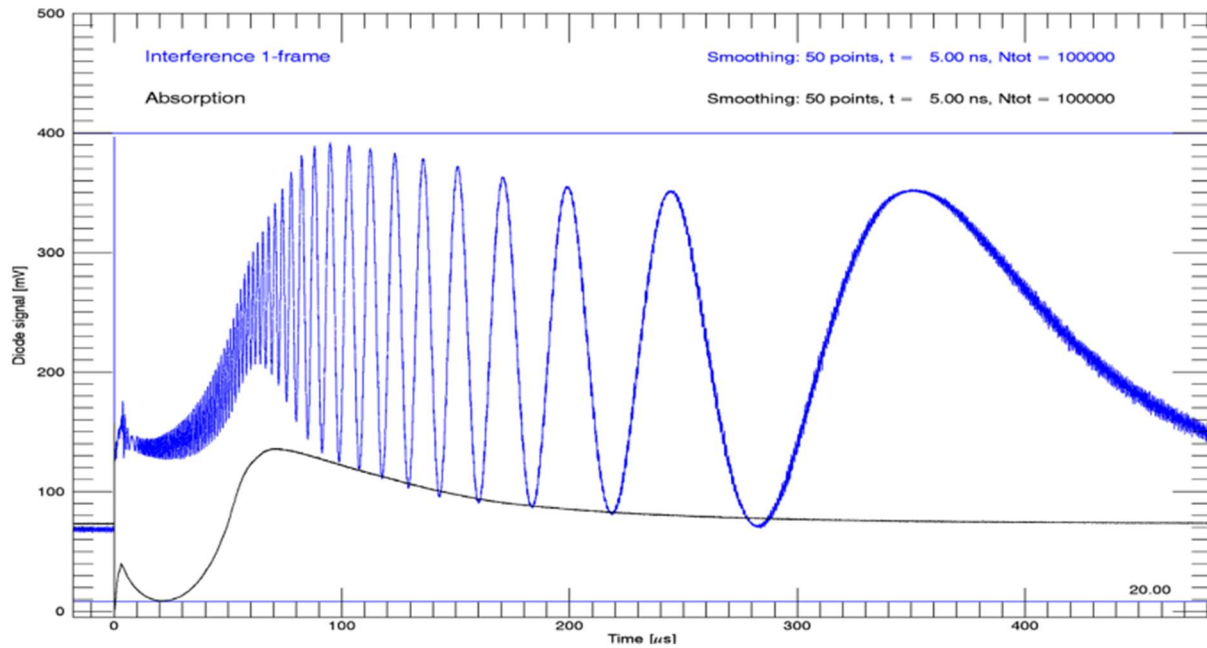
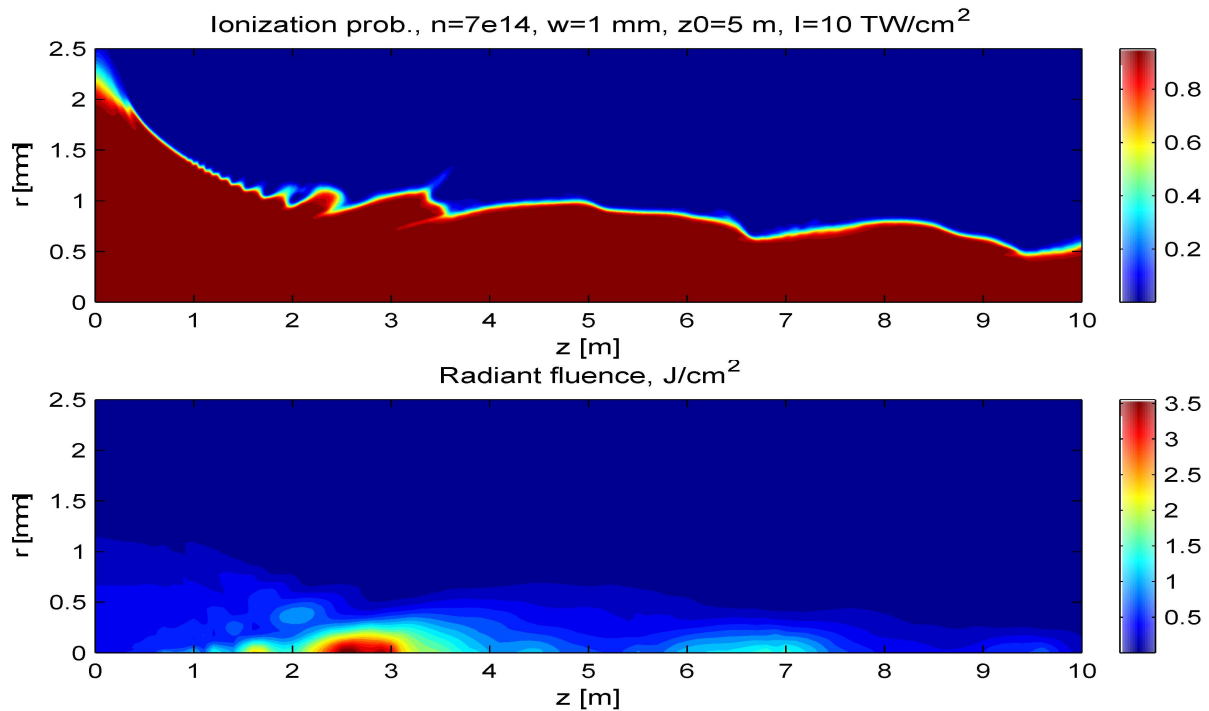


Fig.2. An example of an interferometry signal measured by the fast detector with a cosine fitting curve: $I_{interf}(t) = I_{tr}(t) + I_{ref} + 2\varepsilon\sqrt{I_{tr}(t)I_{ref}} \cos(\varphi_0 + \varphi_1(t)e^{-t/\tau})$

Modeling of propagation of an ionizing femtosecond laser pulse in Rb vapors. — In 2017 we investigated the propagation of an ultrashort, ionizing laser pulse through rubidium vapor, a project associated with the previously mentioned AWAKE experiment. An initial calculation that employed a relatively simple atomic model to calculate the effect of the ultrashort pulse on the rubidium atoms and to compute the optical response of the atoms was perfected in



two respects. First, the atomic model was made more elaborate by including a more precise description of the internal atomic structure, using more atomic levels for the calculation. Instead of the very simple four-level atomic model, an 18-level and a 10-level model was developed and their accuracy evaluated. It was confirmed that the approximation that uses the 10 lowest lying atomic levels of rubidium is accurate enough for computing the optical response, yet it is still simple enough to be used in propagation calculations. Next, the propagation calculations (using the original, four level model) were generalized to include two spatial dimensions, one along the propagation direction and one perpendicular to it. Assuming cylindrical symmetry, we started studying the propagation of the ionizing laser beam in order to evaluate the intensity and focusing requirements to produce a 10 m long plasma channel with very close to 100% ionization in its central region. Self-channeling of the ultrashort laser pulse, as well as a nontrivial pulsing of the plasma channel radius was observed in the calculations, (see Fig.3), where the ionization probability dependence on the propagation length and dependence of the radiant fluence of the ionizing field versus propagation length are presented.

Figure 3. The ionization probability and ionizing pulse radiant fluence versus propagation length.

Grants and international cooperation

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

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

Collaboration with the Technical University of Kaiserslautern, Kaiserslautern, Germany

Collaboration with the University of Bourgogne, Dijon, France

R-O. ITER and fusion diagnostic development

Gábor Veres, Tétény Baross, Livia Beri, Tamás Ilkei, Jenő Kádi, Gábor Nádas, Domokos Nagy, Réka Nagy, József Németh, Miklós Palánkai, László Poszovecz, Bálint Z. Szabó, Gábor Tari, Mátyás Tóth, András Vargyas, Erik Walcz, András Zsákai



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

In 2017 we delivered two large beam emission spectroscopy diagnostic equipment to two European fusion laboratories: to the MAST Upgrade tokamak in the UK and to the Wendelstein 7X stellarator in Germany (Fig. 1). This involved a substantial amount of engineering, manufacturing, testing and commissioning works.

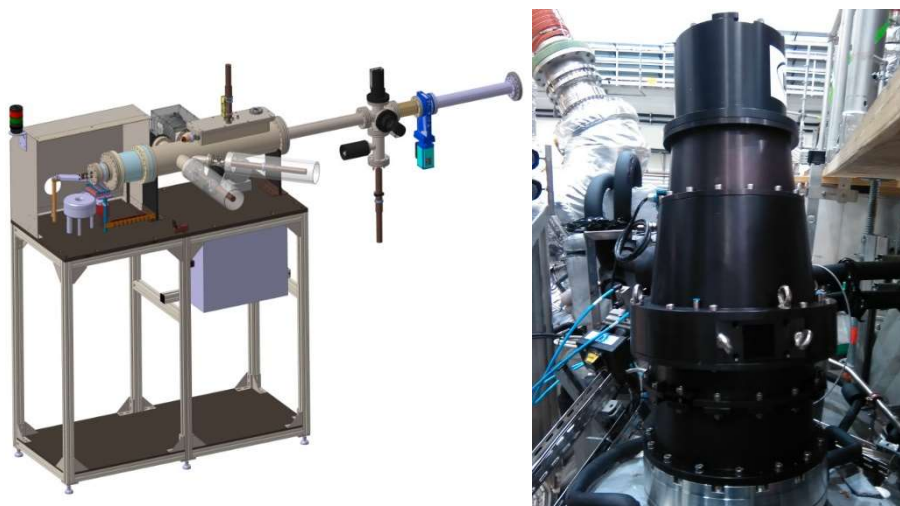


Figure 1. The alkali beam injector for W7X and its observation system

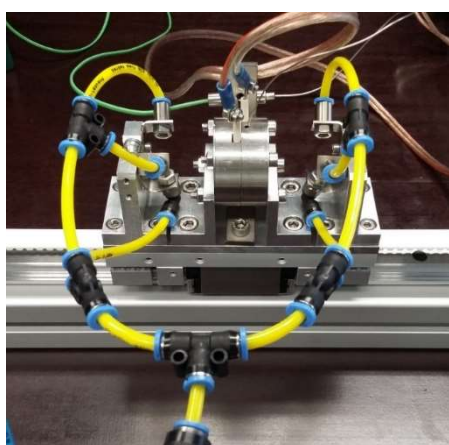


Figure 2. The movable oven for TIEMF measurements

In the Tokamak Services for Diagnostics project that is responsible for the development of the electrical infrastructure for signal transmission in the vacuum vessel, the group successfully carried out a series of qualification experiments to qualify the Mineral Insulated (MI) cables for ITER. These included resistivity, cross-talk, thermal and mechanical load, thermal induced electromotive force (TIEMF) generation and vacuum tightness measurements (Fig. 2).

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

Grants

F4E-FPA-328 Tokamak Services for Diagnostics (G. Veres, 2012-2018)

F4E-FPA-384 Diagnostic Development: ITER Bolometers (G. Veres, 2014-2018)

EUROfusion (G. Veres, 2014-2020)

International cooperation

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

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

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

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See also: R-R.2

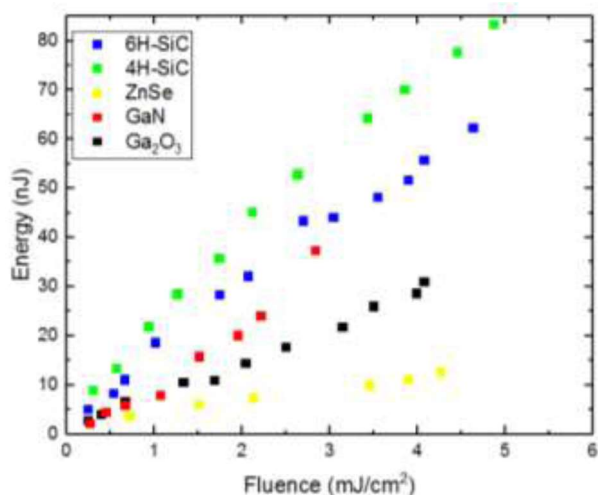
See also: R-H NA49 Collaboration, R-Q Jet Collaboration

R-P. Laser plasma

István B. Földes, Márk Aladi[#], Imre Ferenc Barna, Zsolt Kovács[#], Mihály Pocsai[#]



Generation of THz radiation by a KrF laser. — Large-Aperture Photo-Conductive Antenna (LAPCA) is a perspective intense terahertz (THz) source. It possesses various unique properties, such as the relatively low frequency (< 0.3 THz) of the central spectrum. This is especially interesting in studying nonlinear THz effects, where efficient acceleration of carriers plays an important role. In LAPCA, the THz field is extracted from the bias field. Therefore, wide bandgap semiconductors - which have high breakdown voltage - are excellent candidates as substrate for intense THz generation using LAPCA. However, the challenge is that wide bandgap semiconductors must be driven using lasers with high photon energy (or short wavelength). In this regard, the KrF laser seems to be ideal for this purpose. Experiments were carried out using the 40 mJ/500 fs KrF laser of the University of Szeged together with the researchers of INRS (Canada). Experiments were carried out with



semiconductors of band gaps from 2.7 to 4.8 eV. The results using 16.4 kV/cm show that the THz increases with increasing laser fluence, not reaching saturation. The optimal semiconductor was 4H-SiC with 3.23 eV band gap demonstrating the advantage of using a KrF laser (Fig. 1). Further experiments to increase conversion with higher bias in vacuum are planned.

Figure 1. Energy of THz pulses generated from different semiconductor LAPCAs as a function of the UV fluence.

Fourier filtering integrated to the HILL laser system. — Fourier-filtering was reported earlier to produce improvement both in the temporal and the spatial distribution of the KrF laser pulse. It uses the nonlinear phase-shift in the Fourier plane introduced by the self-generated plasma in a pulsed gas jet. Now the system has been integrated to the laser system which gives >70 mJ energy in 500fs pulses on the 248 nm wavelength in a 1.5 times diffraction limited beam. The intensity contrast with this method is 10^{11} , thus when focusing it to 10^{18} W/cm² intensity the prepulse will not generate significant amount of ions via photoionization, i.e. the main pulse may hit a steplike solid state surface. It can be noted that due to the direct amplification there will be no coherent pedestal in the picosecond scale.

Photoionization of rubidium atoms. — We investigate the ionisation processes of rubidium in strong infra-red laser fields via ab initio calculations. The bound and the continuum states are described with Slater orbitals and Coulomb wavepackets, respectively. The bound state spectrum has been calculated with the variational method and reproduced the experimental

data within a few percent accuracy. Using this approach ionisation processes can be studied successfully. Investigation the effects of the shape and the parameters of the pulse to the photoionisation cross section and the energy spectrum of the ionised electron(Fig. 2) may provide a valuable contribution at the design of laser and plasma based novel accelerators, e.g. the CERN AWAKE experiment. The above-threshold ionization(ATI) peaks are clear to see in Fig. 2.

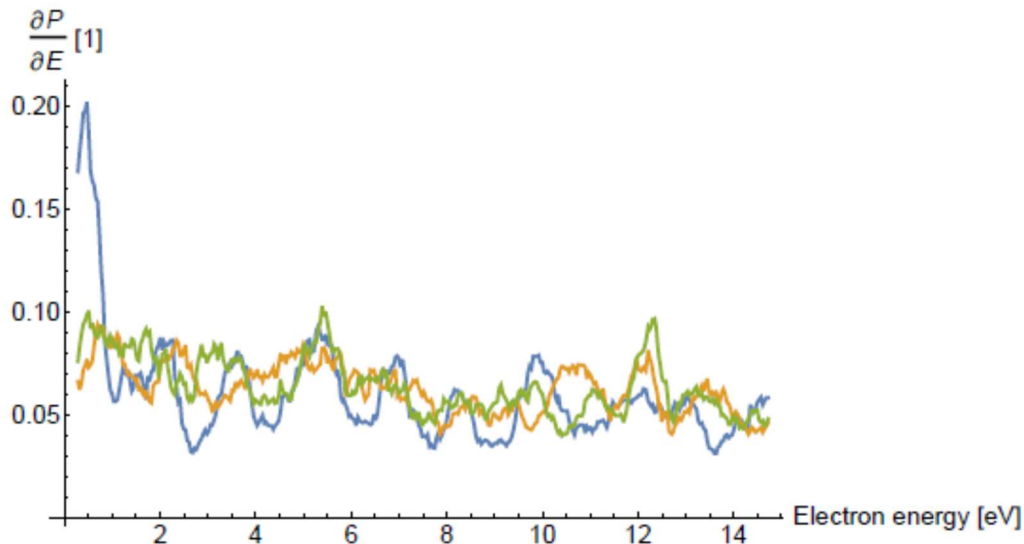


Figure 2. The energy spectrum of the ionized electron. The blue, orange and green lines are for $I = 10^{12}$, $2,5 \cdot 10^{13}$ and $8,1 \cdot 10^{13}$ W/cm², respectively.

Grants

EUROFUSION, Enabling Research ToIFE project, “Preparation and Realization of European Shock Ignition Experiment” project

VEKOP-2.3.2-16 participation

International cooperation

Max Planck Institute of Quantum Optics (MPQ), Garching, Germany.

Institut national de la recherche scientifique (INRS), Montreal, Canada.

AWAKE Experiment CERN.

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R-Q. Beam emission spectroscopy

Dániel Dunai, Gábor Anda, Attila Bencze, A. Búzás[#], Sándor Hegedűs, Tibor Krizsanóczy, Máté Lampert[#], G. Pokol, Dániel Réfy[#], Balázs Tál, M. Vécsei, Sándor Zoletnik



Installation of a 60keV diagnostic beam and observation system on the Wendelstein 7-X stellarator in Germany. — The BES research group designs, manufactures, installs and operates BES diagnostics in several major fusion devices worldwide. The main project of 2017 was the installation of a new BES diagnostic on the Wendelstein 7-X (W7-X) stellarator in Greifswald. The W7-X device is the largest and most advanced stellarator type fusion experiment. The new BES diagnostics will provide unique high spatial and temporal resolved edge density measurements as well as fluctuation analysis possibilities.

The injector, the vacuum and control system were designed and manufactured and tested at Wigner RCP and were delivered to Greifswald in May. After an extensive test procedure the injector was installed at its final place in the torus hall during the summer. The observation system, which applied a novel design – where special fiber bundles are used in the optics - was also manufactured and tested in Wigner RCP labs. After a successful installation of the observation system the diagnostic could take part in the measurement campaign. Our colleagues are also operated the diagnostics and are responsible for the data analysis as well.

The capabilities of this new diagnostic, which were demonstrated with great success, will allow us to participate in the physics program of the W7-X project. The fast density profiles could resolve the island structures, and will also show the evolution of the edge plasma density profile. The microsecond resolution will reveal the underlying and flow patterns in the scrape-off layer plasma (SOL) and in the edge region of Wendelstein 7-X plasmas.



Figure 1. The installed 60keV alkali BES system with the German and the Hungarian team.

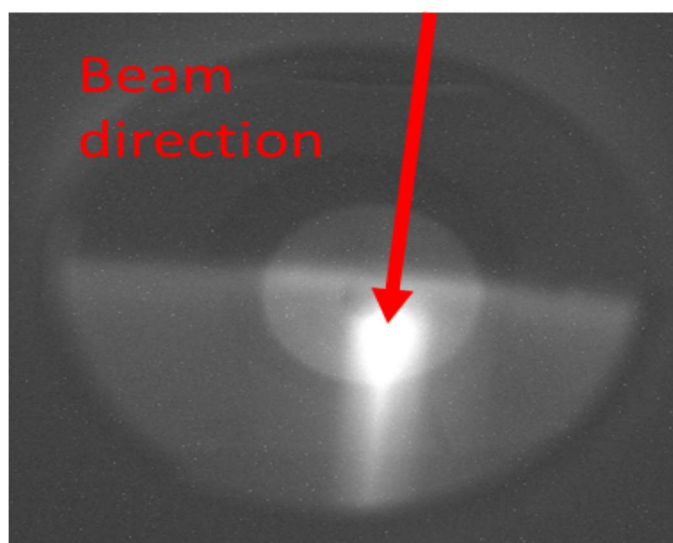


Figure 2. Sodium beam in the plasma.

Beam Emission Spectroscopy measurement results from various experiments. — Beside the installation of the new diagnostic we also participated in the physics programs of various fusion experiments by operating BES diagnostics. We've measured in China, Korea, UK, Germany and the Czech Republic in 2017. A few results are recalled from these experiments

A new confinement regime is being investigated as a candidate for a limit cycle oscillation (cLCO) at the COMPASS tokamak in Prague, appearing near the L-H transition, and identified by a low frequency ($\sim 3\text{-}5$ kHz), divertor $D\alpha$ oscillation. The outstanding performance of the COMPASS Lithium beam emission spectroscopy (Li-BES) diagnostic system enables us to resolve the phenomenon in more detail, namely the edge density profile, flow velocity and turbulence amplitude modulation. Our analysis revealed that the cLCO close to the L-H transition at COMPASS modulates the electron density profile at the pedestal mostly at the foot part. The density fluctuations in the 50-200 kHz band in the pedestal are also modulated, the fluctuation amplitude is approximately in opposite phase to the density gradient. The flattening of the profile happens simultaneously with density increase in the SOL. The poloidal flow velocity of turbulence is also modulated by the cLCO. The density pedestal dynamics are similar to our findings at the JET M-mode and the ASDEX Upgrade I-phase in the previous year.

Since the commissioning of the Hydrogen beam emission spectroscopy diagnostic on the KSTAR tokamak (Daejeon, Korea) in 2012, it has been operated in all latter campaigns. Similarly to the previously described W7-X diagnostics, these measurements mainly focused on the edge plasma and the SOL plasma outside the last closed flux surface. In our latest work in 2017 we proved that the diagnostic is feasible to measure intermittent events both in the SOL and in the edge plasma as well. By utilizing our measurement technique the dynamics of these positive and negative density fluctuations were resolved and studied in detail. It was found that the results agree with measurements done on other tokamaks with different diagnostics, and provide new information to the Langmuir probe measurements on KSTAR. Our future work is going to focus on subtracting the effects of spatial smearing by developing new data analysis techniques.

Grants

Eurofusion Grants

International cooperation

Culham Centre for Fusion Energy (Culham, UK),

Institute of Plasma Physics (Prague, Czech Rep.),

Max Planck Institute for Plasma Physics (Greifswald, Germany),

Institute of Plasma Physics – ASIPP, (Hefei, China),

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See also R-O.4, R-R.7

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TCV Team

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See also: R-R ASDEX Upgrade Collaboration

R-R. Pellet and video diagnostics

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



Video diagnostics system at Wendelstein 7-X (W7-X) — A 10-channel overview video diagnostic system was developed for W7-X superconducting stellarator, based on self-developed Event Detection Intelligent Cameras (EDICAM). The main aim of the system is to monitor almost the entire inner wall, and detect dangerous events automatically. Additionally, making use of the non-destructive feature of the EDICAM's sensor, scientific observations with up to 50 kHz frame rate can be simultaneously carried out, without affecting the low frame rate overview. For the second campaign of W7-X (OP1.2a), spanning from September to December 2017, an inertially cooled island divertor was installed, allowing plasma discharges to span over 25 s. EDICAMs could be successfully used to follow the evolution of the strike-lines (high heat flux areas) on the divertors. As EDICAMs are sensitive for visible light, they could be used to identify hot-spots. Hot-spots appear where (part of) the plasma gets closer to an in-vessel structure where normally no heat load is expected; they produce tremendous amount of visible light due to an enhanced level of plasma-wall interaction, while the heat flux is still not too high. This allowed us to detect hot-spots and the emergence of strike lines well before (1-2 seconds!) the affected components'

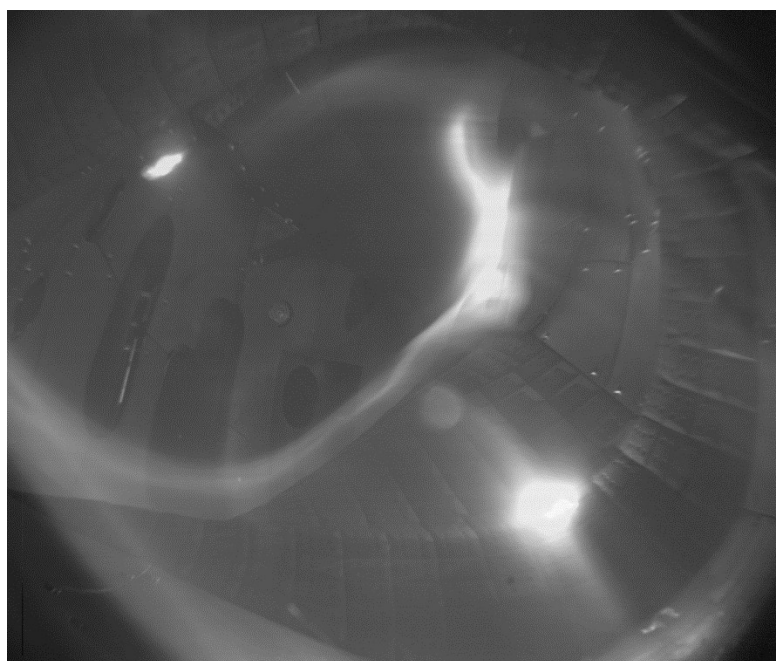


Figure 1. Hot spot as detected by the EDICAM. In this case no counter-measures were carried out, so the affected component (carbon heat shield tile) was heated up to several 100 °C.

temperature had risen above the sensitivity threshold for IR cameras, thus demonstrating the safety functionality of the EDICAM system (Fig. 1). An additional upgrade will allow us to automatically broadcast warnings to the plasma control system in such cases – this will be demonstrated in the next (OP1.2b) campaign. Two of the ten video channels were equipped with ultra-fast framing Photron cameras, for dedicated studies. One of the fast cameras was used to monitor pellet injection, both from the inboard and the outboard. It was observed that pellets are decelerated and even

stopped during the pellet-plasma interaction process, presumably due to a rocket-effect

caused by asymmetric ablation. It was also observed that pellet cloud drift, unlike in tokamaks, points not only to the outboard direction, but to any direction, and mainly outward from the plasma (i.e. inboard direction for inboard launch and outboard direction for outboard launch). Using a special view with higher photon sensitivity, the other fast camera was used to detect filaments – these radially localized structures, elongated along magnetic field lines, are closely related to plasma turbulence. Filaments were observed in all plasmas with high enough intrinsic radiation level; they appeared mainly in the region affected by the divertor, where a C-III interference filter could also be used to increase the contrast (Fig. 2).

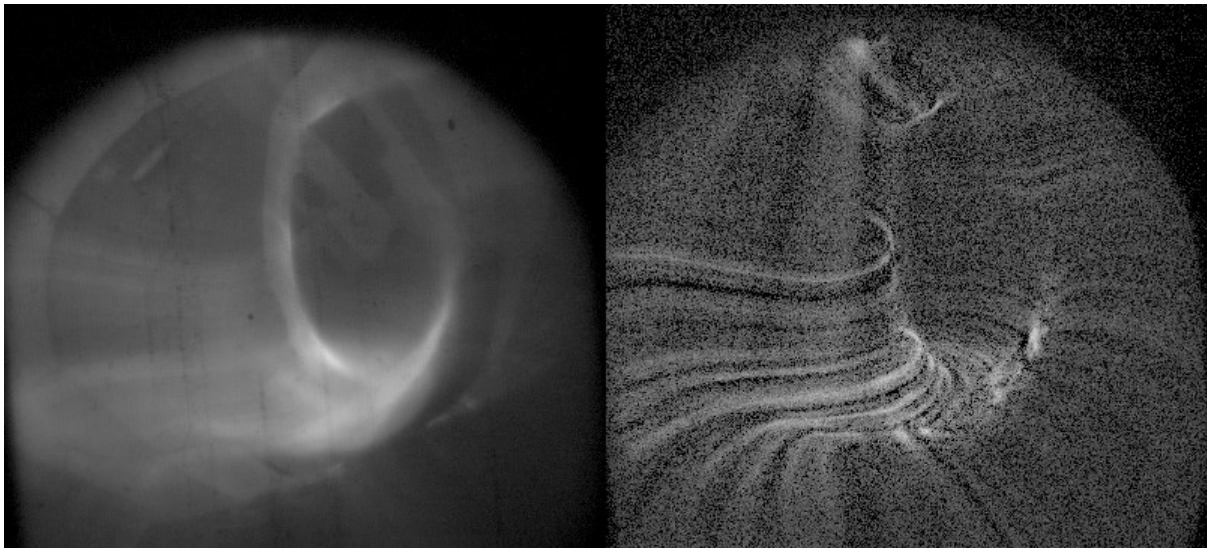


Figure 2. Filaments in a diverted W7-X plasma discharge. Image processing algorithms and interference filters can be applied on the raw fast camera images (left) to enhance the visibility of the filaments (right).

EDICAM diagnostic development for JT-60SA — The development of a single channel EDICAM system for the Japanese superconducting tokamak, JT-60SA, has been started in 2017. The EDICAM will be part of the overview visible video diagnostic system, monitoring the torus interior from five tangentially viewing channels. The requirements are harsh: 80° field-of-view, with a depth-of-field of 5 m (3-8 m away from the first lens). Additionally, the system for this experiment also includes the diagnostic port plug (immersion tube), in other words a part of the tokamak vacuum vessel is also to be delivered. In 2017 we focused on the design of the system; designing the optics was a real challenge, since the light rays collected by the tangential view have to be ‘bent’ by 40° to fit into the radial port plug. This task is really conflicting with the above-mentioned wide-angle view, but the problem could be solved by using a double reflecting prism. In parallel, the mechanics design was also developed, strongly linked together with the optics design (Figure 3). Both designs have been finished successfully, and construction can be started in early 2018, as expected. The project is funded by Fusion for Energy, in the framework of the Broader Approach agreement.

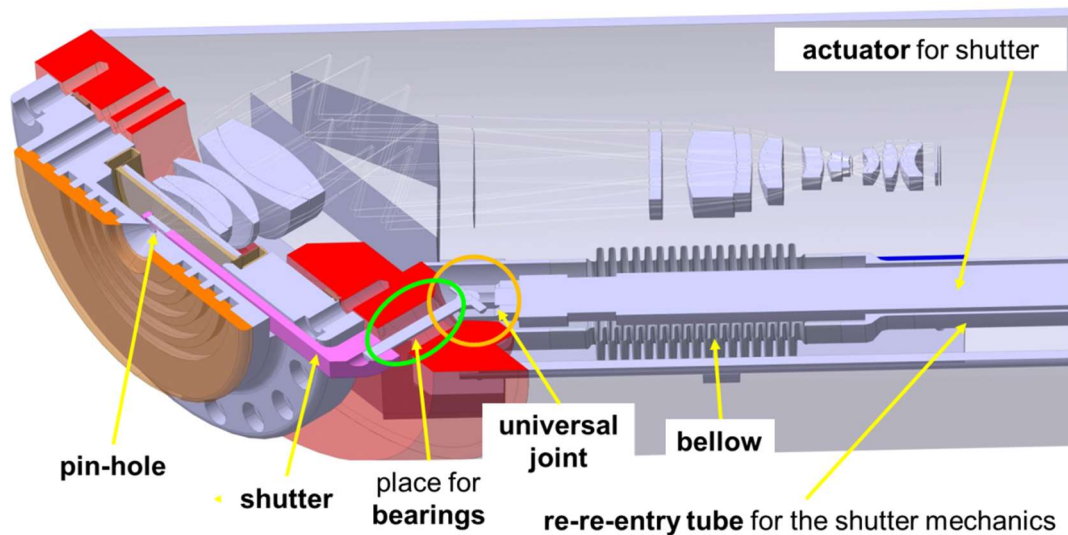


Figure 3. CAD and optics design of the JT-60SA video diagnostic port for EDICAM.

Grants

EUROfusion: WP Medium-Size Tokamak 1 (G. Kocsis, 2016-2017)

EUROfusion: WP JET 1 (G. Kocsis, 2016-2017)

EUROfusion: WP Stellarator 1 (T. Szepesi, 2016-2017)

EUROfusion: WP SA (T. Szepesi, 2016-2017)

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)

National Institutes for Quantum and Radiological Science and Technology, Naka, Japan (T. Szepesi)

Publications

Articles

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ASDEX Upgrade Team

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W7X Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2016, here we list only a short selection of appearances in journals with the highest impact factor. Wigner authors in the Collaboration are: Cseh G, Kocsis G, Szabolics T, Szepesi T

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See also: R-Q JET Collaboration

R-S. Space physics

Andrea Opitz, Zsófia Bebesi, Melinda Dósa[#], Géza Erdős, Lajos Földy, Antal Juhász, Károly Kecskeméty, Péter Király^A, Zoltán Németh, Klaudia Szabó, Károly Szegő^A, Mariella Tátrallyay^A, Anikó Timár[#]



The main focus of our research group is space plasma physics, we study plasma processes in our Solar System through spacecraft observations and modeling. We are involved in numerous space missions at all stages from design to data exploitation in collaboration with the Space Technology research group. The Rosetta mission (2004/2014-2016) has provided us with a huge amount of data about the cometary plasma. In 2017 we took farewell of the Cassini spacecraft that orbited Saturn for 13 years, and started to prepare for the next mission to a giant planet and its moons: the JUICE spacecraft, which targets Jupiter and its satellites. We use previous solar mission results to develop reliable solar wind prediction tools both in house and in international collaboration as part of the Europlanet Planetary Space Weather Services team.

Modeling dust delivery from Enceladus to the moons of Saturn. — The active geysers in the south polar region of Enceladus are sources of dust particles that sustain the vast E-ring of Saturn, extending out beyond Titan at 20 Saturn radii. The dynamics of the small micron and submicron particles escaping from Enceladus is primarily set by Saturn's gravity, plasma drag, radiation pressure and electromagnetic forces. We developed simulations to follow different sized (0.1-5 micron) dust particles from Enceladus till their ultimate demise: being ejected from Saturn's magnetosphere, or hitting one of its moons. We determined the expected size, speed and spatial distributions of the impacting particles and identify their predicted anisotropies bombarding the leading/trailing hemispheres of the moons, possibly offering an explanation for their observed brightness features (Fig. 1).

Cometary Physics. — We calculated the diamagnetic cavity boundary distance around Comet 67P/Churyumov-Gerasimenko using various methods. We found that the global outgassing rate determines the position of the boundary with local pressure variations being suppressed, while the rapid changes in the external solar wind pressure at the position of the comet can explain the intermittent nature of the cavity crossing events (Fig. 2).

Interplanetary space. — The heliospheric magnetic field was investigated by the analysis of near-earth interplanetary measurements. It was shown, that structures recurrent with the solar rotation are persistent for a long time, both in the polarity (magnetic sectors) and the magnitude of the magnetic field. The origin of those structures are different, and also, the rotation period of the magnetic field enhancements, associated to Corotating Interaction Regions is slightly smaller than that of the magnetic sectors. The different rotation period suggests a major re-arrangement of the solar magnetic field during the declining phase of the solar cycles.

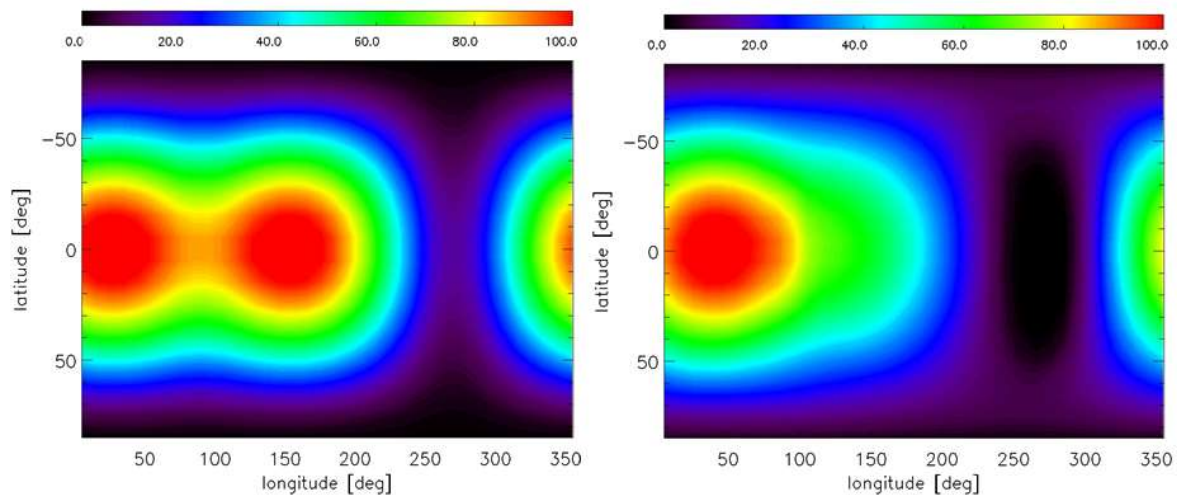


Figure 1. The color plates show the E ring dust deposition map on the surface of moons Enceladus (left) and Titan (right). The longitude is measured from the anti-Saturnian direction and the 90 degrees marks the leading side of the moons. The modeled dust deposition rates are: 3400 kg/day for Enceladus and 460 kg/day for Titan. (Other moons, Mimas, Tethys, Dione and Rhea were modeled also.)

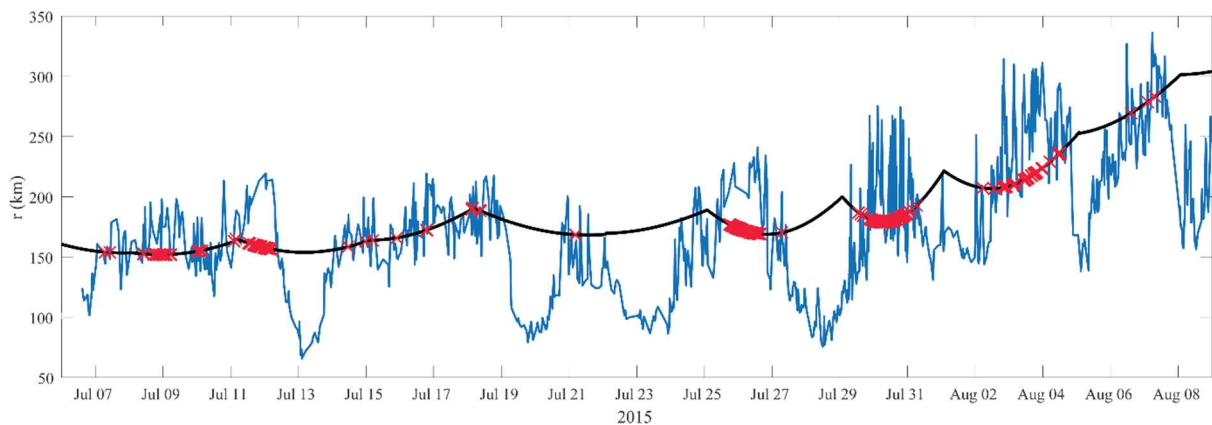


Figure 2. Calculated cavity distance in July and August of 2015. The red signs mark the observed cavity crossing events, the black line is the distance of the Rosetta spacecraft from the cometary nucleus, and the blue line is the calculated distance of the cavity boundary from the nucleus.

Suprathermal ions in the heliosphere. — By comparing the intensity peaks observed in the fluxes of suprathermal He, C, O, and Fe ions during the last two solar maxima we found marked differences and suggested that these ions were accelerated to suprathermal energies under different conditions in the solar corona.

Grants

EU H2020 Europlanet-RI (K. Szegő and A. Opitz, 2015-2019)

ESA PECS Cluster Science Data System (M. Tátrallyay, 2015-2017)

János Bolyai Research Scholarship (Z. Németh, 2016-2019)

International cooperation

International team of the NASA Cassini Plasma Spectrometer (CAPS), (K. Szegő, Z. Németh)

International team of the NASA Cassini Magnetometer (MAG), (G. Erdős)

International team of the NASA STEREO Plasma Spectrometer (PLASTIC), (A. Opitz)

International team of the ESA Rosetta Plasma Consortium (RPC), (K. Szegő, Z. Németh)

International team of the ESA Cluster mission (M. Tátrallyay)

International team of the ESA BepiColombo Particle Detector (SERENA), (K. Szegő)

International team of the ESA Solar Orbiter Magnetometer (MAG), (G. Erdős)

International team of the ESA JUICE Magnetometer (J-MAG), (G. Erdős)

International team of the ESA JUICE Particle Environment Package (PEP), (K. Szegő)

Europlanet2020-RI, integrating the European planetary science community (K. Szegő, A. Opitz)

University of Colorado, Boulder, USA (A. Juhász)

Lomonosov Moscow State University, Russia (K. Kecskeméty)

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See also: R-T.2

R-U. NAP I-B PATTERN Research Group

András Telcs, Balázs Újfalussy, Gergő Orbán, Marcell Stippinger



The focus of the group activity was the analysis of population activity of neurons.

Within that framework the group investigated the position coding of hippocampal grid cells, the activity of V1 neurons during reach task of behaving monkey, response dependence of stimulus in V1 and their higher order statistics as well as in vitro calcium imaging of 600+ hippocampal cells.

Robust and efficient coding with grid cells. — The neuronal code arising from the coordinated population activity of grid cells in the rodent entorhinal cortex can uniquely represent space across large distances but the precise conditions for efficient coding are unknown. A number-theoretic analysis of grid coding is presented and an upper bound on the distance that a population of grid cells can represent without error is derived. It is shown that in the absence of neuronal noise, the capacity of the system would be extremely sensitive to the choice of the grid periods. However, when the accuracy of the representation is limited by neuronal noise, the capacity becomes gradually more robust against the choice of grid scales as the number of modules increases and remains near optimal even for random scale choices. It is revealed that robust and efficient coding can be achieved without parameter tuning in the case of grid cell representation.

Population activity statistics dissect subthreshold and spiking variability in V1. — Response variability, as measured by fluctuating responses upon repeated performance of trials, is a major component of neural responses, and its characterization is key to interpret high dimensional population recordings. Response variability and covariability display predictable hinges upon changes in stimulus and cognitive or behavioural state, providing an opportunity to test the predictive power of models of neural variability. Still, there is little agreement on which model to use as a building block for population level analyses, and models of variability are often treated as a subject of choice. We investigate two competing models, the doubly stochastic Poisson (DSP) model assuming stochasticity at spike generation, and the rectified Gaussian (RG) model tracing variability back to membrane potential variance, to analyse stimulus-dependent modulation of both single-neuron and pairwise response statistics. Using a pair of model neurons, we demonstrate that the two models predict similar single-cell statistics. However, DSP and RG models have contradicting predictions on the joint statistics of spiking responses. To test the models against data, we build a population model to simulate stimulus change-related modulations in pairwise response statistics. We use single-unit data from the primary visual cortex (V1) of monkeys to show that while model predictions for variance are qualitatively similar to experimental data, only the RG model's predictions are compatible with joint statistics. These results suggest that models using Poisson-like variability might fail to capture important properties of response statistics. We argue that membrane potential-level modelling of stochasticity provides an efficient strategy to model correlations.

Grant

NAP-B: KTIA_NAP_13-2-2015-0007 Analysis of neural patterns and their interaction rules in diverse cerebral cortex states (2015-)

R-V. Neurorehabilitation and motor control

József Laczkó, András Arató^A, Lilla Botzheim[#], Szabolcs Malik, Norbert Márkus^A, Mariann Mravcsik



Control and biomechanics of human limb movements, were studied to reveal hidden features of coordinated muscle activities and joint rotations. Spatiotemporal coordination of selected anatomical points of the body and electromyograms of selected muscles were recorded during limb movements of able-bodied participants. Muscle activity patterns were established, based on evaluation and statistical analysis of measured data. Such patterns were used to substitute missing neural control of spinal cord injured individuals through multichannel functional electrical muscle stimulation (FES). As a practical application in medical rehabilitation, several lower-limb paralyzed individuals with complete spinal cord injury (SCI), performed cycling movements against various loads on a stationary bike. These “trainings” were performed regularly twice a week, at the National Institute for Medical Rehabilitation. Two other SCI participants with denervated muscles performed cycling movements on a special tricycle equipped by a 4 channel electrical stimulator for denervated muscles. This kind of cycling were performed in open air track and the average cycling distance (across trainings and participants) was 2.16 km and the average cycling speed was 4.7 km/h. Power and energy output of the complete SCI participants were measured. The paralyzed people who participated in this FES assisted rehabilitation program were very motivated and enjoyed the physiological and psychological benefits and that they used their own paralyzed muscles to drive a stationary bike or tricycle and were able to produce mechanical work by active muscle force, even if their muscles were not controlled by their brain, but by artificial control through an external device. These cycling movements are advantageous for cardiovascular and respiratory well-being and can't be done without FES.

Control of cycling upper limb movements were also investigated in young, able bodied people. Variances (and stability) of these movements were analyzed. Three joint angles (shoulder, elbow, wrist) and four muscles (biceps, triceps, anterior delta, posterior delta) were studied in each arm (dominant and non-dominant). There were no significant differences in the joint angular variances, observed in the two arms. It is concluded that at kinematic level the neural control is equally stable for the two arms in this motor task. Muscle synergies were established applying dimension reduction methods (non negative matrix factorization) and it was found that muscle activity vectors in the 4D muscle space can be well estimated from 2 modules (synergies) because the variance accounted for by 2 muscle synergies was over 93%. There were no significant differences between the two arms in this respect either, reflecting the speciality of cycling movements (Fig. 1).

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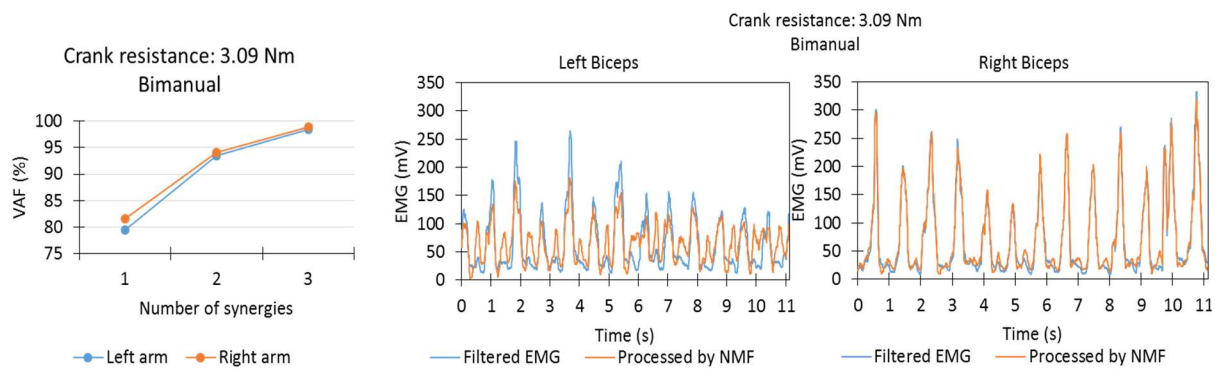


Figure 1. The variance of muscle activities (EMG) was largely explained by 2 synergies as the variance accounted for (VAF) by 2 synergies was over 93% in both arms (left panel). Measured left and right biceps activities are approximated by activities assembled from 2 synergies

Another motor task was investigated in able bodied people and in individuals who suffered stroke. The participants performed point-to-point reaching tasks: they moved their hand from a central starting position to targets in the horizontal plane. The smoothness (or amount of jerkiness) of the movement was investigated. The jerk of hand movement and its dependence on terms related to angular velocities, accelerations and jerks were analyzed. We showed that contribution of such terms to the jerk of the hand differs in healthy people and people who suffered severe stroke. The revealed differences may reflect deficits in neural control and impaired ability of stroke survivors to compensate for multi-joint interaction torques.

The research and development of assistive devices were continued for helping blind people to use braille input devices and mobile phones. The MOST (Mobile Slate Talker) devices for the blind and deaf-blind has been further advanced due to the challenges given by continuously changing operating system.

Grants

Austrian – Hungarian Scientific and Educational Cooperation Action Fund, Project number: 94ou7, Development of rehabilitation protocols for spinal cord injured people (J. Laczko, 2016-2017)

International cooperation

Medical University Vienna, Center for Medical Physics and Biomedical Technics (Prof. Winfried Mayr, Wien Austria, J. Laczko, Wigner RC, Budapest).

Rehabilitation Institute of Chicago (Prof. R. Scheidt and F. Mussa-Ivaldi USA, J. Laczko Wigner RC)

INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS*

* **Abbreviations in the researcher lists of the scientific projects:**

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A: associate fellow

E: professor emeritus

S-B. Complex systems

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The research activity of Complex Systems research group in 2017 covered various topics in the field of cooperative behavior, phase transitions and nonequilibrium dynamics of systems with many degrees of freedom.

Entanglement entropy of composite quantum spin chains. — The entanglement entropy in clean, as well as in random critical quantum spin chains is well known to have a logarithmic scaling with the size of the subsystem. We considered a composite, antiferromagnetic XX chain that consists of a clean and a random part, and found a double-logarithmic scaling of the half-chain entanglement entropy: $S \sim \ln \ln(L)$. We also considered the case, when the disorder penetrates into the homogeneous part in such a way that its strength decays with the distance l as $\sim l^{-\kappa}$. For $\kappa < 1/2$, the entropy scales logarithmically with a modified prefactor as $S(\kappa) \simeq (1-2\kappa)S(\kappa=0)$, while for $\kappa \geq 1/2$, we recover the double-logarithmic scaling. These results were explained by strong-disorder RG arguments. We also studied the half-chain entanglement entropy across a symmetric, extended random defect, where the strength of disorder decays algebraically on both sides of the interface. In the whole regime $\kappa \geq 0$, we found a logarithmic scaling of the entropy, but the variation of the prefactor with κ is non-monotonic and discontinuous at $\kappa=1/2$.

Quantum relaxation of lattice bosons with cavity-induced interactions. — The coupling of cold atoms to the radiation field within a high-finesse optical resonator induces long-range interactions which can compete with an underlying optical lattice. The interplay between short- and long-range interactions gives rise to new phases of matter including supersolidity (SS) and density waves (DW). We have shown that for hard-core bosons in one dimension, the ground-state phase diagram (see Fig. 1) and the quantum relaxation after sudden quenches can be calculated exactly in the thermodynamic limit. Remanent DW order is observed for quenches from a DW ground state into the superfluid (SF) phase below a dynamical transition line. After sufficiently strong SF to DW quenches beyond a static metastability line, DW order emerges on top of remanent SF order, giving rise to a dynamically generated supersolid state.

Proof of phase transition in homogeneous systems of interacting bosons. — Using the rigorous path integral formalism of Feynman and Kac, we proved London's eighty-year-old conjecture that during the superfluid transition in liquid helium, Bose-Einstein condensation (BEC) takes place. The result is obtained by proving first that, at low enough temperatures, macroscopic permutation cycles appear in the system, and then showing that this implies BEC. We found also that, in the limit of zero temperature, the infinite cycles cover the whole system, while BEC remains partial. Via the equivalence of $1/2$ spins and hard-core bosons the method extends to lattice models. We showed that, at low enough temperatures, the spin- $1/2$ axially anisotropic Heisenberg models, including the isotropic ferro- and antiferromagnet and the XY model, undergo magnetic ordering.

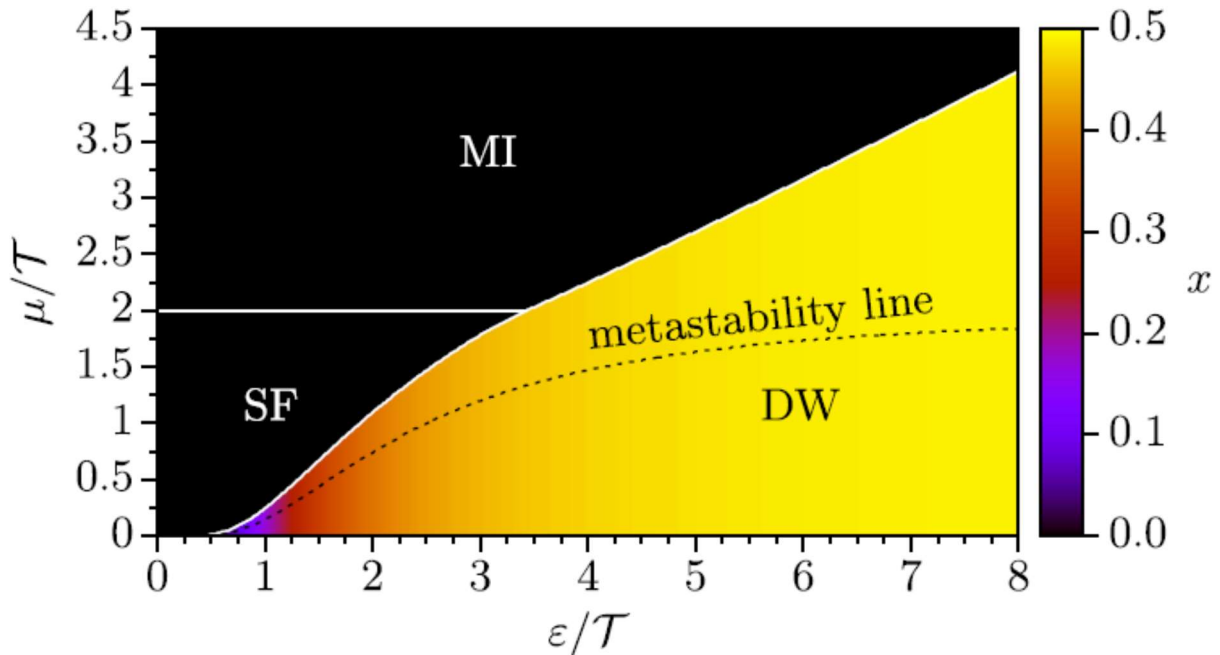


Figure 1. Phase diagram of the Bose-Hubbard model with cavity-induced infinite-range interactions. \mathcal{T} , μ , ε , and x denote the tunneling constant, the chemical potential, the strength of cavity-induced interactions, and the density-wave order parameter (imbalance), respectively. MI, SF, and DW stand for Mott insulator, superfluid, and density wave, respectively.

Critical behavior of the contact process near an extended defect. — The contact process is a simple stochastic lattice model of epidemic spreading. We considered its inhomogeneous variant, where the deviation of the local control parameter from the bulk value tends to zero with the distance from the surface as $\lambda(l) - \lambda(\infty) = Al^{-s}$. In the marginal case, $s = 1/\nu_{\perp}$, where ν_{\perp} is the correlation-length critical exponent, Monte Carlo simulations show a rich surface critical behavior. For weaker perturbations, $A < A_c$, the transition is continuous and the order-parameter critical exponent varies continuously with A . For $A > A_c$, the phase transition is of mixed order: the order parameter is discontinuous but, at the same time, the temporal correlation length diverges, with different exponents on the two sides of the transition. This behavior in the mixed-order regime was explained in the frame of a scaling theory.

Grants

OTKA K-109577: Ordering and dynamics in many-body systems (F. Iglói, 2014-2017)

International cooperation

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

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

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

Institut Néel (Grenoble, France) Critical behavior of systems with long-range interactions (F. Iglói)

Université Saclay, CEA, CNRS (Saclay, France) Dynamics of random quantum systems (F. Iglói)

TU München (München, Germany), Entanglement entropy of disordered quantum wire junctions (R. Juhász)

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S-E. Non-equilibrium alloys

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



Interface properties of nanoscale multilayers. — Artificial multilayers and hetero-structures of nanoscale layers are essential parts of information technology as well as many other technical applications. Since these multilayers are prepared by depositing layer by layer the appropriate amount of different atoms, the interface structure is determined by stochastic processes taking place at the actual, continuously changing surface of the structure. This way the width, the crystal structure, the atomic composition and the associated physical properties of the interface can be largely different when A atoms are deposited over a layer of B atoms or, vice versa, when B is deposited over A.

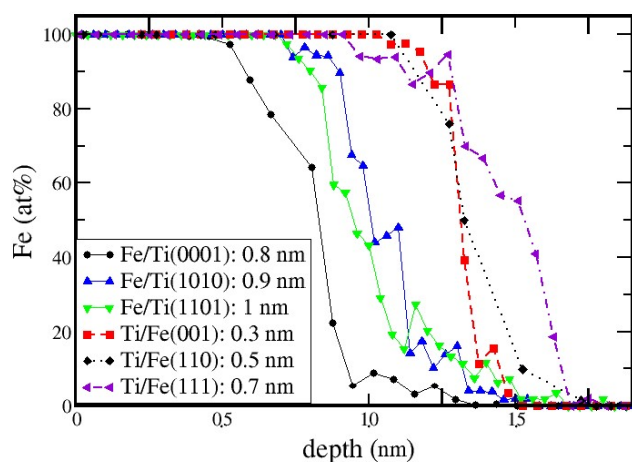


Figure 1. Concentration profiles across the Fe-on-Ti and Ti-on-Fe interfaces as calculated from MD simulations for different orientations of the substrate layer. The substrate orientations which belong to the different curves and the thickness of the respective interface alloy are indicated in the inset.

The largest intermixing takes place in case of the Fe(111) substrate orientation, but the interface width (0.7 nm) still remains below the Fe-on-Ti values. Altogether, from the simulations we can conclude that the intermixing is asymmetric with respect to the interchange of the constituents of the film and the substrate.

In our study, a significant difference of the Ti-on-Fe and the Fe-on-Ti interfaces are undoubtedly revealed both by molecular dynamics simulations of the layer growth (in collaboration with the Research Institute for Materials Science, Centre for Energy Research, HAS) and by experimental investigations. The calculated concentration depth profiles for different substrate orientations are displayed in Fig. 1. The Fe-on-Ti interfaces are slightly intermixed and the interface broadening depends on the orientation of the substrate, although the variation is small. In the Ti-on-Fe case, no atomic mixing can be seen for the Fe(001) substrate orientation, but the interface is slightly wavy which results in a 0.3 nm intermixing in the

The experimental studies were made by conversion electron Mössbauer spectroscopy (CEMS) complemented by cross-sectional transmission electron microscopy (TEM) and X-ray reflectometry (XRR). The Ti/Fe/Ti trilayer samples were prepared by evaporation in high vacuum onto Si single crystal substrate using iron metal highly enriched in the ⁵⁷Fe Mössbauer

resonant isotope. In order to determine the phase fractions within the top (Ti-on-Fe) and bottom (Fe-on-Ti) Fe interface, Ti/⁵⁷Fe/Ti/Si and Ag/⁵⁷Fe/Ti/Si sample pairs were compared by exploiting the non-mixing property of Fe and Ag. Analyzing the spectra of Ag/⁵⁷Fe/Ti samples provides information on the Fe-on-Ti interface, since the Ag/Fe interface is chemically sharp and the Ag layer causes only a small and well documented change in the hyperfine parameters of ⁵⁷Fe within the atomic layers nearest and next-nearest to the Fe-Ag interface. Additional spectral components appearing in the Mössbauer spectra of Ti/⁵⁷Fe/Ti samples reveal the specific properties of the Ti-on-Fe interface.

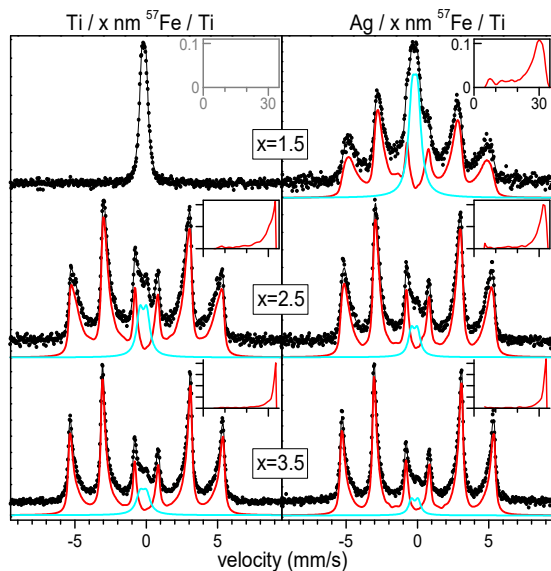


Figure 2. Room temperature Mössbauer spectra of Ti/⁵⁷Fe/Ti and Ag/⁵⁷Fe/Ti sample pairs with varying thickness of the ⁵⁷Fe layer, as indicated in the figure. The sub-spectra belonging to paramagnetic amorphous alloy and ferromagnetic crystalline alloy components are indicated by blue and red lines, respectively.

interfaces, respectively. The scaling of the interface width may be model dependent, but a strong asymmetry of the Ti-on-Fe and the Fe-on-Ti interface widths is undoubtedly experimentally verified by the Mössbauer and the X-ray reflexivity (XRR) data. The TEM and XRR studies have been carried out in collaboration with the Peter Grünberg Institut, Forschungszentrum Jülich (Jülich, Germany).

Grants

OTKA K-101456 Mössbauer and Magnetic Study of Intermetallic Compounds (I. Vincze, 2012-2017)

OTKA K-112811 Magnetic Multilayers Modified by Amorphous Alloys (J. Balogh, 2015-2019)

International cooperation

Department of Physics, Shiga University of Medical Science (Shiga, Japan) (J. Balogh)

From the Mössbauer results shown in Fig. 2 one can conclude that the bottom and the top interface of a Fe layer in between Ti layers are very different both in the extent and in the ratio of the amorphous and the crystalline alloys appearing at the interface. The Fe-on-Ti interface is about three times thicker than the Ti-on-Fe interface and the ratio of the Fe-rich bcc alloy is larger than that of the Ti-rich amorphous alloy. The Ti-rich amorphous alloy has a higher ratio than the crystalline alloy in the thin Ti-on-Fe interface, which probably does not form a continuous layer.

Surprisingly, the TEM experiments do not show the marked asymmetry of the Fe interfaces, probably due to the averaging of the signal across the specimen thickness in the view direction and a possible modest heating in spite of all the care taken during the sample thinning, but the XRR measurements also indicate a significant asymmetry. The fitted roughness values of 0.86 nm and 0.23 nm result in 2.0 and 0.54 nm “10-90” interface widths for the Fe-on-Ti and Ti-on-Fe

Peter Grünberg Institut, Forschungszentrum Jülich (Jülich, Germany) (J. Balogh)

Publications

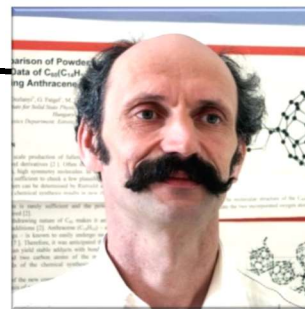
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See also: R-L.1, S-I.2

S-F. Laboratory for advanced structural studies

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LASS carries out research in three areas: carbon based materials, the theory of phase transformations and x-ray-related methods. In the last year we have reached significant results in all of these fields.

Carbon based systems

Lately, various carbon based materials became the center of intensive research. Earlier we concentrated on fullerenes and related compounds. Recently, metal organic framework materials (MOF), carbon nanotubes and nanotube-based hybrid systems are our center of interest.

Metal-organic frameworks. — Metal organic frameworks are coordination polymers with high porosity. These crystalline, high-symmetry materials consist of metal-containing nodes and rigid organic linkers. Formerly, we developed a new MOF family with Zn-based secondary building units (SBUs) and 1,4-cubanedicarboxylate linkers. This year, we started a new family of MOF-s with the same Zn-containing nodes, but with a previously unknown spiroheptanedicarboxylate linker. We prepared the organic precursor in a racemic form and demonstrated

the formation of the new MOFs. We made ready the raw material for chromatographic separation of the enantiomers. The goal of the experiment is the preparation of chiral MOFs, suitable for separation of various racemic mixtures.

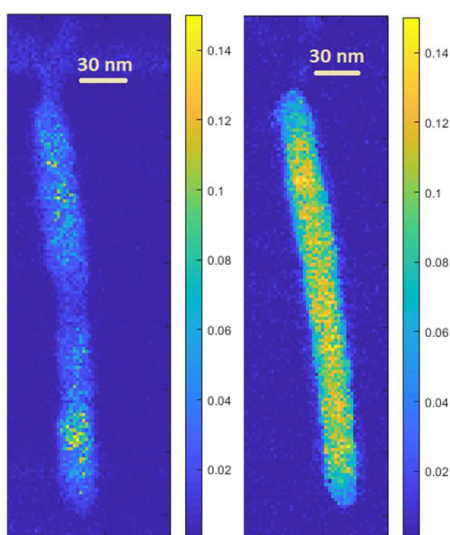


Figure 1. Spatial distribution of the boron nitride phonon-polariton mode (left) and the infrared-active defect mode (right) in a multiwall boron nitride nanotube.

Infrared spectroscopy on carbon based systems. — We changed the focus of our research to include two new topics: near-field infrared spectroscopy and microscopy of various nanotubes and optoelectronic properties of organic perovskite-based solar cell materials. We succeeded in determining the semiconducting or metallic character of individual carbon nanotubes below 10 nm in diameter. In the case of boron nitride nanotubes, we mapped the defect distribution with a spatial resolution of a few nanometers (Fig. 1).

We combined methylamine lead iodide perovskite with carbon nanotubes to obtain hybrid structures for possible application as photovoltaic devices. We

[#] Ph.D student

proved the charge transfer from the perovskite to the carbon nanotube layer upon illumination. These observations may lead to new solar cells with the perovskite as active layer and the carbon nanotubes as hole-transporting layer.

Theory of phase transformations

Hydrodynamic theory of freezing – Nucleation and polycrystalline growth. — Structural aspects of crystal nucleation in undercooled liquids are explored using a nonlinear hydrodynamic theory of crystallization we proposed recently, which is based on combining fluctuating hydrodynamics with the phase-field crystal (PFC) theory. We have shown that in our hydrodynamic approach not only homogeneous and heterogeneous nucleation processes are accessible, but also growth front nucleation, which leads to the formation of new (differently oriented) grains at the solid-liquid front in highly undercooled systems. Formation of dislocations at the solid-liquid interface and interference of density waves ahead of the crystallization front are responsible for the appearance of the new orientations at the growth front that lead to spherulite-like nanostructures (Fig. 2).

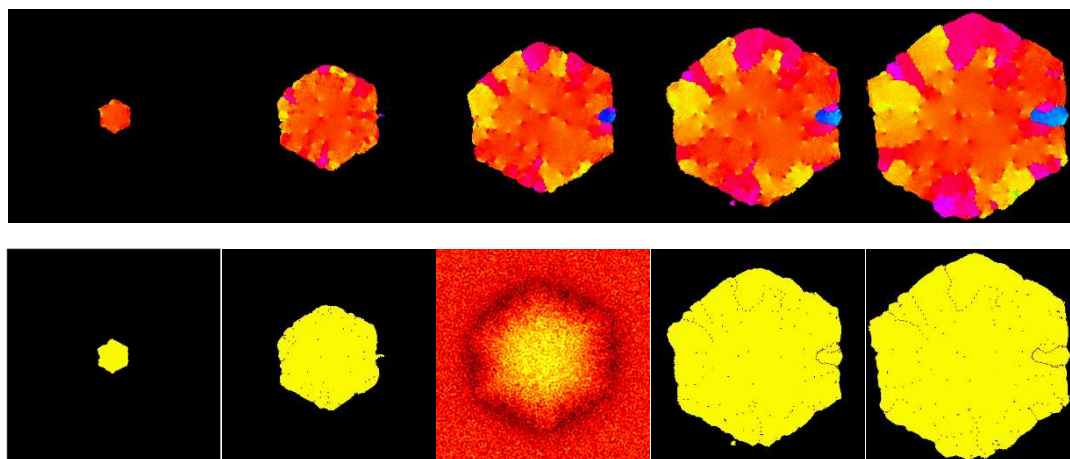


Figure 2. Polycrystalline growth in the hydrodynamic model of freezing. Snapshots of the orientation field (upper row), the Voronoi map (bottom row), and coarse-grained density (bottom row central panel: lighter colour denotes higher density) taken at dimensionless times $t = 900, 2100, 2900, 3400,$ and 3900 are shown. Note the spatial variation of the orientation field due to the dislocations shown as red-blue pairs of dots (atoms of 7 and 5 neighbours) in the Voronoi map, and the small crystallite formed close to the interface in the 4th panel from the left. This indicates two mechanisms for growth front nucleation: (i) nucleation of dislocations at the interface, and (ii) crystal nucleation ahead of the growth front.

Grain coarsening in two-dimensional phase-field models with orientation field. — Contradictory results were published regarding the form of the long-time grain size distribution (LGSD) that characterizes grain coarsening in two-dimensional systems: While experiments and the PFC model indicate a log-normal distribution, other works including studies based on phase-field simulations that rely on coarse-grained fields, like the multi-phase-field and orientation field (OF) models, yield significantly different distributions. We investigated this problem, and demonstrated for the OF models that an insufficient resolution of the small-angle grain boundaries leads to a log-normal distribution close to those seen in the experiments. Our work also indicates that the LGSD is critically sensitive to the details of

the evaluation, and raises the possibility that the differences among the LGSD results from different sources originate from differences in the detection of small-angle grain boundaries.

Topological defects in two-dimensional orientation-field models. — In 2D, a continuous scalar field is used to represent crystallographic orientation. The respective order parameter space is the unit circle, which is not simply connected. This property has important consequences for the multigrain structures: (i) triple junctions may be singular; (ii) for each pair of grains, there exist two different interfacial solutions that cannot be continuously transformed to each another; (iii) if both solutions appear along a grain boundary, a topologically stable singular point defect forms between them. While (i) can be interpreted in the classical picture of grain boundaries, (ii) and, therefore, (iii) cannot. To overcome these problems, we proposed two solutions. The first is based on a three-component unit vector field, while in the second we utilize a two-component vector field with an additional potential. In both cases, the additional degree of freedom makes the order parameter space simply connected, which removes the topological stability of these defect.

X-ray-related methods

We have continued our studies on structure determination by inside x-ray sources. We have carried out a series of experiments at ESRF, and measured atomic resolution holograms and also Kossel line patterns. The atoms which we used as point sources were excited by a very intense, synchrotron-generated focused X-ray beam. The diffraction patterns and the holograms were detected by a new 2D position sensitive detector allowing the collection of higher quality data than in earlier measurements. The evaluation of the data is under way. This type of measurements open the way to single-pulse structure determination at X-ray free-electron lasers.

Grants

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

OTKA K-115504. Structure determination of biological particles with x-ray free electron laser (M. Tegze 2015- 2019).

NKFI K-115959, Pattern formation in far-from equilibrium systems (L. Gránásy, 2016–2019).

NKFI SNN-118012 Correlated electrons in confined molecular systems (K. Kamarás 2016-2019)

NKFI PD-121320 Spectroscopic study of low-dimensional materials (Á. Pekker 2016-2019)

NKFI FK-125063 Spectroscopic study of chemically modified low-dimensional materials (Á. Pekker 2017-2021)

NKFI NN-127069 Pb-free perovskite solar cells with long-term stability (K. Kamarás 2018-2020)

ESA PECS Contract No. 40000110759/11/NL/KML: GRADECET - Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2015–2017).

VEKOP-2.3.3-15-2016-00001 Determination of atomic structure of nanosystems (K. Kamarás 2016-2018)

VEKOP-2.3.2-16-2016-00011 Strategic workshop for the technological challenges of renewable energy systems (K. Kamarás 2017-2020)

International cooperations

Institut de Physique de la Matière Complexe, EPFL, Lausanne, Switzerland, Prof. László Forró

Institut Jozef Stefan, Ljubljana, Slovenia, Prof. Denis Arcon

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German Aerospace Center (DLR), Linder Höhe, 51147 Cologne, Dr. Mathias Kolbe

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See also: S-D.1, S-D.2

S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Kálmán Tompa^E



Thermodynamical characterization of protein-water interactions in aqueous solution. — Proteins are dissolved by water through hydrogen bonds, long-range Coulomb forces, and hydrophobic forces. To shed light on the effect of these forces, we performed wide-line ^1H NMR measurements in aqueous solutions of thymosin- β_4 (T β_4), stabilin C-terminal domain (CTD), and their 1:1 complex. Based on a thermodynamic approach, we characterized quantitatively the potential barriers which hinder the motion of water molecules in interaction with the protein.

We suggest that the interaction sites of stabilin CTD belonging to the rather hydrophilic parts of the solvent-accessible surface are involved in the interactions holding the complex together. Exceptions are the lowest-energy potential barriers or interaction centers of thymosin- β_4 , which are absent in the complex. This can be interpreted as they are not present in the complex and they are engaged in making bonds necessary for complex formation. Stabilin CTD lacks such low-energy potential barriers. The constant amount of mobile water per amino acid residue vs. potential barrier data (Fig. 1) at low energies are attributed to ordered protein structural patterns.

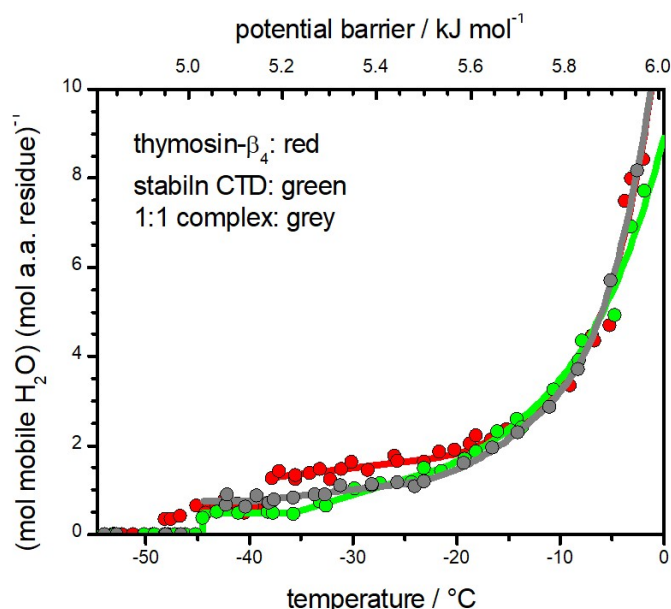


Figure 1. Melting diagram, i.e. the number of mobile hydration water molecules per amino acid residue as a function of temperature (lower abscissa) and of the potential barrier hindering the motion of water molecules (upper abscissa).

The ratio of heterogeneous binding interface derived from the actual energy scale of the motions or interactions of water molecules showed that the individual proteins thymosin- β_4 , stabilin CTD and also their complex have highly heterogeneous bonds with the mobile water molecules. The dynamical characterization by the heterogeneity ratio values of the binding interface led to the conclusion that the studied proteins have ordered components ranging to 10% to 20%. Helical structures are considered as ordered parts seen by wide-line NMR.

^E Professor Emeritus

The comparison of the amount of mobile water per amino acid residue values for the proteins in the potential barrier independent section (Fig. 1) suggests that the complex has the most open structure and that stabilin CTD is the most compact. The continuous distribution of potential barriers found above the section of constant amount of mobile water is characteristic to disordered proteins or protein regions. The protein-water interactions, which are activated closer to 0 °C, hydrate more pronouncedly hydrophilic parts of the protein surface. It can be suggested that they are involved in the interactions holding the complex together. Approximately 40% of the water bonding sites of free thymosin- β 4 gets involved in the bonds holding the protein complex together. The interaction centers of thymosin- β 4, which form the complex can be the electrostatic interactions by which thymosin- β 4 binding to stabilin CTD is stabilized. A small part of the protein-water interaction sites occupied by mobile water molecules bound to stabilin CTD and experiencing potential barriers higher than the start of the quadratic part of the melting diagram disappear for the complex. It can be suggested that these interaction sites are involved in the interactions holding the complex together.

The general picture of the melting diagrams shows that thymosin- β 4 and stabilin CTD are disordered both in their free and bound states. The ratios of heterogeneity to homogeneity of these proteins and their complex are close to 1, indicating again that they are intrinsically disordered proteins.

Grants

Research contract with the HAS, Research Centre for Natural Sciences, Institute of Enzymology

International cooperation

VIB Structural Biology Research Center (SBRC)

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S-H. Partially ordered systems

Tamás Börzsönyi, Ágnes Buka^E, Nándor Éber, Katalin Fodor-Csorba^A, Antal Jákli, István Jánossy^A, Dániel Nagy, Péter Salamon, Ellák Somfai, Balázs Szabó[#], Tibor Tóth-Katona



Granular materials – Flow, jamming and segregation phenomena in sheared systems. — Segregation is often observed in granular mixtures due to size or weight difference of the grains. It is well known that heavier or smaller grains migrate downwards in a granular shear flow. We have shown, that grains differing only in surface friction (size and weight is the same) also segregate when sheared, where smooth grains accumulate in the lower regions of the shear zone (Fig. 1). Moreover, when gravity is negligible to other (compressional) forces, the sample still segregates with the smooth grains leaving the shear zone.

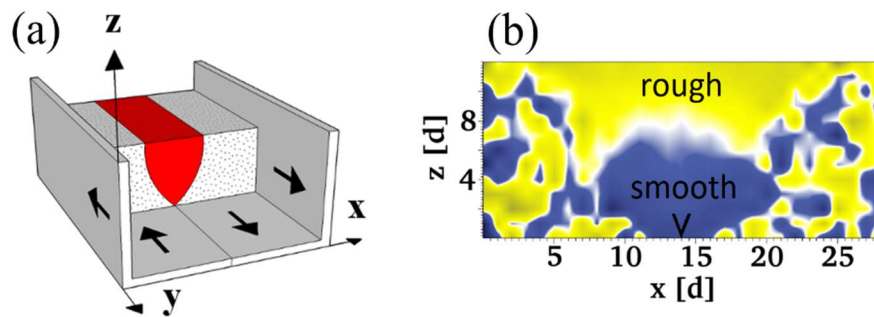


Figure 1. A mixture of smooth and rough beads is sheared. Smooth beads migrate to the bottom of the shear zone due to kinetic sieving.

The flow of elongated grains has been also studied in experiments and numerical simulations. We have experimentally shown, that the flow rate of a hopper is slightly decreased and clogging probability is higher for rod like particles compared to spheres. In numerical simulations, the effective friction of an assembly of frictionless spherocylinders was a non-monotonic, but predominantly decreasing function of the particle aspect ratio.

Two distinct strain amplitudes have been identified in soft glassy materials, such as emulsions, foams, suspensions and pastes, close to the jamming transition. Numerical simulations of oscillatorily sheared soft sphere packings revealed that as the strain amplitude is increased, the initially elastic systems undergo a softening transition, at which both the elastic and loss moduli drop and reach a new plateau. Increasing the strain amplitude further causes yielding, marked by diffusive particle trajectories.

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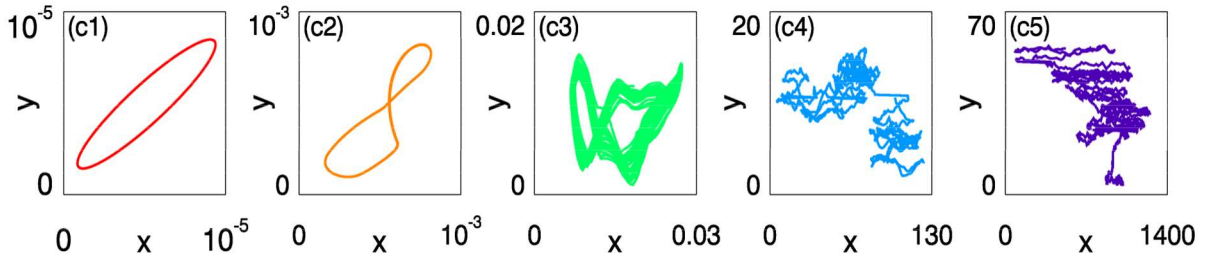


Figure 2. Representative particle trajectories in oscillatory shear. For increasing shear amplitude (left to right), the elliptic trajectory corresponding to linear elasticity becomes non-periodic, but still bounded (softening), then diffusive (yielding).

Liquid crystals. — Tunable optical gratings based on the flexoelectric effect were created in a bent-core nematic liquid crystal. The wavelength of the structure was controlled by the applied d.c. voltage, as demonstrated by polarizing microscopy and light diffraction techniques (Fig. 3): higher voltage yields shorter wavelength. Visibility of the diffraction orders depended on the polarization of the illuminating laser beam (Fig. 4). The dynamical response of the system to switching between voltage levels were also explored. The characteristics and the mechanisms of switching were found to be different, depending on whether the lower voltage level is below or above the threshold of pattern onset. In both cases, the response to increasing voltage levels was much slower than that to decreasing ones.

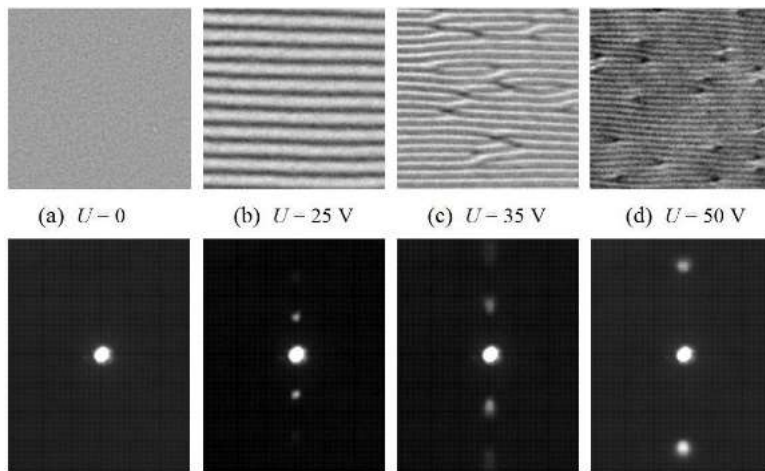


Figure 3. Microphotographs and diffraction patterns of flexodomain gratings at increasing applied voltages.

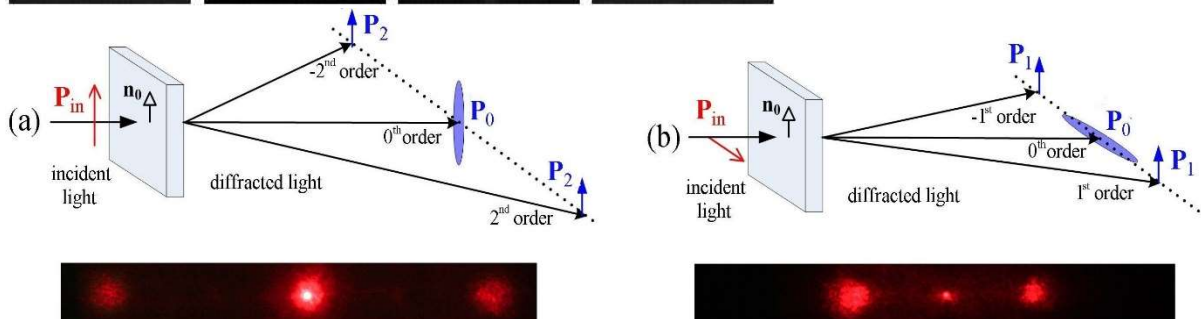


Figure 4. Diffraction geometries and the corresponding diffraction images at (a) extraordinary and (b) ordinary illumination.

Liquid crystal composite materials. — Structural transitions under the combined action of magnetic and electric fields have been monitored in 6CHBT and 6CB liquid crystal-based

ferronematics, obtained by doping the nematics with spherical and rod-like magnetic nanoparticles in low ($\leq 10^{-4}$) volume concentrations. Based on the experimental data, the type of the anchoring at the liquid crystal–nanoparticle interface (rigid or soft), as well as the mutual orientation of the magnetic moment of the nanoparticles and the nematic director have been determined.

Studies of the effect discovered the previous year, namely the increase of the alternating current magnetic susceptibility of ferronematics, induced by a dc bias magnetic field applied in the isotropic phase, which vanishes irreversibly when the ferronematic is cooled down to the nematic phase, have been continued. With the optimization of the ferronematic composition, the range of the d.c. bias magnetic field to which the ferronematic is sensitive without saturation was increased by about two orders of magnitude. This finding paves a way to application possibilities such as low magnetic field sensors or basic logical elements for information storage.

Grants

NKFI K 116036: Flow and rheology of non-spherical particles (E. Somfai, 2016-2020)

NKFI FK 125134: Tunable topology of confined soft matter (P. Salamon, 2017-2021)

NKFI PD16 121019: Interfacial topology of anisotropic soft matter, (P. Salamon, 2016-2019)

International cooperation

COST Action IC1208: Integrating devices and materials: a challenge for new instrumentation in ICT (Management Committee Member: N. Éber, 2013-2017)

Ecole Supérieure de Physique et de Chimie Industrielles de Paris (France): Rheology of elongated grains and suspensions of fibers (T. Börzsönyi, 2016-2017)

RIKEN (Wako, Japan): Creation, active control, and possible application of topological defects in advanced soft matter systems (Á. Buka, 2016-2018)

Jožef Stefan Institute (Ljubljana, Slovenia): Microfluidic systems based on anisotropic soft matter (P. Salamon, 2016-2018)

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See also: S-L.6, S-L.7

S-I. Electrodeposited nanostructures

László Péter,^E Imre Bakonyi^E, Vandri Ahmad Isnaini[#], Katalin Németh,
Lajos Pogány^A, Sándor Zsurzsa[#]



Oscillating electrochemical reactions. — Samples containing alternating Co-rich and Mn-B-O layers were prepared by oscillating electrochemical reaction in collaboration with the Institute of Physical Chemistry of the Bulgarian Academy of Sciences. The preliminary cyclic voltammetric study of the solution containing CoSO_4 , MnSO_4 and H_3BO_3 revealed that the manganese-containing layer is formed by a precipitation-like process due to the alkalination of the cathode vicinity during the hydrogen evolution.

A detailed analysis of the current oscillation was performed by using fast Fourier transformation. The oscillation was stable typically for more than 20 minutes. The current oscillation was anharmonic and exhibited a double maximum pattern. A few current oscillations are depicted in Fig. 1.a with the fast Fourier transform of the current–time function of a 80 s section in Fig. 1.b.

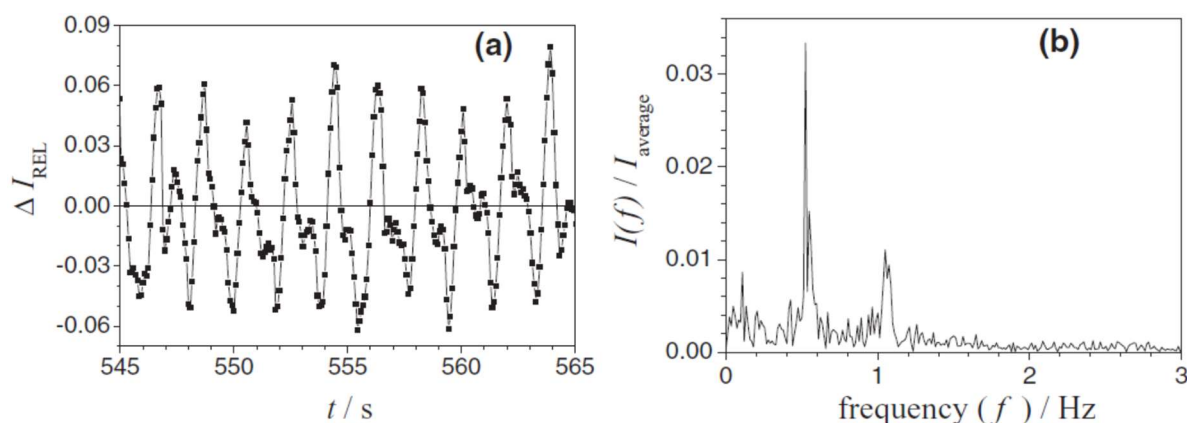


Figure 1. (a) Typical current oscillations obtained and (b) the fast Fourier transform of an 80-second-long section of the current–time function that comprises the data shown in Fig.1(a).

The stability of the oscillation was characterized by the ratio of the two characteristic frequency maxima and the full width at the half maxima of the peak in the fast Fourier spectra. It can be seen in Fig. 2 that the current oscillation does not only prevail for a long time but it is also stabilized, as the decrease in the width of the frequency peaks in time indicates.

The magnetic analysis of the deposits revealed a superparamagnetic behavior of the samples. The size of the magnetic entities as calculated from the Langevin fit of the magnetization

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^A Associate fellow

curves was in accord with the magnetic layer thickness calculated from the current density and the length of the oscillation period.

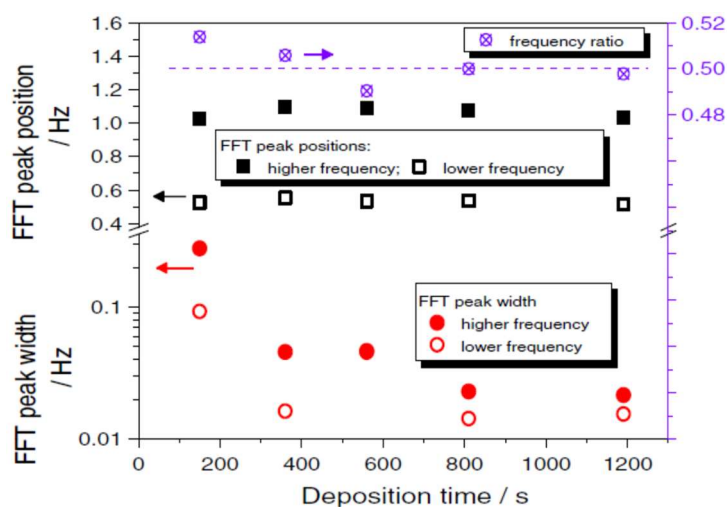


Figure 2. Key parameters of the stability of the electrochemical oscillation.

Magnetism and electronic structure of Ni-metalloid amorphous alloys. — The paramagnetic (PM) to ferromagnetic (FM) transition has been previously investigated on numerous $(\text{Ni}_{100-x}\text{Fe}_x)$ -MD alloys upon the introduction of Fe where MD can represent a combination of various metalloid elements (P, B, Al, Si), while keeping the metal/metalloid ratio constant. Adding a sufficient amount of Fe to a Pauli PM Ni-MD alloy matrix first induces a spin-glass (SG) state at low temperatures which goes over to a PM state at higher temperatures. Beyond a critical Fe content, x_c , the SG state transforms to a FM state upon increasing the temperature. By plotting the characteristic transition temperatures as a function of the Fe content, a magnetic phase diagram (Fig. 3) can be constructed for each Ni-Fe-MD system which has a multicritical point (MCP) at x_c . It has been now shown that by using the reported magnetic phase diagrams of various Ni-Fe-MD alloy systems, the critical Fe content, x_c , for the onset of ferromagnetic order scales inversely with the density of states at the Fermi level, $N(E_F)$, of the parent Ni-MD matrix. This means that the higher the $N(E_F)$, the lower the critical Fe content to induce ferromagnetism in the Ni-MD matrix. This is because a higher $N(E_F)$ leads to a higher Stoner enhancement factor, S , which characterizes the tendency of the matrix to become ferromagnetic. If S is higher for a Ni-MD matrix, a smaller amount of Fe atoms is able to develop an exchange interaction with each other and with the Ni atoms to drive the system to an FM state. Along this line, the critical Fe concentration was found to scale also with S , and the same was found to hold also for the multicritical temperature, T_{MCP} .

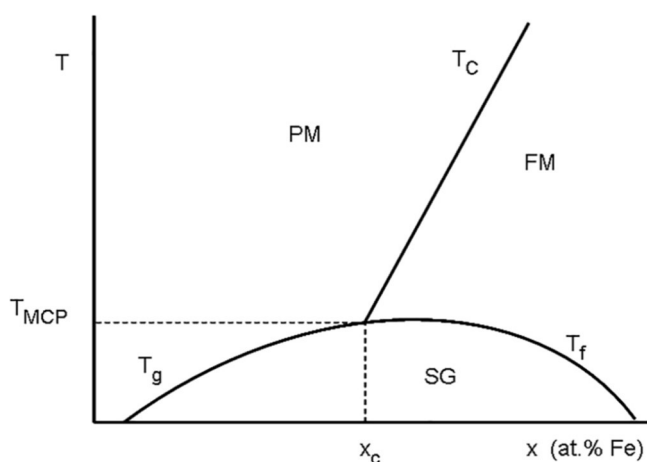


Figure 3. Schematic view of the magnetic phase diagram for $(\text{Ni}_{100-x}\text{Fe}_x)$ -MD amorphous alloys.

Corrosion studies. — Long-term corrosion tests were performed for welded 18Ni-10Cr austenitic stainless steel pipes. The model experiment simulated the impact of the differential ventilation conditions with a large cathode/anode surface area ratio and the enhanced corrosion sensitivity of the welded area. The schematic picture of the experimental setup is shown in Fig. 4. The 46-day-long experiment revealed that under the differential ventilation conditions, pitting corrosion can occur also at the time scale of months on a material that is designed to be in service for

decades. It was also found that the solute in the corrosion medium (a boric acid solution that is analogous to some bath used in the nuclear industry) cannot prevent the occurrence of microbiologically induced corrosion processes since the reproduction of bacteria and their biofilm-forming activity is not blocked.

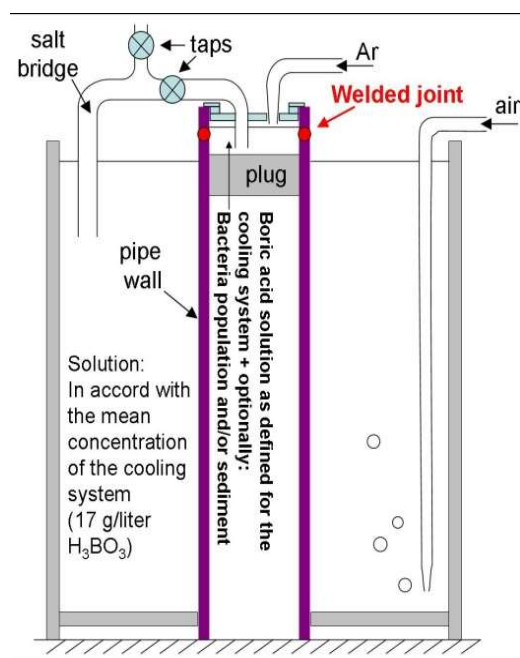


Figure 4. Setup of the corrosion test device with the application of differential ventilation conditions and a high cathode/anode surface area ratio. The height of the device was 1 meter.

Grants

Research Cooperation Project "Periodic magnetic nanostructures by electrochemical approaches: a novel route towards the fabrication of magnonic crystals" supported by the Humboldt Foundation Research Group Linkage Programme between the Wigner RCP and the Leibniz Institute IFW-Dresden (Hungarian project leader: I. Bakonyi, 2017-2019)

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EK-G-SZ-0009/2017, Centre for Energy Research, HAS: "Electrolytic hydrogenation of zirconium samples" (research contract, 2017)

International cooperation

COST Action MP1407 (17 COST and 3 non-COST countries): Electrochemical processing methodologies and corrosion protection for device and systems miniaturization: e-MINDS (Management Committee members: I. Bakonyi and L. Péter, 2015-2019)

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See also: R-M.4, S-E.2

S-L. Nanostructure research by neutron scattering

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The research group has been involved in several research projects and various user measurements performed at the neutron scattering instruments operated by the members of the Group: Small-Angle Neutron Scattering (SANS) instrument, Time of Flight (TOF) spectrometer, Three-axis spectrometer, Reflectometer and PSD Diffractometer. Some of the results are specified below.

Study of desiccation-tolerant desert cyanobacterium, *Leptolyngbya ohadii* by means of small-angle neutron scattering. — Cyanobacteria (or blue-green algae), the first photosynthetic organisms capable of producing oxygen, the ancestors of chloroplasts of vascular plants, appeared about 3 billion years ago and contributed significantly to the transformation of our globe to a habitable planet. These organisms can be found in the most diverse terrestrial and aquatic habitats – from hot springs to the Antarctic climate and from the oceans and fresh water lakes to only temporarily moistened rocks and desert soils. In order to acclimate to these different habitats and to adapt to rapidly changing environmental conditions (temperature, illumination intensity, availability of nutrients and water), different cyanobacteria evolved different, multilevel regulatory mechanisms, the details of which are not well understood.

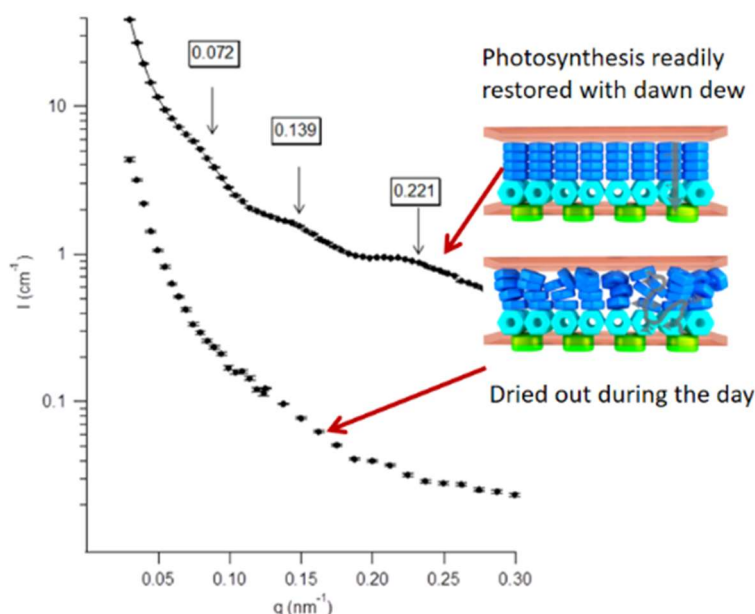


Figure 1. Hydrated and dry state of the multilamellar thylakoid membrane system.

A desiccation-tolerant desert cyanobacterium, *Leptolyngbya ohadii*, a keystone species in desert sand crusts was studied. *L. ohadii* spends most of the daytime in the desiccated state in strong sunshine, surviving extremely harmful conditions. Recovery of photosynthesis can occur immediately upon the addition of water (in nature, e.g. predawn dew deposition).

Desiccation and rehydration in photosynthetic organisms are complex processes; it is important to reveal their structural background. As revealed by small-angle neutron scattering, in the hydrated state, the multilamellar thylakoid membrane system (responsible

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for the conversion of light energy to chemical energy in the cell) displayed three peaks in the SANS profile: one peak at $q=0.072 \text{ nm}^{-1}$ and two additional, higher harmonic features at 0.139 and 0.221 nm^{-1} . These values can be interpreted as the repeat distance (RD) $\approx 87 \text{ nm}$ of thylakoid membranes. In the desiccated state, these peaks were completely lost. The scattering intensity decreased dramatically due to the loss of water and no Bragg peak could be discerned between 0.05 and 0.1 nm^{-1} ; instead, a broad shoulder emerged between 0.10 and 0.15 nm^{-1} , which can be assigned to a $20\text{-}30 \text{ nm}$ shrinkage in the RD (Fig. 1).

Neutron spin echo (NSE) spectrometry using very cold neutrons (VCN). — The concept of spin echo spectrometer on very cold neutrons (wavelengths $\lambda \sim 10\text{-}30 \text{ nm}$) to provide extra high resolution in energy transfer ($\Delta E \sim 10^{-13} \text{ eV}$) has been proposed. Measurements of spin echo signals at different wavelengths were realized using broadband spin flippers in combination with Fourier-analysis of λ -spectrum. The application of very cold neutrons should extend the spin echo time diapason radically, $t \sim 10^{-12}\text{-}10^{-3} \text{ s}$. This promises to open a set of novel scientific areas including the spectroscopy of chemical reactions and catalytic processes, conformational transitions in polymers and biological molecules, dynamic modes in carbon structures (fullerenes, nanotubes, graphenes) at scales from few nanometers to microns.

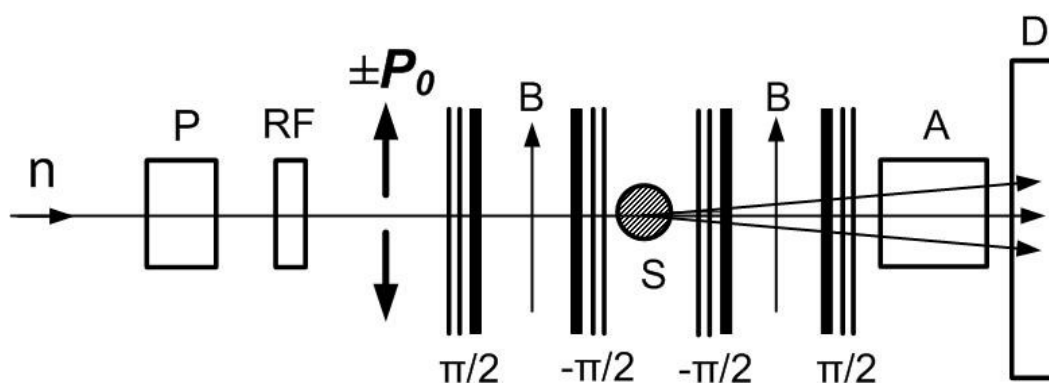


Figure 2. NSE-VCN-spectrometer: neutron beam (n), polarizer (P), radiofrequency flipper (RF), $\pm\pi/2$ -flippers forming the borders of precession fields (B), sample (S), analyzer (A), detector (D).

Spin echo spectrometry based on very cold neutrons promises excellent opportunities in studies of molecular, polymeric, biological objects and systems in extra wide range of times from picoseconds to milliseconds at which their complicated dynamics is revealed. New scientific fields for research open up in comprehensive analysis of chemical reactions and catalysis phenomena, subtle features of conformational and structural transformations in biological molecules and their living structures by using very high energy resolution $\sim 10^{-13} \text{ eV}$ in neutron inelastic scattering experiments based on the proposed principles of wide-band spin-echo technique. The creation of such advanced NSE-instrument (Fig. 2) is considered in connection with the development of intense source of ultra and very cold neutrons on WWR-M reactor at the Petersburg Nuclear Physics Institute using the principles of deep cooling of neutrons in superfluid helium.

Stabilization of detonation nanodiamonds (DND) hydrosol in physiological media with poly(vinylpyrrolidone) (PVP). — A simple method of stabilization of detonation nanodiamonds with negative ζ -potential in isotonic aqueous-saline media was realized by means of complex formation with poly(vinylpyrrolidone). The stability conditions of the

complexes were defined and their structure was determined by neutron scattering. The obtained hydrosols of nanodiamond particles stable in physiological medium may be used in biological researches and in medicine as drug carriers.

The reliable evidences for the formation of stable DND-PVP complexes in hydrosol were obtained with particle sizes 30-35 nm when the ratio of weight concentrations of the component reached $r = C_{PVP}/C_{DND} \sim 0.5$. In the range of $r = 0.3 \div 0.5$, complexes with sizes 30-35 nm are formed, stable in isotonic NaCl solution. At lower r , the amount of PVP is not sufficient to form such complexes, and at larger r , PVP forms a more dense shell around DND particles, resulting an increase of their stability in aqueous-saline media. With the use of PVP, the cluster chain structure formed by the DND particles was observed. It was possible to achieve the stability of such structures of DND particles in isotonic solutions for a long period of time (several months) by varying the amount of PVP in the system. The studied systems are promising for use in medicine due to their high stability in isotonic media. The use of PVP will allow to introduce the drugs to DND-PVP complexes, which will be stable drug carriers.

Cultural heritage-related studies with the aid of neutrons. — Firing conditions in old-fired clay bricks were studied by means of small-angle neutron scattering. Masonry and chimney brick samples (Úpice, 1876, Telé, 1950) from Czech Republic, were compared to samples of raw clay from the sites of the original quarries. Bricks produced with different raw materials could be distinguished on the basis of the fractal exponent of the scattering surface of pores.

Firing temperature of archaeological pottery wares was determined by means of neutron scattering. A series of control samples with known firing conditions revealed linear correlation between firing temperature and p -exponent of the Porod-approximation of SANS intensity versus momentum transfer curves. Based on this correlation, the firing temperatures of 17 archaeological ceramic samples from the Early Medieval site of Keszthely have been determined in a non-invasive manner.

Scientific analysis of the ceramic artefacts (20 pcs) of the 6th century AD cemetery of Szólád (Hungary) was carried out. During the pottery analysis thin-section petrography (resulting in mineralogical data), Prompt-Gamma Activation Analysis and Neutron Activation Analysis (resulting in major and trace elemental composition) was made. These methods allowed to apply two different statistical models where both types of data (qualitative mineralogical and quantitative chemical) were incorporated into the analysis (“mixed-mode”): multidimensional scaling (MDS) and multifactorial analysis (MFA). They were studied separately, together or weighted. The aim of the analyses was to distinguish different material groups based on their mineralogical and chemical composition which refer either to local or import pottery production. The analyses resulted in two separate material groups, both of local origin, and four individual vessels, which could be defined as import production.

Optimization of new borosilicate glasses for conditioning High-Level-Waste (HLW) materials. The immobilization process of HLW materials in borosilicate glasses is generally accepted in the literature. Stable and compact structure, multi-component matrix glasses with a compact structure, namely borosilicate-based glasses doped with 30wt% CeO₂, Nd₂O₃ and Eu₂O₃ lanthanides were investigated. They were used for chemical modelling of the actinides, with the aim to clear up the correlation between structural characteristics and to find answer for a possible incorporation of Ce, Nd and Eu elements. Based on neutron and X-ray diffraction measurements combined with Reverse Monte Carlo simulation, a

comprehensive structural study of the glasses was done. The special interest of this system lies in the different glass forming mechanisms of SiO_2 and B_2O_3 . The shortest second-neighbour distances obtained for the (Si,B)-Ce, (Si,B)-Nd and (Si,B)-Eu pair correlation functions suggest that lanthanide ions take part partially as network former in the structure. These pronounced correlations show that Ce, Nd and Eu atoms can be incorporated in the matrix glass structure.

Hybrid silica materials with ordered pore structure. — Hybrid silica materials have been synthesized and studied by a variety of experimental methods including scattering techniques. The materials were prepared using organically modified precursors with methyl and aminopropyl functional groups, as well as using templating surfactant molecules with different alkyl tail lengths. These additives influence the pore structure, ordering and the chemical nature of pore surface such as hydrophobicity, which allow to control and tailor the properties of the materials for various applications. The methyl-modified materials were tested for their drug-uptake and -release properties, and a strong correlation between the methyl content and the *in vitro* dissolution rate of ketoprofen has been achieved, demonstrating the potential applicability of such co-condensation type of synthesis for practical applications.

The microstructure of ODS steels processed by friction steel welding (FSW), friction steel welding, has been investigated by methods of small-angle neutron scattering with magnetic contrast variation, and electron microscopy. The particle size distribution of the nano-sized yttrium oxide and its derivatives (Fig. 3) shows a strong change with the parameters of the welding process. The relative number of particles in the range of 2-80 nm decreases, partially dissolves in the stir zone with respect to the base material, and this effect is stronger in the case of higher tool rotation speed, i.e., higher heat input during the welding.

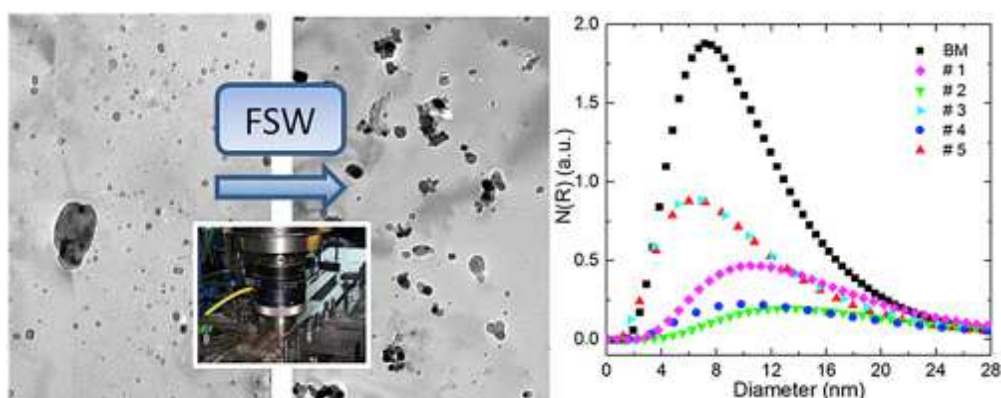


Figure 3. Representative TEM images and the statistically correct size distribution of the ceramic precipitates.

Grants

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

H2020-IPERION CH-2014-2015: 654028 (L. Rosta, 2015-2019)

H2020-654000, SINE2020 Science & Innovation with Neutrons in Europe in 2020 Training (L. Rosta, 2015-2019)

HAS complementary support

International cooperation

HAS Romania Academic exchange, Institute of Chemistry Timisoara

TÉT DST-India, Bhabha Atomic Research Centre, Mumbai

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See also: R-L.6, S-M.1, S-M.4,S-M.6

S-M. Neutron optics

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



Neutron instrumentation development. — Members of the group actively participated in the detailed design work of two instruments for the European Spallation Source (ESS) in Lund, Sweden: BIFROST indirect neutron spectrometer and NMX macromolecular single-crystal diffractometer. Both are new type instruments, the first ones in their class. The final design of the neutron optics systems of the instruments (neutron guide systems, choppers and detectors) are finalized by means of analytical calculations completed at our department. Researchers of the Neutron Spectroscopy Department investigated the robustness of the neutron guide system against misalignment and waviness of the neutron mirrors and the movement of the floor, features indispensable both in the optimization of the guide system and in the design of radiological shielding.

In the frame of the EU-H2020 BrightnESS project, researchers of the group have performed the optimal principal design of the ESS Test Beamline, the first equipment to receive neutrons and produce results at the ESS facility currently being built at Lund.

We have developed, successfully tested at the Budapest Research Reactor and applied during an experiment series at the JEEP-II reactor of IFE Kjeller, Norway a compact, mobile equipment for energy-sensitive imaging of neutron sources. The key components are the mask with pinhole and chopper unit as well as a four-layer, double-readout solid boron converter



Figure 1. TOF large sample positioning system

neutron detector. Neutron adsorber materials, system geometry and parameters have been optimized to accommodate the high count rate and good resolution specific for the intended application.

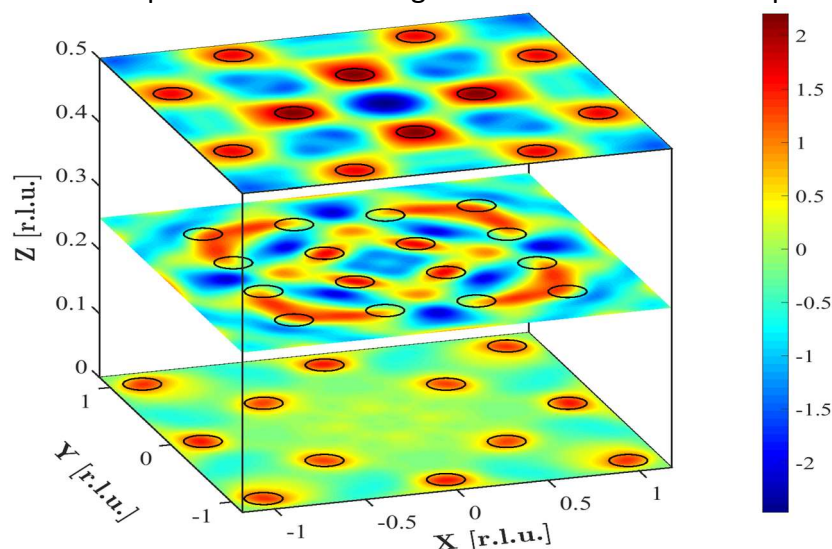
A further development is the equipment for positioning large samples at the time-of-flight (TOF) diffractometer (Fig. 1), a sample environment equipment indispensable for fulfillment of archeometry tasks in the frame of the EU-H2020 Iperion project.

We coordinated the instrumental part of the Hungarian In-Kind contribution to the ESS, including design and production of neutron optical elements and shielding as well as engineer and physicist secondment provisions.

[#] Ph.D student

^E Professor Emeritus

Neutron holography. — In 2017, we continued the research started earlier on the topic of magnetic holography. Neutrons possess magnetic moment, thus they interact with the magnetic moments of the atoms in the sample. The latest investigations revealed the possibility to use this interaction to measure the local magnetic structure around selected atoms in the sample. We described the magnetic hologram previously and showed that the radial component of the atomic magnetic moments can be obtained by applying the Helmholtz-Kirchoff integral transformation to holograms measured in a special experimental arrangement. In 2017, we found a correlation method which can be used to determine the three components of the magnetization vectors. The optimal experimental parameters



(neutron spin direction, neutron wavelength and required statistics) were obtained by model calculations (Fig. 2).

Figure 2. The z-component of the magnetic moments of Cu atoms in CuCr_2O_4 , obtained by applying the proposed correlation method on the simulated magnetic hologram.

Structural investigation of

hybrid silica gels. — The similarities and the differences on the physicochemical characteristics of the organic–inorganic hybrid silica gels derived from two-vinyl substituted (Vinyl – triacetoxo / - triethoxo silica (VTAS/VTES)) precursors were studied. NaF and NH_4F catalysts were applied to promote the gelification. For both silica precursors the use of NH_4F catalysts resulted in higher specific surface area. Using VTES, higher degree of vinyl substitution could be obtained, but the silica gel specific surface areas are lower compared to the corresponding samples obtained with VTAS. The increasing quantity of the vinyl substituents causes a decrease in primary particle size, pore number and sizes, but an increasing hydrophobicity no matter if VTAS or VTES were used. Further investigation will be made to determine how structural modification of the silica hybrid silica support will influence the activity of immobilized guest molecules (porphyrins, drug or enzymes).

An international symposium was organized dedicated to the memory of our passed colleague, László Cser, in the frame of the yearly meeting of the International Scientific Advisory Committee of the Budapest Research Centre. Co-workers, friends, colleagues, former and actual PhD students held lectures to honor his life-long scientific activity.

Grants

TÉT_13_DST-1-2013-0017 Development and technology transfer for marketable components of cold neutron moderator and beam extraction systems at advanced neutron sources (L. Rosta, 2015-2017)

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

International cooperation

European Spallation Source ERIC, Paul Scherrer Institut, Helmholtz-Zentrum Berlin, Forschungszentrum Jülich, Helmholtz Zentrum Geesthacht, Linköping University, Lund University, Universidade de Aveiro, University of Messina, Institute of Chemistry Timisoara of Romanian Academy, Université Ibn Tofail l'Université Cadi Ayyad, Elettra Synchrotron Trieste, JEEP-II reactor of IFE Kjeller.

Publications

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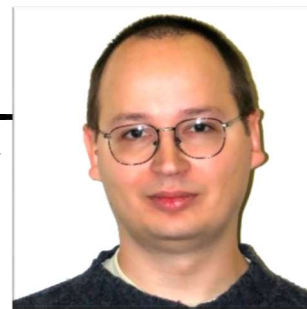
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See also: R-L.6, S-L.6, S-L.7, S-L.23, S-L.24

S-N. Laser applications and optical measurement techniques



Attila Tibor Nagy, Aladár Czitrovsky, Kárpát Ferencz, Zoltán György Horváth^A, Péter Jani^A, Attila Kerekes, Szilvia Kugler, Lénárd Vámos

Aerosol drug delivery/deposition in human lungs. — The MMAD (mass median aerodynamic diameter) of the Symbicort® Turbuhaler dry powder inhaler (DPI) and the aerosol particle deposition in the upper airways was studied in case of different inhalation waveforms. For the detection of the aerosol size distribution, the Aerosol Particle Sizer (APS) Spectrometer was used. The effect of the breathing pattern on the MMAD was determined after the upper airways. With the help of the stochastic lung deposition model (SLDM), the amount of deposited particles in the lung was quantified. It was found that approximately 10% of the particles from the DPI deposit in the upper airways. The lung deposition of the drug from the DPI was calculated to be between 18 and 63% of the nominal dose, depending on the inhalation time and the peak inhalation flow.

Vibrational (Raman and infrared) spectroscopy based methods have been developed to determine the distribution of inhalation drugs (and other aerosols) in human airway replicas. The tested medication was introduced by metered dose inhaler into a realistic human lung tract prepared by 3D printing from computer tomographic data of human respiratory system. The deposited material was collected with silicon substrates attached to the hollow airway's walls in different points. The analysis of the substrates was performed by Raman and infrared spectroscopic mapping of drug's characteristic peak intensities over the surface. The method was verified by comparison with optical microscopic images recorded on the same surface area.

Study of optical properties of aerosols. — We have participated in the A-LIFE ERC project of the University of Vienna with PI Prof. Bernadett Weinzierl. The project is aimed at investigating the properties of absorbing aerosols (in particular mineral dust – black carbon (BC) mixtures) to characterize the aging and mixing of light-absorbing aerosol layers during their lifetime, to assess the contribution of individual aerosol components, in particular mineral dust and BC to the radiative forcing (RF) of mixed absorbing aerosol layers, to implement complex particle morphologies in RF estimates, and to investigate potential links between the presence of absorbing particles, aerosol layer lifetime and removal. We participated in the project by applying an optical method for the measurement of the optical and physical properties of ambient aerosols, which was developed by us in cooperation with the University of Vienna.

Optical thin film structures for advanced ultrafast applications. — We have continued our research concerning the development of optical thin film structures (high reflectors, output couplers, beam splitters, triple-band antireflective coatings etc.) for advanced femtosecond laser sources producing energetic light pulses in the near- and middle-infrared wavelength ranges. We have produced successfully sampling beam splitters on sapphire substrates for

^A Associate fellow

the French company Fastlite, working perfectly in their MIR laser system installed at ELI ALPS in Szeged already. We have developed new type of negative- or zero-dispersion multilayer mirror structures for our Japan partner also. The new laser mirror structures developed by us are very important in the development of new ultrafast high-power lasers which are able to shift the limits of the higher harmonic generation from the soft X-ray range to the hard X-ray range.

Optical measurement techniques serving the development of medical laser systems. — We have been involved in a project where the participants conduct research and development activities aiming at developing prototype instruments for medical surgery applications based on ultrashort pulse and fibre lasers. We have studied the light scattering and absorption properties of model tissue materials using different lasers and detection techniques. We have studied the surgical smoke that is generated upon the interaction of intense laser light and model tissue materials. In the frame of this study, we measured the size distribution of the surgical smoke with optical particle counter, aerodynamic particle counter and condensation particle counter, we measured the spread of the generated aerosols using laser Doppler anemometer, and collected samples with a cascade impactor for further analysis.

Grants

EAC - European Aerosol Conference (A. Czitrovsky)

EXMET Academic Excellence Program - Development of interferometric measurement methods and its applications (A. Czitrovsky, 2015 - 2017)

HAS - Wigner RCP Infrastructural Developments, establishing a service laboratory for optical measurements (A. Czitrovsky, 2014-2017)

HAS - Wigner RCP Infrastructural Developments - Photon counting detectors (A. Nagy, 2016 - 2017)

LASRAM Engineering - Wigner RCP Development of medical laser systems using fibre lasers and femtoseconds pulse lasers (A. Nagy, A. Czitrovsky 2016-2018)

OPTILAB - WIGNER RCP No. WG-04/2016

International cooperation

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

University of Vienna (Nagy Attila Tibor) – Bernadett Weinzierl, ERC A-LIFE project

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

Uzhhorod National University (Uzhhorod, Ukraine), (Czitrovsky Aladár)

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5. Kugler Sz, Kerekes A, Nagy A, Czitrovsky A: Porinhalátorok kiülepedésének vizsgálata különböző légzési paraméterek esetén (Investigation of the deposition of the drugs from dry powder inhalers under different breathing conditions, in Hungarian). In: *Proc. XIII. Hungarian Aerosol Conference (Pécs, Hungary, 19-20 April 2017)* Ed.: Schmeller G, Pécsi Tudományegyetem ISBN:978-963-429-127-5, 2017 pp. 43-44
6. Nagy A, Kerekes A, Kugler Sz, Czitrovsky A: Aeroszol gyógyszerkészítmények méreteloszlásának időfelbontásos vizsgálata realisztikus légzési feltételek esetén (Time resolved measurement of the size distribution of aerosol medications under realistic breathing conditions, in Hungarian). In: *Proc. XIII. Hungarian Aerosol Conference (Pécs, Hungary, 19-20 April 2017)* Ed.: Schmeller G, Pécsi Tudományegyetem ISBN:978-963-429-127-5, 2017 pp. 37-38

S-O. Femtosecond lasers for non-linear microscopy

Róbert Szipőcs, Norbert Kiss[#]



Coherent anti-Stokes Raman Spectroscopy (CARS) microscopy; Stain-free histopathology.

— Basal cell carcinoma (BCC) is the most common malignancy in Caucasians. Non-linear microscopy has been previously utilized for the imaging of BCC, but the captured images do not correlate with standard hematoxylin and eosin (H&E) staining. This year we have developed a novel algorithm to post-process images obtained from dual vibration resonance frequency (DVRF) CARS measurements to acquire high-quality pseudo H&E images of BCC samples (Fig. 1). We adapted our CARS setup to utilize the distinct vibrational properties of CH_3 (mainly in proteins) and CH_2 bonds (primarily in lipids). In a narrow-band setup, the central wavelength of the pump laser is set to 791 nm and 796 nm to obtain optimal excitation. Due to the partial overlap of the excitation spectra and the 5-10 nm FWHM spectral bandwidth of our lasers, we set the wavelengths to 790 nm (proteins) and 800 nm (lipids). Non-resonant background from water molecules also reduces the chemical selectivity which can be significantly improved if we subtract the DVRF images from each other. As a result, we acquired two images: one for “lipids” and one for “proteins” when we properly set a multiplication factor to minimize the non-specific background. By merging these images, we obtained high contrast H&E “stained” images of BBCs. Non-linear microscope systems upgraded for real time DVRF CARS measurements, providing pseudo H&E images can be suitable for *in vivo* assessment of BCC in the future.

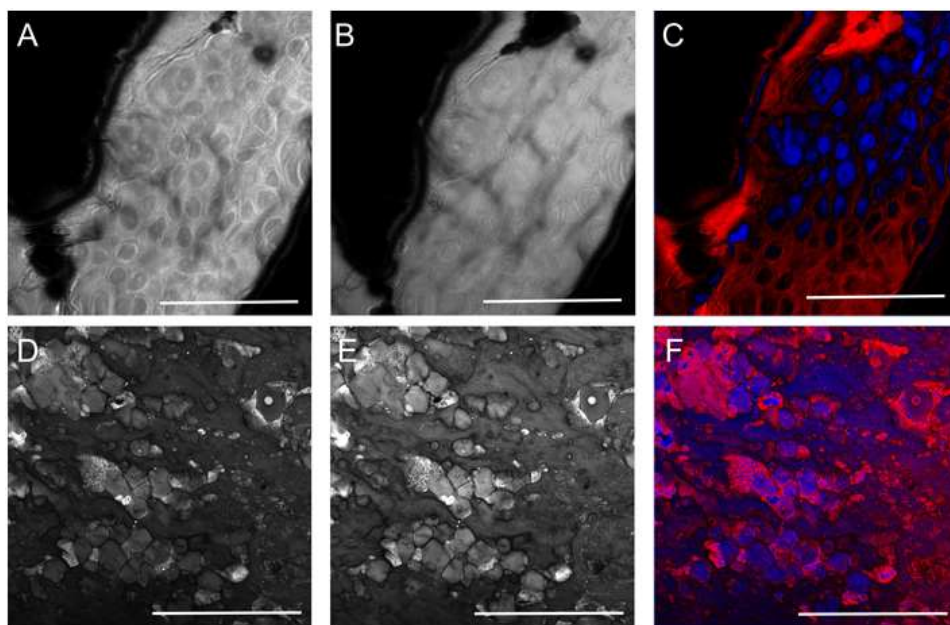


Figure 1. CARS images of mouse epidermis (A-C) and human basal cell carcinoma (D-F). A, D: “ CH_2 ” images; B, E: “ CH_3 ” images; C, F: merged color DVRF-CARS images (red: CH_2 - CH_3 , blue: CH_3 - CH_2). Scale bar: 50 μm .

[#] Ph.D student

Multimodal stain-free mosaic imaging of malignant tumour in the skin – BCCs often have poorly defined borders, the clinical assessment of the tumor margins can be challenging. Therefore, there is an emerging demand for efficient *in vivo* imaging techniques for the evaluation of the tumor borders of BCC prior to and during surgeries. This demand might be met in the near future by non-linear microscopy techniques (such as auto-fluorescence (AF) and second harmonic generation (SHG) mosaic imaging) utilizing our novel, fibre-laser based, hand-held 3D nonlinear microscope system (*FiberScope*).

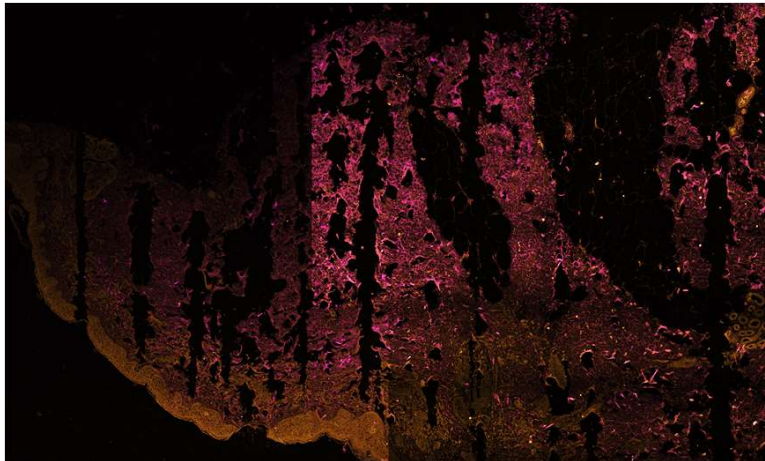


Figure 2. Multimodal (AF+SHG) mosaic image of human basal cell carcinoma comprising 6x10 microscope images with an overall area of 2,5x 4.2 mm². Yellow: detected AF signal, purple: SHG signal of collagen.

This year, we have measured AF and SHG signal of collagen on 10 *ex vivo* healthy control and BCC skin samples and compared

the images by different quantitative image analysis methods. These included integrated optical density (IOD) measurements on AF and SHG images and application of fast Fourier transform (FFT), CT-FIRE and CurveAlign algorithms on SHG images to evaluate collagen structure. In the BCC samples, we found significantly lower IOD of both the AF and SHG signals and higher collagen orientation index utilizing FFT. CT-FIRE algorithm revealed increased collagen fiber length and decreased fiber angle while CurveAlign detected significantly higher fiber alignment of collagen fibers in BCC. These results are in line with previous findings which describe pronounced changes in the collagen structure of BCC. In the future, these novel image analysis methods could be integrated in our *FiberScope* imaging system for sensitive and specific identification of BCC.

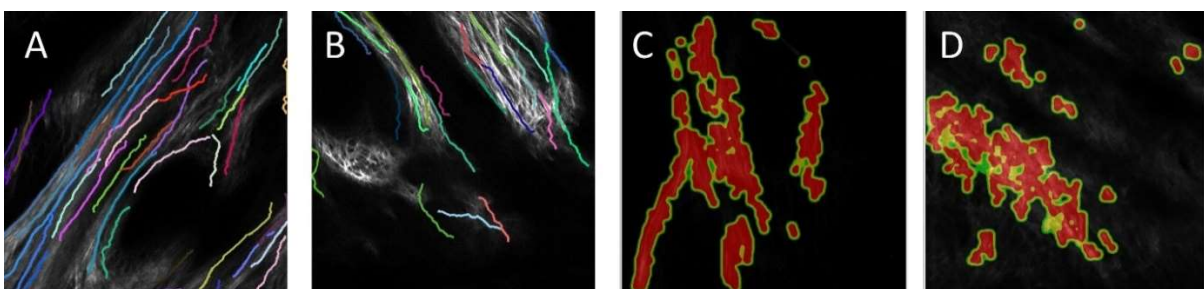


Figure 3. Normal human skin (A, C) and basal cell carcinoma (B, D) collagen SHG images processed by different numerical algorithms. Image size: 420x420 μ m².

Grants

KTIA_13_NAP-A-I/16 National Brain Research Program, - Neuronal myelination and nitric-oxide dynamics studied by CARS microscopy (R. Szipőcs, 2014-2017)

Publications

Article

1. Lőrincz K, Haluszka D, Kiss N, Gyöngyösi N, Bánvölgyi A, Szipócs R, Wikonkál NM: Voluntary exercise improves murine dermal connective tissue status in high-fat diet-induced obesity. **ARCH DERMATOL RES** 309:(3) 209-215 (2017)

S-Q. Crystal physics

László Kovács, László Bencs, Gábor Corradi^A, Gabriella Dravecz, István Földvári^A, Ivett Hajdara, Laura Kocsor[#], Krisztián Lengyel, Gábor Mandula, Ágnes Péter^A, Katalin Polgár^A, Zsuzsanna Szaller, Éva Tichy-Rács[#]



Crystal growth of niobates. — A series of Fe+Ti double-doped stoichiometric LiNbO_3 (LN) crystals has been grown to optimize/balance photorefractive and wave-guiding properties. Rare-earth (Er, Nd, Yb) and transition-metal (Fe, Ti) doped over-threshold stoichiometric LN crystals have been grown for IR spectroscopic studies showing that these dopants (M) may also incorporate at Nb sites forming $\text{M}_{\text{Nb}} - \text{OH}^-$ -type complexes like optical-damage-resistant (Mg, Zn, In, Sc, Hf, Zr, Sn) ions.

Spectroscopy of lithium yttrium orthoborate ($\text{Li}_6\text{Y}(\text{BO}_3)_3$, LYB) single crystals. — Czochralski grown LYB:Dy crystals suitable for scintillator and laser communication systems (Fig. 1) have been characterized by temperature and polarization dependent FTIR absorption and luminescence measurements. Up to the $^4\text{I}_{15/2}$ multiplet, all Stark levels split by low-symmetry crystal field could be determined. The most intense luminescence was detected at 577 nm ($^4\text{F}_{9/2} \rightarrow ^6\text{H}_{13/2}$ transition).



Figure 1. High optical quality LYB crystal doped with Dy.

Coherent Yb-pair emission in $\text{Li}_6\text{Y}_{1-x}\text{Yb}_x(\text{BO}_3)_3$ crystals ($x=0.01, 0.05, 0.20$) was successfully generated using laser excitation at ≈ 972 nm. At 6 K, the emission showed a detailed structure containing at least 13 band components in the 470-540 nm range. The laser intensity dependence of the integrated area of the spectra was explained by an energy transfer mechanism via Yb^{3+} chains in the crystal lattice.

Spectroscopy of the tissue-equivalent dosimeter material lithium tetraborate (LTB). — Luminescence studies of Mn doped LTB single crystals complemented by EPR analysis in the 33 GHz Q-band revealed rechargeable Mn^{2+} centres incorporated in the lithium sublattice, compensated by mobile lithium vacancies. Both electrons and holes created by ionising radiation are trapped by Mn^{2+} centres, their recombination accounting for the thermoluminescent readout of the radiation dose.

Spectroscopy of LiNbO_3 :Yb nano-powders. — LN nano-powders have been prepared by high-energy ball milling from bulk crystals, using alumina, steel or tungsten carbide vials. The type of mills, number of balls (1 or 2), milling time and the ball-to-powder ratio has been varied to produce the smallest grain size. After resonant irradiation at $\lambda=980$ nm, a fluorescent signal with a lifetime of 0.5 ms at ≈ 40 K, but surviving also at RT was found in a LiNbO_3 :Yb nano-powder with a characteristic grain size of 390 nm. Using a saturation spectroscopic method in KBr- LiNbO_3 :Yb pellets with characteristic size of 390 nm, the population relaxation kinetics

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[#] Ph.D student

and magnetic field splitting of the spectral hole was determined for the ${}^2F_{7/2} - {}^2F_{5/2}$ transition of Yb^{3+} . The same processes were studied for 70 nm pellets as well, but only a single strong spectral hole component with a lifetime longer than 10 h was found instead, that could only be erased by a 30 min annealing of the sample above 90 K.

Transient absorption of small polarons and excitons in $\text{LiNbO}_3:\text{Mg}$. — Picosecond absorption in the 0.3–1.05 eV *mid-infrared* region induced by 100 fs pumping pulses with 2.5 eV photon energy was attributed to free electrons originating from hot electron-hole pairs undergoing phonon-assisted dissociation and cooling, as well as their subsequent trapping as Nb^{4+} polarons at regular Nb sites. The concentrations of hot, cold, and polaronic charge carriers could be derived based on a kinetic model. Long-lived absorption in the *near infrared and visible* region could be interpreted as due to the survival of trapped polarons and pinned excitons near lattice defects, respectively (Fig. 2).

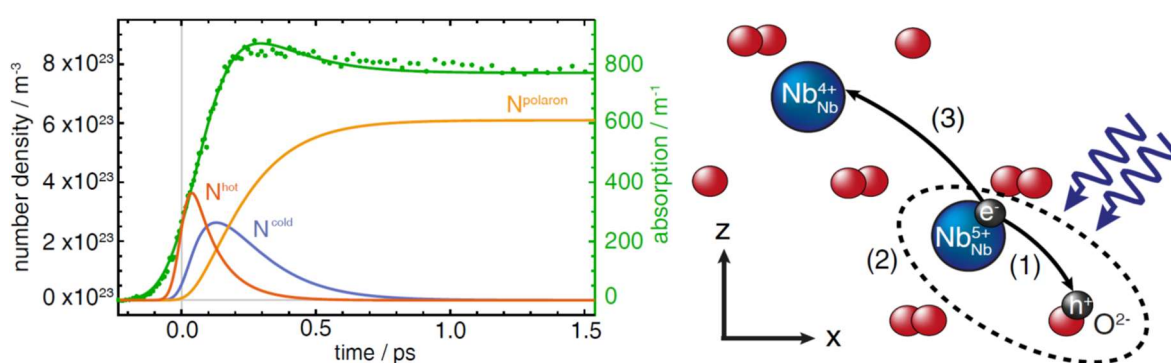


Figure 2. Left: subpicosecond pulse-induced two-photon absorption in $\text{LiNbO}_3:\text{Mg}$ (green) and the resulting number densities of hot, cold and polaronic carriers (orange, blue and yellow lines, respectively). Right: early recombination (1), excitonic stabilisation (2) and dissociation (3) of hot electron-hole pairs located on neighboring matrix ions of the LiNbO_3 lattice.

Dielectric parameters of lithium tantalate (LiTaO_3) in the terahertz range. — The refractive indices and absorption coefficients of congruent, stoichiometric and 0.5 or 1.0 mol% Mg-doped LiTaO_3 crystals have been investigated using polarization dependent terahertz time-domain spectroscopy in the 0.3–2.0 THz range. The data were successfully fitted by a three-term Lorentz oscillator model. Stoichiometry was shown to have a significant influence, while Mg had a much smaller effect. LiTaO_3 can be a promising THz generator material due to the lack of the three-photon absorption at 800 nm.

Analytical methods for environmental and advanced materials. — The distributions of mass, water-soluble inorganic salts and mineral elements of size-segregated aerosols, precursor gaseous pollutants, black carbon, and nanoparticles over the Southern North Sea have been studied. The nano-aerosol count, originating from ocean-going ships, peaked at lower diameters (≈ 28 nm) than those observed for smaller (e.g. fishing) boats (45–50 nm) and depended also on weather conditions.

Solid phase extraction with high-resolution continuum-source graphite-furnace atomic absorption spectrometry has been developed for speciation of inorganic As in geothermal, well and pretreated water samples from four Hungarian waterworks. Total As in well waters varied between 40–120 $\mu\text{g/L}$. Occurrence of As(III) in well waters exceeded 80% of the total

As, while As(V) was predominant ($\approx 90\%$) in pretreated waters, but below the health limit value of the 98/83/EC Council Directive ($10 \mu\text{g/L}$).

Grants

NKP-2017-00001 (2017-2020, Creating and sharing quantum bits and development of quantum information, contributors: L. Kocsor, L. Kovács, K. Lengyel, G. Mandula).

GINOP-2.2.1-15-2017-00070 (2017-2019, Development of a sampler for online monitoring of the moving sedimentary phase of surface water bodies and the establishment of the related material testing and biological systems, consortium leader: AquaTerra, Veszprém, contributors: L. Bencs, G. Dravecz).

International cooperation

Tartu University (Estonia), Spectroscopy of doped borate crystals for quantum optics and dosimetry (G. Corradi, participants: L. Kovács, K. Lengyel and É. Tichy-Rács)

Laser Research Centre of Vilnius University (Lithuania), Coherent rare-earth pair excitation in $\text{Li}_6\text{Y}(\text{BO}_3)_3$ crystals (K. Lengyel)

Publications

Articles

1. Bencs L, Horemans B, Buczyńska AJ, Van Grieken R: Uneven distribution of inorganic pollutants in marine air originating from ocean-going ships. *ENVIRON POLLUT* **222**: 226-233 (2017)
2. Buzády A, Unferdorben M, Tóth G, Hebling J, Hajdara I, Kovács L, Pálfalvi L: Refractive index and absorption coefficient of undoped and Mg-doped lithium tantalate in the terahertz range. *J INFRARED MILLIM TE* **38**:(8) 963-971 (2017)
3. Kijatkin C, Eggert J, Bock S, Berben D, Oláh L, Szaller Zs, Kis Zs, Imlau M: Nonlinear diffuse fs-pulse reflectometry of harmonic upconversion nanoparticles. *PHOTONICS* **4**:(1) 11/1-14 (2017)
4. Kovács L, Arceiz Casas S, Corradi G, Tichy-Rács É, Kocsor L, Lengyel K, Ryba-Romanowski W, Strzep A, Scholle A, Greulich-Weber S: Optical and EPR spectroscopy of Er^{3+} in lithium yttrium borate, $\text{Li}_6\text{Y}(\text{BO}_3)_3:\text{Er}$ single crystals. *OPT MATER* **72**: 270-275 (2017)
5. Kovács L, Kocsor L, Szaller Z, Hajdara I, Dravecz G, Lengyel K, Corradi G: Lattice site of rare-earth ions in stoichiometric lithium niobate probed by OH^- vibrational spectroscopy. *CRYSTALS* **7**:(8) 230/1-9 (2017)
6. Mihucz VG, Bencs L, Koncz K, Tatár E, Weiszbürg T, Zárny Gy: Fast arsenic speciation in water by on-site solid phase extraction and high-resolution continuum source graphite furnace atomic absorption spectrometry. *SPECTROCHIM ACTA B* **128**: 30-35 (2017)
7. Mihucz VG, Enesei D, Veszely A, Bencs L, Pap-Balazs T, Ovari M, Strelci C, Zárny Gy: A simple method for monitoring of removal of arsenic species from drinking water applying on-site separation with solid phase extraction and detection by atomic absorption and X-ray fluorescence based techniques. *MICROCHEM J* **135**: 105-113 (2017)

8. Romet I, Buryi M, Corradi G, Feldbach E, Laguta V, Tichy-Rács É, Nagirnyi V: Recombination luminescence and EPR of Mn doped Li₂B₄O₇ single crystals. ***OPT MATER*** **70**: 184-193 (2017)

S-R. Nanostructures and applied spectroscopy

Miklós Veres, Péter Baranyai, Arnold Gucsik, László Himics, Margit Koós^A, Malik Al-lami[#], István Rigó[#], Sára Tóth, Tamás Váczi



Color centers in nanodiamond. — Among the numerous optically active defects (color centers), studied in nanosized diamond (ND), the silicon-vacancy (SiV) center is a promising candidate for utilization in different fields like quantum computing and cryptography, nanoscopy, medicine or cell biology. Most applications are based on the intensive and narrow zero-phonon emission line (ZPL) of the mentioned color center, which can be detected in near infrared wavelength region, around 1.68 eV (738 nm). However, the asymmetric lineshape of the SiV ZPL may restrict the spectral parameters important for different applications and prohibit the determination of the real ZPL characteristics by traditional spectroscopic techniques.

Micro-photoluminescence measurements performed on a high number of CVD nanodiamond films containing SiV centers showed that the undesirable asymmetric tail on the low-energy side of the ZPL is related to another optically active defect (so-called GR1 center) being present in the nanodiamond structures as well. Regions with relatively high GR1 content and with well-distinguishable zero-phonon lines related to different optically active defect structures can be localized by mapping of the ND film with an appropriate excitation wavelength (Fig. 1).

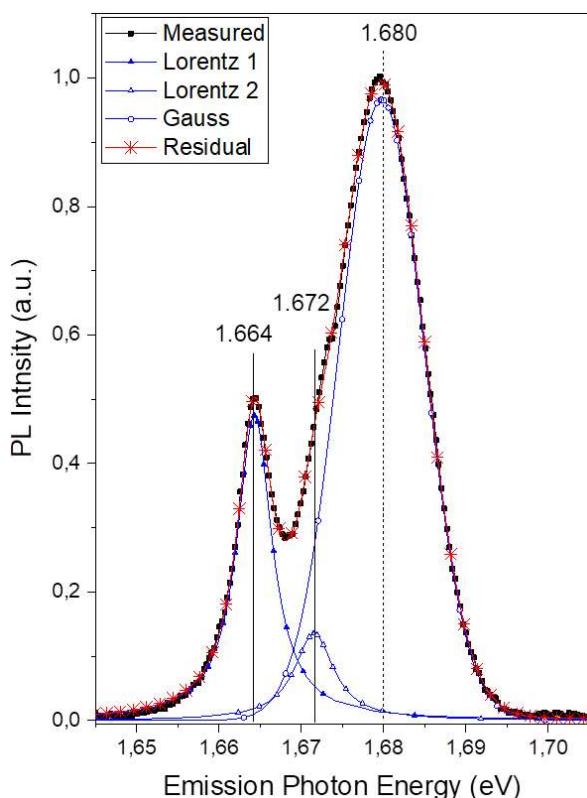


Figure 1. Fine-structured emission spectrum of CVD nanodiamond film around the SiV center ZPL region excited by 635 nm and recorded at room temperature. The deconvoluted peaks correspond to SiV center ZPL (1.680 eV) and the double ZPL of the GR1 defect (1.664 eV and the weak shoulder at 1.672 eV).

Preparation of new tetragonal silicon polymorphs by ultrashort laser pulses. — Tetragonal polymorphs of silicon were created successfully by irradiation of microcrystalline silicon powder with femtosecond laser pulses (800 nm center wavelength with 1 kHz repetition rate and 42 fs pulse duration) in air at room temperature. Surface enhanced Raman spectroscopy and, in collaboration with the Research Institute for Materials Science, Centre for Energy

^A Associate fellow

[#] Ph.D student

Research, HAS and the Research Centre for Natural Sciences, HAS, transmission electron microscopy (TEM) measurements were carried out to prove the presence of bt8 (Fig. 2) and t32* (Fig. 3) Si phases.

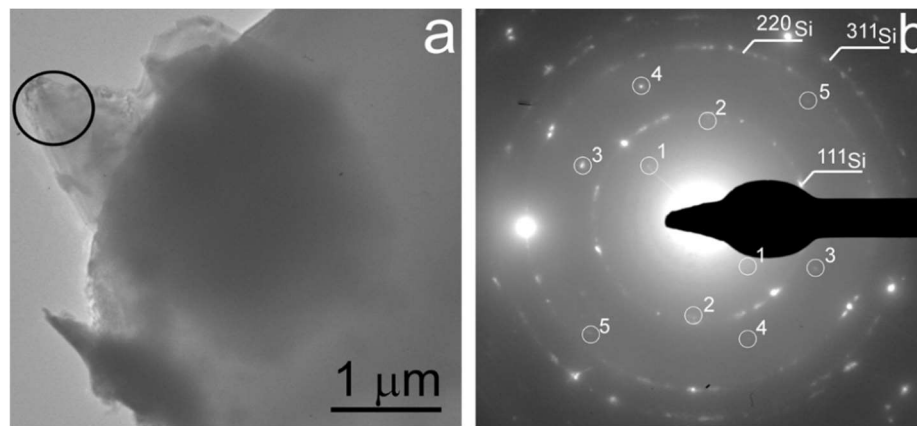


Figure 2. TEM image of bt8 Si polymorph. In addition to ordinary cubic Si, weak extra reflections occur with the following d spacings: 4.70 (1), 3.37 (2), 2.60 (3), 2.38 (4), 2.10 (5) Å. These extra reflections are consistent with $\{101\}$ (1), $\{200\}$ (2), $\{211\}$ (3), $\{220\}$ (4) and $\{301\}$ (5) reflections of bt8 Si.

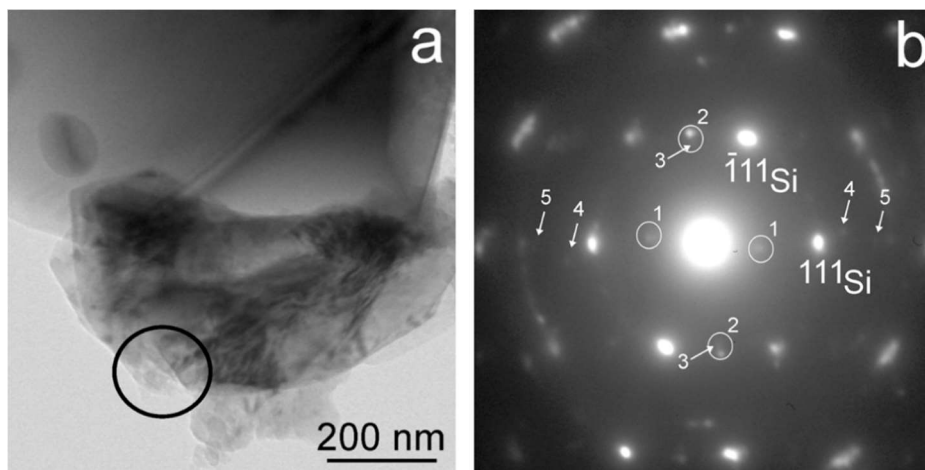


Figure 3. TEM image of t32* Si polymorph. In addition to ordinary cubic Si, there are two sets of strong reflections with 6.60 (1) and 3.20 (2) Å. These strong reflections and their measured angles are consistent with $\{110\}$ and $\{0-12\}$ of t32* Si grain. The additional weak reflections with 3.63 (3), 2.65 (4), 2.16 (5) Å can be interpreted with $\{211\}$, $\{311\}$ and $\{013\}$ of t32* Si.

Grants

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

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

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

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

NVKP_16-1-2016-0043: Development of fluorescent dyes and high resolution, fast scanning 3D microscope for the treatment of epilepsy (M. Veres, 2017-2019)

VEKOP-2.3.2-16-2016-00011: Strategic workshop for the technological challenges of renewable energy systems (M. Veres, 2017-2020)

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

COST CA16101: MULTI-modal Imaging of FOREnsic SciEnce Evidence - tools for Forensic Science (M. Veres, 2017-2020)

International cooperation

University College London, Department of Chemistry, Christopher Ingold Laboratories, London UK (s. Tóth)

Saint Petersburg National Research University of Information Technologies, St. Petersburg, Russia (S. Tóth)

Universität Kassel, Kassel, Germany (L. Himics)

Uzhhorod National University, Uzhhorod, Ukraine (M. Veres)

V. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine (M. Veres)

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

University of Birmingham, Birmingham, United Kingdom (M. Veres)

Max Planck Institute for Neurobiology, Martinsried, Germany (M. Veres)

Okayama University of Science, Okayama, Japan (A. Gucsik)

Max Planck Institute for Astronomy, Jena, Germany (A. Gucsik)

University of Arizona, Tucson, USA (A. Gucsik)

Institut für Mineralogie und Kristallographie, Universität Wien, Vienna, Austria (T. Váci)

Publications

Articles

1. Csarnovics I, Veres M, Nemeč P, Latif MR, Hawlova P, Molnar S, Kokenyesi S: Surface patterning in GeSe amorphous layers. *J NON-CRYST SOLIDS* **459**: 51-56 (2017)
2. Kereszturi A, Gyollai I, Kereszty Zs, Kiss K, Szabó M, Szalai Z, Ringer M, Veres M: Analyzing Raman – Infrared spectral correlation in the recently found meteorite Csátalja. *SPECTROCHIM ACTA A* **173**: 637-646 (2017)
3. Kondrat O, Holomb R, Csik A, Takats V, Veres M, Mitsa V: Coherent light photo-modification, mass transport effect, and surface relief formation in As_xS_{100-x} nanolayers: Absorption edge, XPS, and Raman spectroscopy combined with profilometry study. *NANOSCALE RES LETT* **12**: 149/1-10 (2017)
4. Kondrat O, Holomb R, Mitsa V, Veres M, Tsud N: Structural investigation of As-Se chalcogenide thin films with different compositions: Formation, characterization and

- peculiarities of volume and near-surface nanolayers. **FUNCTIONAL MATERIALS** 24:(4) 547-554 (2017)
5. Vejpongsa I, Suvachittanont S, Klinklan N, Thongyen T, Veres M, Szymanski WW: Deliberation between PM1 and PM2.5 as air quality indicators based on comprehensive characterization of urban aerosols in Bangkok, Thailand. **PARTICUOLOGY** 35: 1-9 (2017)
 6. Zhuk DI, Burunkova JA, Denisyuk I Yu, Miroshnichenko GP, Csarnovics I, Tóth D, Bonyár A, Veres M, Kokenyesi S: Peculiarities of photonic crystal recording in functional polymer nanocomposites by multibeam interference holography. **POLYMER** 112: 136-143 (2017)

See also: S-N.2, S-N.3

THE RESEARCH LIBRARY

Anikó Kutnyánszky, Szabolcs Bálint, Andrea Harsányi, Emese Szabó, Ilona Verle



The library's main task is to provide information resources and materials for the research centres and institutes of the Hungarian Academy of Sciences (HAS). Although it is jointly financed by all of the user institutes, it is developed and managed by the Wigner Research Centre.

On 31 December 2017 the stock of the library consisted of 61 536 print monographs and conference proceedings, 65 electronic books with remote access, 41 202 periodical issues and 40 893 research reports. From the 200 newly acquired print books that were added to the collection 146 were purchased, 53 were donated, and 1 item was meant for provisional deposit. As a result of the increased amount of funds that the library received this year for collection development, 109 items of all monographs were bought on the library's budget as compared to 91 copies paid by research groups.

In 2017 we had a subscription for 17 print periodical titles and the issues of 8 additional titles were donated to the library. There were 95 electronic journals with full-text access available for the researchers via individual subscriptions, and the library also had access to as many as 14 246 online periodicals in the scientific databases sponsored by the Electronic Information Service National Programme. Incorporated in this programme, 39 new journal titles published by the Royal Society of Chemistry (RSC) were made available for our researchers from this year on. In addition to the new subscription complimentary vouchers were offered to the library to support authors in making their articles open access published in one of the RSC journals.

The library has its own website, where direct links are provided to the subscription-based and open access e-journals. Besides, the website serves readers with updates on library services and the online resources, as well as information on events, free trial periods or new subscriptions and acquisitions. According to the records, the website was visited 24 234 times during the year, including the number of queries in the online catalogue.

From the library stock 562 print items (books, journal issues and reports) were borrowed by more than 200 registered users on the campus, and the due date of 543 items was renewed during the year. In addition, 353 user requests were fulfilled by the library staff downloading the online versions of articles or scanning printed materials.

Within inter-library loan services 102 library items were provided to our registered users in either print or electronic format, and we successfully completed 60 document requests made by other libraries and external partners. In 2017 we had a network of 30 partner institutes in Hungary and abroad.

This year we finished the inventory that was started in 2012, and after an interval continued from 2015 onwards. During the procedure the total library stock, approx. 100 000 library

items were checked on the shelves against the catalogue records. In the final part of the revision process we went through the stock of periodicals and the research reports published by our institute, which was completed by the end of the first quarter of the year. A final report was made in April and then approved by the head of the Research Centre. According to this report 179 copies of books and 12 issues of periodicals were deleted from the records as missing items. This degree of loss is within the acceptable limit set out by library regulations. All the library records and registers were updated accordingly.

We continued retrospective conversion, adding 2446 records to the online catalogue by processing print catalogue cards of the old stock. 193 records of the new acquisitions were also created and added to the catalogue.

In participation of the digitization project of the Hungarian academic periodicals and materials, the digitization of all journals published before 2000 by the former Central Research Institute of Physics have been completed. The project continues in 2018 with converting reports and preprints into digital format. The files are being released in institutional and also academic databases for a wider community.

The earlier version of Library Rules and Regulations has been revised and updated. Some changes have occurred, among other things, regarding the scope of users who can register without a sponsor's guarantee, and the charges of lost or damaged items.

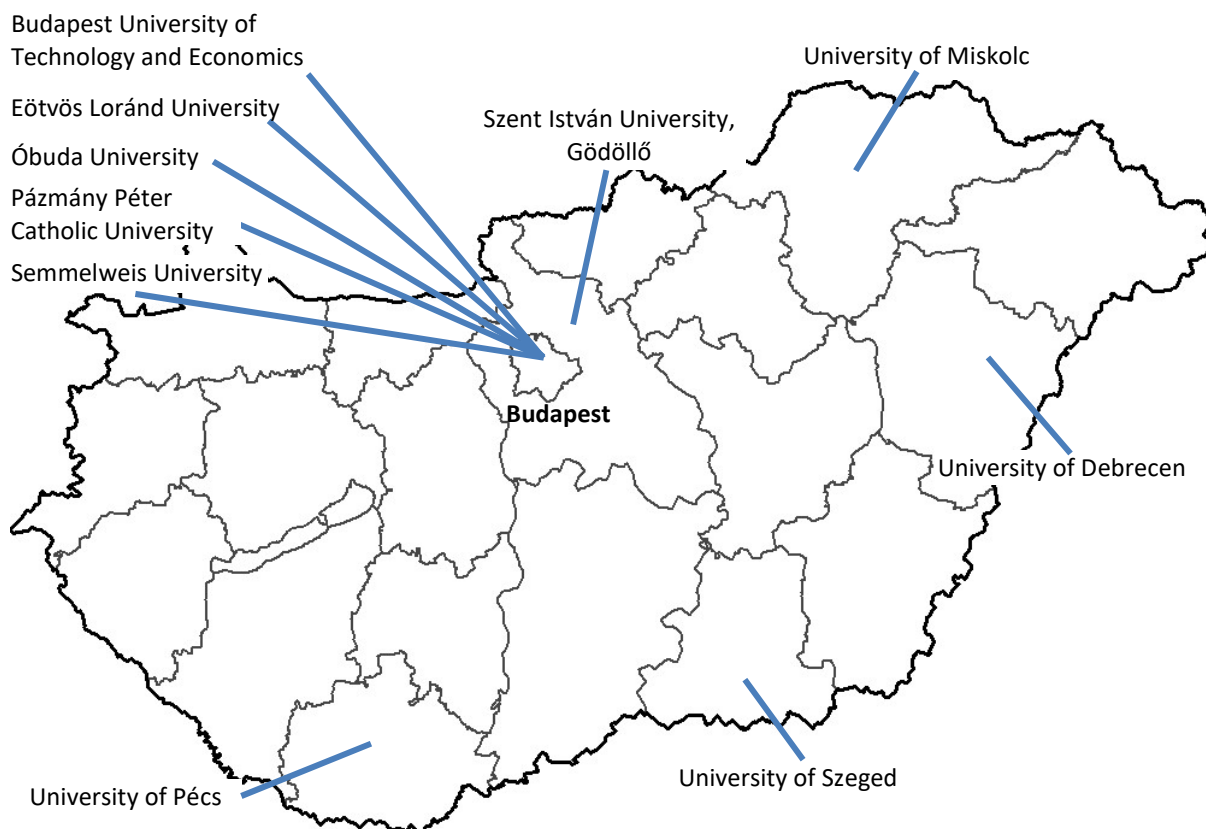
Following the practice of the previous years, a training session was held again in September 2017 for 20 participants to introduce young researchers to the library services, especially to the use of online resources and scientific databases.

Two of our colleagues have successfully completed a course on 'Copyright law in the library', organized by the National Széchényi Library. Members of the library team participated in 23 professional events and conferences during the year, and some visits were paid to other libraries, like the Library of the Alfred Rényi Institute of Mathematics, the Library of the Konkoly Observatory, the Library of the Andrásy University, and the Library of the Hungarian National Museum.

The library went through some remodelling and refurbishment. The walls in most of the rooms got freshly painted and some old window frames were replaced by new ones. One room was discarded, another one was divided into two, making room for a small kitchen. New shelves were bought to store the current periodicals and the dissertations in the reading room.

SUPPLEMENTARY DATA

Education



Graduate and post-graduate courses

Eötvös Loránd University, Budapest

- Advanced biostatistics (Z. Somogyvári)
- Algebraic field theory I.-II.-III. (P. Vecsernyés)
- Atomic and molecular physics (P. Udvarhelyi)
- Computational neuroscience (Z. Somogyvári)
- Computational neuroscience (B. Újfalussy)
- Conformal field theory (Z. Bajnok)
- Electrodeposition of metals (L. Péter)
- Introduction to gravitational theory and high-energy physics (G.G. Barnaföldi, M. Vasúth)
- Introduction to cognitive science, (P. Érdi)
- Introduction to general relativity (M. Vasúth)
- Introduction to gravitation and high energy physics (M. Vasúth)
- Investigation of the inner structure of compact stars (G.G. Barnaföldi)
- Macromolecules (S. Pekker)
- Many-body problem I-II. (G. Szirmai)
- Materials science in chemistry (L. Rosta)
- Mathematical models of the nervous system (G. Orbán)
- Nanophase metals (I. Bakonyi)
- Neutron Physics (M. Markó)
- Nuclear solid-state physics I-II (D.G. Merkel, D.L. Nagy)

- Optics and relativity theory (J. Cserti, Gy. Dávid, D. Varga)
- Physics of jets (P. Lévai)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Physics of low temperature plasmas (Z. Donkó)
- Quantum-information theory (L. Diósi)
- Raman spectroscopy in Earth sciences (T. Vácz)
- Selected chapters from high-energy experimental physics (multiple lecturers, including A. László, D. Varga)
- Selected topics in experimental high-energy physics (F. Siklér, R. Vértesi)
- Solid state research I (I. Tüttő)
- Solid state physics (I. Tüttő)
- Solid state theory I (I. Tüttő)
- Statistical learning in the nervous system (M. Bányai, M.E. Gáspár, D.G. Nagy, G. Orbán)
- Statistical physics (G. Szirmai)
- String theory (Z. Bajnok)
- Superconductivity (I. Tüttő)
- The phase-structure of the strongly interacting matter (P. Lévai)
- The physics of the solar system (K. Szegő)
- Topological Insulators (J. Asbóth)

Bonn University (Germany)

- Introduction to topological insulators and their implementations in artificial matter setups (J. Asbóth)

Budapest University of Technology and Economics

- Group theory in solid state physics (G. Kriza)
- Chapters from experimental high temperature plasma physics (G. Kocsis, T. Szepesi)
- Infrared and Raman spectroscopy (K. Kamarás)
- Interacting spin-systems in real materials (K. Penc)
- Introduction to fusion plasma physics. (S. Zoletnik, D. Dunai)
- Introduction to irreversible thermodynamics (P. Ván)
- Introduction to physics for chemical engineers (A. Csóré)
- Introduction to theoretical plasma physics (A. Bencze)
- Mechanics I.-II. (A. Virosztek)
- MHD in low dimensional systems (A. Bencze)
- Modeling higher level brain functions (M. Bányai, M.E. Gáspár, D.G. Nagy, Orbán)
- Modern solid state physics (A. Virosztek)
- Neutron and synchrotron radiation for condensed matter studies (L. Temleitner)
- Neutron physics (M. Markó)
- Nuclear fuel cycle (M. Fábián)
- Physics of low temperature plasmas (Z. Donkó)
- Quantum Optics (J. Asbóth and P. Domokos)
- Queing theory (A. Telcs)
- Spectroscopy and the structure of matter (K. Kamarás)
- Superconductivity (G. Kriza)

- Theoretical solid state physics (A. Virosztek)
- Theory of magnetism I.-II. (A. Virosztek)
- Variational methods in the basics laws of physics (T.S. Biró)

Semmelweis University, Budapest

- Learning and navigation (Z. Somogyári, Systems Neuroscience Summer School)
- Neocortex: from structure to function (L.Négyessy, Systems Neuroscience Summer School)
- Neuroinformatics (M. Bányai)

Óbuda University, Budapest

- Chemistry and physics of polymers (S. Pekker)

Pázmány Péter Catholic University

- Neoromorph movement control (J. Laczkó)

Subotica Tech - College of Applied Sciences (Serbia)

- Physics (F. Bazsó)

University of Debrecen

- Particle physics 1 and 2 (D. Horváth)
- Particle physics exercises (D. Horváth)
- Structure and experimental test of the standard model 1 and 2 (D. Horváth)

University of Pécs

- Building materials (A. Len)
- Control and regulation technology, (J. Laczkó)
- Control systems (J. Füzi)
- Digital Control (J. Füzi)
- Electronics (J. Füzi)
- Geometry and visualisation (J. Laczkó)
- Introduction to algebra and number theory (J. Laczkó)
- Statistical physics (K. Szlachányi)
- Theoretical mechanics (K. Szlachányi)
- Materials science (A. Len)
- Mechanics - dynamics (A Len)
- Neurobioinformatic programming (J. Laczkó)
- Non-destructive methods for building materials sttudy (A. Len)
- Numerical methods (P. Ádám)
- Open quantum systems (P. Ádám)
- Physics (A. Len)
- Probability theory (P. Ádám)
- Quantum information processing by quantum opticsl means (T. Kiss)
- Resonant light-matter interaction (P. Ádám)
- Theoretical physics III. (P. Ádám)

University of Szeged

- Applications of statistical physics (F. Iglói)
- Introduction to the physics of laser plasmas (I. Földes)
- Introduction to statistical physics (F. Iglói)
- Linear algebra for physicist (L. Fehér)
- Mathematical methods in physics I.-II. (L. Fehér)
- Statistical physics (F. Iglói)

University of Veterinary Medicine, Budapest

- Biophysics (Z. Szőkefalvi-Nagy, both in Hungarian and in English, two courses)

Budapest Semester in Cognitive Science

- Neural computation (M- Bányai)
- Statistical models of brain function (G. Orbán)
- Cognitive neuroscience (L. Négyessy)

Laboratory practices and seminars

Eötvös Loránd University, Budapest

- Advanced physics laboratory (M. Varga-Kófaragó, R. Vértesi)
- Differential equations I-II (T. Gombor)
- Electromagnetism II (M. Lájér)
- Experiments on liquid crystals (Á. Buka, N. Éber, P. Salamon)
- Graphical processors for scientific applications (D. Berényi and M.F. Nagy-Egri)
- Laboratory practice (T. Pusztai)
- Laboratory practice on neutron scattering (L. Almásy, A. Len, M. Fábrián, L. Rosta, T. Veres, Gy. Török)
- Magnetism (J. Balogh)
- Magnetohydrodynamic waves, part of the course “Advanced physics laboratory” (A. Opitz)
- Materials science in chemistry (L. Rosta)
- NMR and Cherenkov photometry, nuclear analytics laboratory (P. Pósfay)
- Particle and nuclear physics detectors laboratory (G. Hamar, D. Varga)
- Probability theory (M. Korniyik)
- Quantum mechanics A, (M. Lájér)
- Raman spectroscopy, part of the course Laboratory practice in biophysics (M. Veres)
- Solid state physics, materials science laboratory practice – NMR (M. Bokor)
- Stochastic processes (M. Korniyik)
- The theory of C++ programming (G. Biró)

Budapest University of Technology and Economics

- Engineering thermodynamics 2 (R. Kovács)
- Independent task I. (L. Bencs)
- Infrared and Raman spectroscopy (K. Kamarás)
- Laboratory practice (M.A. Kedves, B. Raczkevi)

- Laboratory practice on neutron scattering (L. Almásy, A. Len, M. Fábrián, L. Rosta, T. Veres, Gy. Török)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)
- SUMTRAIC Summer School (D. I. Réfy)
- Thermodynamics and Heat Transfer (R. Kovács)
- Thermal physics (P. Ván)

Semmelweis University, Budapest

- Education of medical technicians (Z. Horváth)

University of Pécs

- Control and regulation technology, (J. Laczkó and M. Mravcsik)
- Control systems (J. Füzi)
- Diagnostics – SEM laboratory practice (A. Len)
- Geometry and visualisation (J. Laczkó)
- Introduction to algebra and number theory (J. Laczkó)
- Linear algebra (I. Márton)
- Mathematical methods in physics IV. (P. Ádám)
- Mechanics – dynamics - seminar (A. Len)
- Neomorph movement control. (J. Laczkó and L. Botzheim)
- Probability theory (B. Nagy)

University of Szeged

- Calculus (G. Pusztai)
- Elements of complex and real functions and their applications (G. Pusztai)
- How to bring the Sun to Earth, the ITER experiment (D. I. Réfy)
- Laboratory for graduate BSc student (I. Földes)
- Linear algebra for physicists (L. Fehér)
- Mathematical methods in physics I. (L. Fehér)
- Physics practice for 3rd year BSc students (I. Földes)
- Statistical Physics (G. Roósz)
- Summer practice in the HILL laboratory, high intensity laser-plasma interactions (I. Földes)

Diploma works

Eötvös Loránd University, Budapest

- L. Ábrók, Study of electron-phonon Interaction in rare earth doped single crystals (BSc, supervisor: Zs. Kis)
- D. Datz: Near-field infrared nanospectroscopy (MSc, supervisor: Á. Pekker)
- B. Horváth: Numerical modeling of radiofrequency discharges (BSc, supervisor: A. Derzsi)
- G. Kasza, New results in hydrodynamically describing collisions in heavy-ion-physics (M.Sc, supervisor: T. Csörgő)
- D. Kálmán, Numerical modeling of granular materials (MSc, supervisor: E. Somfai)

- M. Máté, Simulation of strongly correlated systems with tensor network state methods (MSc, supervisors: Ö. Legeza, Sz. Szalay)
- I. Stark, Causality analysis and simulation of epileptic neural data (MSc, supervisor: Z. Somogyvári)
- K. Szabó, Space weather at Mars (BSc, supervisor: A. Opitz)
- Á. Takács: Investigation of the hadronization in the non-extensive statistical approach (Supervisors: G.G. Barnaföldi and G. Papp)
- L. Vanó, Experimental study of the effect of the resonant magnetic perturbation on the edge plasma (MSc, supervisor: D. Dunai)
- M. Vass: Experimental determination and numerical computation of electron transport coefficients in CO₂ (BSc, supervisor: Z. Donkó)
- TÁ. Vámi, Reconstruction of data recorded with the prototype of the new CMS pixel detector (BSc, Supervisor: V. Veszprémi)

Budapest University of Technology and Economics

- G. Balassa, Multiple scattering in high-energy heavy-ion collisions (Supervisor: Gy. Wolf)
- A. Biricz, Two dimensional turbulent electrolyte flow in periodic magnetic field, (BSc, supervisor: A. Bencze)
- N. Galbiczek, Two-component polytrope equation of state of neutron stars in relativistic model and the mass-radius correspondence (BSc, Supervisor: M. Vasúth)
- Á. Gera, Optimizing the mechanical structure of proportional detectors (BSc, supervisor: D. Varga)
- I. Gujás, Investigation of incorporation of Na, Cl and Cs ions into basalt rock (BSc, supervisor: M. Fábrián)
- A. Incze, Supporting real-time ultrafast video diagnostics development for plasma physics experiments, (BSc, supervisor: T. Szepesi)
- B. Móricz, Separating silicon carbide nanoparticles by size (MSc, supervisors: Ádám Gali, Dávid Beke)
- D.B. Nagy, Modeling the flow of non-spherical granular materials (MSc, supervisor: E. Somfai)
- G. Nyitrai, Mechanical analysis of a detector scanner (MSc, supervisor: D. Varga)
- D. Pataki, Theoretical investigation of solid-state single-photon emitters and quantum bits (BSc, supervisor: Ádám Gali)
- D. Unyi, Enhancing synthesis methods of hydroxylated silicon carbide nanocrystals (BSc, supervisor: Dávid Beke)
- J. Venczeli, Analysis of stimulus-dependence of neural answer-statistics in visual cortex (MSc, supervisor: M. Bányai)

Óbuda University, Budapest

- Á. Krolopp, Positioning the objective of the FiberScope nonlinear scanning microscope by the use of stepping motors and digital I/O signals (BSc, supervisor: R. Szipőcs)

Széchenyi István University, Győr

- T. Balázs, Development of ion current beam measurement system (MSc, supervisor: A. Németh)

University of Szeged

- K. Bali, Spatial diagnostics of high-intensity laser beams (BSc, supervisor: I. Földes)
- Á. F. Galzó, Derivation of the integrable systems with the Hamiltonian reduction (MSc, supervisor: L. Fehér)
- Gy. Kovács, Basics of the theory of classical integrable systems, (BSc, supervisor: G. Pusztai)
- B. Mitlasóczki, Scattering problems in quantum mechanics (BSc, supervisor: G. Pusztai)

University of Vienna (Austria)

- F. Gesser, Normative model of episodic memory (Supervisor: G. Orbán)

Ph.D students

Eötvös Loránd University, Budapest

- K. Bajnok, 5-7th century pottery production in Transdanubia (Supervisors L. Rosta, T. Vida and Gy. Szakmány)
- P. Balla, Optical properties of magnetic materials (Supervisor: K. Penc)
- D. Barta, Dispersion of gravitational waves in interstellar media (Supervisor: M. Vasúth)
- Gy. Bencédi, Identification of high-momentum particles with the ALICE detector at the LHC (Supervisor: P. Lévai)
- G. Bíró, Investigation of particle production in high-energy heavy-ion collisions (Supervisors: G.G. Barnaföldi and G. Papp)
- K.Z. Csukás, Initial value formulation of general relativity (Supervisor: I. Rácz)
- D. Datz, Chemical modification and near-field infrared microscopy of two-dimensional materials (Co-supervisor: Á. Pekker)
- A. Dombi, Quantum dynamics of atomic motion in multimode optical resonator fields (Supervisor P. Domokos)
- M. Dósa, Space weather at the inner planets (Supervisor: G. Erdős)
- T. Gombor, Holography and the gauge gravity duality, (supervisor: Z. Bajnok)
- G. Homa, Quantum information and irreversibility (Supervisor: L. Diósi)
- V.A. Isnaini, Magnetic and magnetotransport properties of nanoscale ferromagnetic heterostructures (Supervisor I. Bakonyi)
- Sz. Karsai, Investigation of the strongly-interacting matter in compact stars (Supervisors G.G. Barnaföldi and E. Forgács-Dajka)
- D. Kincses, Search for the critical point of the strong interaction (Supervisor: M. Csanád, co-supervisor: T. Csörgő)
- L. Kocsor, Preparation and characterization of nanocrystals doped by rare earth ions (Supervisors L. Péter and K. Sinkó).
- B. Korbuly, Phase-field modeling of complex polycrystalline patterns (Supervisor: L. Gránásy)
- G. Kónya, Many-body physics in cavity QED (Supervisor P. Domokos)
- M. Lájér, Investigation of the string field theory vertex and boundary extensions of holographic dualities (Supervisors: Z. Bajnok and L. Palla)
- P. Magyar, Response functions and collective excitations of strongly coupled plasmas (Supervisor: Z. Donkó)

- K. Márton, Ultrarelativistic hadron-nucleus collisions at the CERN SPS (Supervisors: A. László and D. Varga)
- M. Máté, Studying strongly correlated systems using quantum information theory and tensor network state methods, (Supervisors: Ö. Legeza, Sz. Szalay)
- D.G. Nagy, Normative model of episodic memory (Supervisor: G. Orbán)
- M.F. Nagy-Egri, Numerical solutions of Einstein equations (Supervisor: I. Rácz)
- É. Oláh, Particle physics teaching in secondary school (within the Teacher's PhD program, supervisors: D. Horváth and D. Varga)
- P. Pósfay, Functional renormalization group method for the description of compact stars (Supervisors: G.G. Barnaföldi and A. Jakovác)
- L. Rátkai, Dynamics of crystalline self-organization within continuum theory (Supervisor: T. Pusztai)
- D. Réfy, Beam emission spectroscopy measurements to support understanding of fusion plasma's H-mode (Supervisor: S. Zoletnik)
- O. Surányi, Study of the strong interaction with the CMS detector at the Large Hadron Collider (Supervisors: F. Siklér, G.I. Veres)
- Zs. Szendi, Hydrodynamical behavior of radiation fields (Supervisors: T.S. Biró and A. Jakovác)
- É. Tichy-Rács, Synthesis, crystallization and spectroscopic investigation of rare-earth alkali borate scintillator materials (Supervisor: K. Lengyel)
- A. Timár, Solar wind effects around a comet - investigations based on Rosetta measurements, (Supervisor: Z. Németh)
- B. Török, Interactions of memory systems (Supervisor: G. Orbán)
- P. Udvarhelyi, Ab initio study of solid state quantum bits for quantum application and sensing (Supervisor: Á. Gali)
- Á. Vida, Mechanical properties of high-entropy alloys (Supervisor: L.K. Varga)
- S. Zsurzsa, Preparation and properties of nanowires (Supervisor: I. Bakonyi)

Budapest University of Technology and Economics

- Cs. Araczkai, Vitrification and structural study of high level waste produced by spent fuel reprocessing (Supervisor: M. Fábrián)
- G. Balassa, Transport code development for heavy ion-simulations (Supervisor: Gy Wolf)
- D. Beke, Fabrication and characterization of silicon carbide nanoclusters (Supervisor: Á. Gali)
- A. Buzás, Investigation of L-H transitions in fusion plasmas (supervisor: A. Bencze)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor: G. Kocsis)
- D.R. Cserpán, Estimation of input signals based on multielectrode array measurements, (Supervisor: Z. Somogyvári)
- A. Csóré, Investigation of paramagnetic point defects in silicon carbide with quantum mechanical simulations (Supervisor: Á. Gali)
- Gy. Károlyházy, Controlled generation of point defects in silicon carbide (Supervisor: Á. Gali)
- R. Kovács, Thermodynamic conditions of wave propagation, dispersion and damping (Supervisor: P. Ván)
- M. Lampert, Turbulent and zonal flow studies in fusion plasmas (Supervisor: S. Zoletnik)

- D. Lucsányi, Diamond-based chronometric detectors and their application in the CERN LHC TOTEM experiment (Supervisor: T. Csörgő)
- Zs. Maksa, Formation of high-entropy alloys (Supervisor: L. Varga)
- D. Nagy, Rheology of non-spherical granular particles (Supervisor: E. Somfai)
- G. Németh, Near-field infrared spectroscopy on two-dimensional systems (supervisor: K. Kamarás)
- F. Podmaniczky, Dynamics of solidification, pattern and defect formation in phase-field crystal theories (Supervisor: L. Gránásy)
- B. Somogyi, First-principles study of silicon carbide nanocrystals (Supervisor: Á. Gali)
- A. Szakál, Investigation of application possibilities of atomic resolution neutron holography (Supervisor: L. Cser)
- T. Szarvas, Wave propagation and modelling of quantum optical processes in structured dielectrics (supervisor: Zs. Kis)
- G. Thiering, Theoretical study of point defects in diamond (Supervisor: Á. Gali)
- T. Veres, Investigation of thin layers for neutron optical applications by neutron reflectometry (Supervisors L. Cser and L. Bottyán)
- Á. Zlatniczki, Analysis of shocks in economical models (Supervisor: A. Telcs)

Óbuda University, Budapest

- D. Földes, Preparation and characterisation of new metal-organic frameworks (Supervisors: É. Kováts and S. Pekker)

Pázmány Péter Catholic University, Budapest

- B. Borbély: Kinematic measurement and analysis of human arm movements. (Supervisors: J. Laczkó and P. Szolgay)
- B. Jákly, Neuromorphic robotic control based on spatio-temporal motion analysis (Co-supervisor: L. Négyessy)

Semmelweis University, Budapest

- Zs. Benkő, Causality analysis of cortical dynamical interactions based on multichannel electrode measurements (Supervisor: Z. Somogyvári)
- N. Kiss: The effects of UV-light radiation on the physiological and pathological processes of the skin, on tumor development and its control mechanisms (Supervisors: N. Wikonkál and R. Szipőcs)
- E. Pálfi, Neural basis of the tactile perception in the somatosensory S1 area (Supervisor: L. Négyessy)

University of Physical Education, Budapest

- P. Katona, The effect of kinematic parameters on the electrical activity of thigh muscles during cycling. (Supervisor J. Laczkó)

Szent István University Gödöllő

- T. Baross, The application of the Hot Isostatic Pressing (HIP) welding for fusion reactor conditions (Supervisor: G. Veres)

University of Debrecen

- J. Karancsi, Search for new particles with the CMS detector at the LHC (Co-supervisor: V. Veszprémi)

University of Pécs

- M. Aladi, High harmonics generation from gases and clusters (Supervisor: I. Földes)
- B. Bódi, Optimization of high harmonic generation (Supervisor: P. Dombi)
- F. Bódog, Optimization of periodic one photon sources (Supervisor: P. Ádám)
- V. Csajbók, Inducing ultrafast currents in dielectrics (Supervisor: P. Dombi)
- D. Jakab: Exotic phases and quantum phase transitions in many-body systems (Co-supervisor Z. Zimborás)
- P. Körber: Proof of the effectiveness of water-repellent injection- methods for a subsequent masonry sealing, on the basis of experimental studies on bricks and mortar, using the scanning electron microscope in the ESEM - mode, as well as in comparison with conventional detection methods (Supervisors A. Len, E.Sz Zoltán)
- G. Mogyorósi, Preparation of nonclassical states with propagating waves (Supervisor: P. Ádám)
- E. Molnár, Preparation of nonclassical states by coherent superpositions (Supervisor: P. Ádám)
- B. Nagy, Controlling photoelectrons on the nanoscale with plasmonic nanoparticles (Supervisor: P. Dombi)
- M. Pocsai, Homogeneous rubidium plasma generation for novel particle accelerators (Supervisor: I. Barna)
- L.Á. Somlai, Study of rotating neutron stars (Supervisor M. Vasúth)
- T. Steffgen: Experimental studies building physics investigations of condensation water on plaster surfaces (Supervisors A. Len, A. Fülöp)
- Á. Varga, Quantum measurement with maximum information (Supervisor: P. Ádám, J. Bergou)
- K. Varga-Umbrich: Study of coherent excitation and ionization of alkali atoms by strong laser pulses. (Supervisor M.A. Kedves)
- A. Walter: Studies on the moisture-dependent spread of injection agents for reinforcing construction materials (Supervisors A. Len and A. Fülöp)
- L. Botzheim, Biological movement control and human-machine interface (Supervisor: J. Laczkó)
- M. Mravcsik, Biological movement control and human-machine interface (Supervisor: J. Laczkó)

Al-Farabi Kazakh National University (Kazakhstan)

- U.U. Almasbek, The synthesis of composite nanoparticles and properties of the nanostructures formed in dusty plasma in electric discharges of different gas mixtures. The synthesis and properties of nanomaterials in complex gas-discharge plasma (Co-supervisor: P. Hartmann)
- R. Masheeva, Computer modeling and investigation of dusty plasmas in external electric and magnetic fields (Co-supervisor: Z. Donkó)

University of Szeged

- M. Al-Lami: Investigation of neuron functions using stimulated Raman scattering (Supervisor M. Veres)

- T.F. Görbe, Integrable many-body systems of Calogero-Ruijsenaars type (Supervisor: L. Fehér)
- Zs. Kovács, Investigation of ions from the Coulomb explosion of clusters and from the TNSA acceleration of thin solid targets (Supervisor I. Földes)
- I. Rigó: Synthesis and characterization of plasmonic nanostructures for surface enhanced Raman spectroscopic applications (Supervisor: M. Veres)
- G. Roósz, Nonequilibrium relaxation in closed quantum systems (Supervisor: F. Iglói)
- H.M. Tóháti, Optical spectroscopy of carbon nanotube-based hybrid materials (Supervisor: K. Kamarás)

Dissertations

Ph.D

D. Beke, Fabrication and characterization of silicon carbide nanoclusters (Supervisor: A. Gali, BME)

A. Dombi, Bistability in the strong coupling regime of Cavity and Circuit Quantum Electrodynamics (Supervisor P. Domokos, ELTE)

R. Kovács, Heat conduction beyond Fourier's Law: theoretical predictions and experimental validation (Supervisor P. Ván, BME)

N. Laczai, Preparation and study of polycrystalline scintillator materials (Supervisor: L. Bencs, ELTE)

K. Lőrincz, Effects of weight gain and physical activity induced weight loss on dermal collagen and subcutaneous fat tissue investigated by in vivo nonlinear microscopy on a mouse model (Supervisor: N. Wikonkál and R. Szipőcs, SE)

I. Márton, Investigation of ultrafast photoemission and electron acceleration induced by ultrashort laser pulses. (Supervisor P. Dombi, PTE)

L. Oláh: Research and development of particle detectors for muon tomography and the CERN ALICE experiment (Supervisors: G.G. Barnaföldi and D. Varga)

G. Roósz: Non-equilibrium dynamics of one-dimensional isolated quantum systems (Supervisor: F. Iglói, SZTE)

B. Somogyi, First-principles study of silicon carbide nanocrystals (Supervisor: A. Gali, BME)

Zs. Steinczinger, Computer modelling investigations concerning the structure of liquid water: the issue of consistency between interaction potentials and measured diffraction data (Supervisor: P. Jóvári, ELTE)

B. Szabados, Investigation of molecular thin films by infrared spectroscopy (supervisor K. Kamarás, ELTE)

R. Ünneper, The ultrastructure and flexibility of thylakoid membranes in different photosynthetic organisms as revealed by small angle neutron scattering (Supervisors: L. Rosta and Gy. Garab, ELTE)

Memberships

- L. Almási — Editorial Board of New Frontiers in Chemistry Journal (Timisoara, Romania)
— CANAM Scientific Selection Panel at NPI Rez, Czech Republic
- 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 — Laser Physics Committee of HAS.
- K. Bajnok — Geochemical, Petrographical and Mineralogical Scientific Board of the Archaeological Commission of the HAS
- Z. Bajnok — Particle Physics Committee of the HAS.
— Coordinator of the Gatis+ Network
- I. Bakonyi — Solid State Physics Committee of the HAS (2011-2020)
— Editorial Advisory Board (2005-), Journal of Materials Science and Technology (Bulgaria, Sofia)
— European Board (2006-), European Academy of Surface Technology (EAST)
— EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
— Management Committee, COST MP 1407 action (2015-2019)
- J. Balogh — Int. Board on the Application of the Mössbauer Effect (IBAME), 2012-2017
- J. Balog — Particle Physics Committee of the HAS
— Chairman of the RMI Scientific Council
- G.G. Barnaföldi — 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
— European Physical Society (EPS)
— Hungarian representative, rapporteur, WG2 QCD Topic Leader of the New Compstar COST MP1304, THOR CA15213, PHAROS CA16214 actions
— IAC member of the ISOTDAQ International School on Trigger and Data Acquisition
— IAC member of the International Conference series of the High-pT Physics for the RHIC/LHC Era
— General assembly of the HAS
— Wigner Intellectual Property Council member

- D. Barta — Virgo Scientific Collaboration
- F. Bacsó — Programme Committee, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
- I. Bányász — Program Committee of Photoptics 2017 and Photoptics 2018 Conferences
- L. Bencs — Editorial Board of International Scholarly Research Notices (Hindawi)
— Work Committee for Environmental Chemistry of HAS
- T.S. Biró — Chairman of the Zimányi Foundation for Physics
— Editor-in-Chief (theory) (2013-) of the European Physical Journal A: Hadrons and Nuclei (Springer)
— Editor of the Wigner Yearbook 2016
— Physics PhD School, TU Budapest (BME)
— Physics PhD School, Eötvös University (ELTE) Budapest
— External member of the ELTE TTK PhD Council
— Nuclear Physics Committee at the HAS
— LOC member of the Zimányi School 2016
— Presidential Publication Committee of the HAS
— Wigner Scientific Council (WTT)
— Natural Sciences Committee of the HAS, Chairman of the Physics 2 section
— Member of the Academia Europaea
- L. Bottyán — Heinz Maier-Leibnitz Zentrum (MLZ) Review Panel Magnetism and Spectroscopy, Elastic Application
- G. Böhm — 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 HAS
- G. Cseh — Hungarian Nuclear Society
- L. Csernai — Editorial Board, International Journal of Modern Physics E - Nuclear Physics (World Scientific)
— Member of the Academia Europaea
— Member, Academia Europaea, Council
— Member of the Norwegian Scientific Academy
— Member of the Norwegian Academy for Technological Sciences
— External Member of HAS (2004)
- T. Csörgő — Chairman, International Advisory Committee, Zimányi Schools on Relativistic Heavy Ion Physics (2017-)
— Member of the Academia Europaea
— Section Committee, Physics and Engineering Sciences, Academia Europaea (2013-)

- Physics PhD School, ELTE, Budapest
 - Institutional Board, PHENIX Experiment, BNL
 - Executive Council, TOTEM Experiment, CERN LHC
 - Editorial Board, TOTEM Experiment, CERN LHC
 - CERN LHC Resource Review Board
 - International Advisory Committee, WPCF 2013 Conference, Acireale, Italy
 - International Advisory Committee, ISMD 2013 Conference, Chicago, USA
 - Principal Investigator, PHENIX - Hungary sub-collaboration (2003-2013)
 - Principal Investigator, TOTEM - Hungary sub-collaboration
 - Editorial Board, TOTEM experiment at CERN LHC
 - Section Committee for Physics and Engineering Sciences, Academia Europaea (London)
 - Professorial Council, Eszterházy Károly University
 - IAC, Workshops on Particle Correlations and Femtoscopy (WPCF series)
- A. Czitrovsky
- Chairman of the Laser Physics Committee of HAS
 - President of the Hungarian Aerosol Society
 - Chairman of the Hungarian EOS Chapter
 - Chairman of the Optical Chapter of OPAKFI
 - ELI-ALPS Scientific Advisory Committee
 - Board of International Aerosol Association
 - Board of European Aerosol Assembly
 - Gesellschaft für Aerosolforschung
 - International Junge Award Committee
 - Editorial Board of Fizikai Szemle
 - Physics PhD School, Pécs University
- L. Diósi
- Editorial Board Member of International Journal of Quantum Foundations (electronic, China)
 - Management Committee of COST Action Quantum Technologies in Space CA15220
 - Foundational Questions Institute FQXi
 - Management Committee of COST Action MP1209 Thermodynamics in the Quantum Regime
- P. Dombi
- Committee of Laser Physics of the HAS
 - International Conference on Photonic, Electronic and Atomic Collisions, ICPEAC Program Committee
 - Conference on Lasers and Electro-Optics/Europe 2017, Program Committee
 - Journal Editor at Scientific Reports (Nature Publishing)
 - COST network “Nanospectroscopy”, MC member
 - Optical Society of America, senior member
 - SPIE (Photonics Society), USA, senior member

- P. Domokos — Science and Engineering Board of the National Research, Development and Innovation Office
 — Doctoral Council of the HAS
 — Bolyai Scholarship Advisory Board of HAS
 — Management Committee of COST Action MP1403 Nanoscale Quantum Optics
 — Management Committee of COST Action CA16221 Quantum Technologies with Ultra-Cold Atoms
 — Corresponding member of HAS (2013)
- Z. Donkó — International Scientific Committee, Conference series “Symposium of the Phenomena in Ionized Gases”, from 2006
 — International Advisory Board, Conference series “Strongly Coupled Coulomb Systems”, 2007-
 — International Scientific Committee, Conference series “Symposium on Application of Plasma Processes,” from 2008
 — Editorial Board, IOP Plasma Sources Science and Technology
- G. Dzsotjan — Committee of Laser Physics of the HAS
 — Doctoral Council of the HAS
- M.F. Nagy-Egri — Virgo Scientific Collaboration
- G. Erdős — National Representative of COSPAR
 — Deputy Chairman of the Committee on Astronomy and Space Physics of HAS
- N. Éber — Editorial Board member of The Open Crystallography Journal (Bentham Open)
 — Editorial Board member of the Journal of Research in Physics (DeGruyter)
 — COST Action IC1208 MC member
- P. Érdi — Board of Governors of the International Neural Network Society
 — International Neural Network Society, senior member
 — IEEE Computational Intelligence Society University Curriculum Subcommittee
 — Editor-in-Chief Cognitive Systems Research
 — Associate Editor of BioSystems
 — Editorial and Programme Advisory Board of the Springer Complexity publishing program
- G. Faigel — XFEL In-kind Review Committee
 — XFEL SAC
 — Member of the HAS
- M. Fábrián — ASTM International, Committee C26 on Nuclear Fuel Cycle
- L. Fehér — International editorial board of Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)

- International editorial board of Journal of Nonlinear Mathematical Physics (World Scientific)
- P. Forgács
 - Particle Physics Committee of the HAS.
 - Doctoral Council, Physics Section of the HAS.
 - Doctoral Council, Doctoral School in Physics, Loránd Eötvös University
- I. Földes
 - EPS
 - User Representative of LASERLAB Europe
 - Access Board of LASERLAB Europe
 - Management Committee, COST MP1208 action
- J. Füzi
 - International Scientific Advisory Council of BNC (Budapest Neutron Centre)
 - Editorial Boardr, Pollack Periodica
 - International DENIM Committee
- Á. Gali
 - Technical Program Committee (2011-), ICSCRM - International Conference on Silicon Carbide and Related Materials
 - Technical Program Committee (2011-), ECSCRM - European Conference on Silicon Carbide and Related Materials
 - Symposium Organiser Board, Symposium ED1: Silicon-Carbide, Diamond and Related Materials for Quantum Technologies, MRS Spring Meeting 2017, Phoenix, USA, 17-21 April, 2017
 - Symposium Organiser Board, Symposium T: Silicon, Germanium, Diamond and Carbon nanostructures and their nanocomposites with other materials. E-MRS Fall Meeting 2017 (Warsaw, Poland, Sep. 18-21, 2017)
- L. Gránásy
 - ESA Topical Team “Solidification of Containerless Undercooled Melts”, SOL – EML
 - The Minerals, Metals, and Materials Society, USA
 - Solid State Physics Committee of HAS
 - Mathematics and Science Committee of AKT
 - International Scientific Committee: SP17: 6th Decennial International Conference on Solidification Processing
 - Member of the Academia Europaea
- D. Horváth
 - Editorial Board of “Fizikai Szemle”
- F. Iglói
 - Science Editor – Europhysics News
 - Editorial Board, European Physical Journal B
 - Statistical Physics Committee of the HAS.
 - Editorial Board of ‘Fizikai Szemle’
 - International Advisory Board of the Middle European Cooperation in Statistical Physics (MECO)
 - Scientific Advisory Committee of the European Physical Journal
- J. Janszky
 - Laser Physics Committee of HAS
 - Member of the HAS

- K. Kamarás — Editorial Board, European Physical Journal B
 — Board of the Condensed Matter Division of the European Physical Society
 — Member of the HAS (2016)
 — Member of the Academia Europaea
- K. Kecskeméty — Committee on Astronomy and Space Physics of HAS
- Z. Kis — Editorial Board of the Physical Review A
- T. Kiss — Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP)
 — COST Action MP1006, MC member
- G. Kocsis — Nukleon Editorial Board
 — EUROfusion JET CDT2 Project Board
 — EUROfusion S1 Project Board
- L. Kovács — Hungarian National Committee, International Union of Crystallography
 — International Advisory Committee of EURODIM and ICDIM Conference series
 — Program Committee of the OMEE Conference series
- P. Kovács — General Assembly of the HAS
- G. Kriza — Solid State Physics Committee of HAS
 — Ph.D. School of Physics, BME
 — Bolyai Fellowship Board, HAS
 — Domus Hungarica Scientiarum et Artium Fellowship Board of the HAS
- N. Kroó — Chairman of the Governing Council of the Hungarian Research Infrastructure Program
 — Chairman of the Rátság High School Prize
 — Chairman of the Research Infrastructure Expert Group of ERA (EC)
 — Chairman of Dennis Gabor International Prize Committee
 — Hungarian UNESCO Committee
 — High Level Expert Group on Digital Libraries and Scientific Publications (EC)
 — Advisory Group on ESOF
 — ELI_ALPS Scientific Advisory Committee
 — Editorial Board, Laser Physics Letters (IOP Science)
 — Member (former Chairman) of the Section of Physical and Engineering Sciences of Academia Europaea
 — Member of the HAS
- K. Kutasi — International Scientific Committee, Conference series “International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment”
 — International Scientific Committee, Conference series of “Central European Symposium on Plasma Chemistry”

- International Scientific Committee, Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases"
- J. Laczkó
 - Society for Neuroscience
 - International Society for Motor Control
- A. László
 - NA61 Collaboration Board
- Ö. Legeza
 - Statistical Physics Scientific Committee, HAS
 - Young Researcher Committee, HAS
 - Secretary of the Statistical Physics Section of Roland Eötvös Physical Society
- P. Lévai
 - Physics PhD. School, ELTE
 - Hungarian CERN Committee
 - CERN Council
 - ESFRI (European Strategy Forum on Research Infrastructure)
 - Committee on Research Infrastructure.
 - Committee on Nuclear Physics.
 - Committee on Particle Physics.
 - International Association of Physics Students, honorary member
 - Member of the Academia Europaea
 - Member of the HAS
- B. Lukács
 - Astronomical and Space Research Committee of the HAS.
- F. Mezei
 - Chairman of the Physical Society Publication Committee
 - American Physical Society
 - 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
 - Member of the Academia Europaea, London
 - Member of the HAS
- A. Nagy
 - Co-chairman of the Working Group Instrumentation in European Aerosol Assembly
- D.L. Nagy
 - Common Coordination Committee of the HAS and the JINR, Dubna, HAS Representative
 - Joint Institute for Nuclear Research, Dubna, Scientific Council
 - Program Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research, Dubna
 - European XFEL, Council
 - FP7 Research Infrastructures Programme Committee, expert
 - Chairman of the International Board of the Applications of the Mössbauer Effect
 - European Synchrotron Radiation Facility, Consortium CENTRALSYNC, Steering Committee

- Hyperfine Interactions, Editorial Board
- International Union of Pure and Applied Physics (IUPAP), Commission on Physics for Development (C13)
- European Physical Society, Council
- European Strategy Forum on Research Infrastructures, Working Group on Regional Issues
- European Science Foundation, Organisation Forum on Research Infrastructures

- J.Z. Nagy — MANT (Hungarian Astronautical Society)
- Z. Németh — Materials Science Work Committee of the HAS
- A. Opitz — Guest editor of Journal of Space Weather and Space Climate: topical issue on 'Planetary Space Weather'
- K. Penc — Solid State Physics Committee of the HAS
- L. Péter — Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
- Council of Graduate School of Chemistry, ELTE (2009-)
- Editor for Electrochemistry (Open Chemistry; formerly Central European Journal of Chemistry; DeGruyter, 2009-)
- Key Reader (Metallurgical and Materials Transactions E, Springer, 2014-)
- COST MP 1407 action, MC and training course coordinator, (2015-2019)
- K. Polgár — Hungarian Advisor to the International Organization for Crystal Growth
- I. Rácz — International Society for General Relativity and Gravitation
- L. Rosta — European Neutron Scattering Association
- European Spallation Source, Steering Committee
- Hungarian ESS Committee
- F. Siklér — Institutional representative at the CMS Collaboration Board
- CMS Publication Committee, Heavy Ions editorial board
- CMS Management Board, as adviser to the Spokesman
- Particle Physics Scientific Committee of the HAS; Representative at the general assembly of the HAS; Member of the Nomination Committee of the HAS
- LHC Research Review Board (LHC RRB), Hungarian delegate
- E. Somfai — IOP
- American Physics Society
- L. Somlai — Virgo Scientific Collaboration
- J. Sólyom — President of the Roland Eötvös Physical Society
- Member of the HAS
- A. Sütő — Statistical Physics Committee of the HAS.

- Zs. Sörlei — Committee of Laser Physics of the HAS
- L. Szabados — Scientific advisory panel of the journal Classical and Quantum Gravity
— Particle Physics Committee of the HAS.
- S. Szalai — Hungarian Space Research Council
— ARTEMIS-H steering
— Rosetta Lander steering
- V. Szalay — CMST COST Action CM1405, MC member
- Zs. Szaller — Thermoanalytical Committee of HAS
- K. Szegő — Committee on Astronomy and Space Physics of HAS
— IAA
— ERC Starting Grant Evaluation Panel
- E. Szilágyi — International Committee of the Conference series of Ion Beam Analysis
— Committee on Solid State Physics, HAS
- R. Szipócs — Optical Society of America
- Z. Szőkefalvi-Nagy — Editorial Board, International Journal of PIXE (World Scientific)
— International Honorary Committee, PIXE
— Committee on Atomic and Molecular Physics and Spectroscopy, HAS
- A. Telcs — Editor for Periodica Polytechnica (BME)
— Editor for Open Mathematics (De Gruyter)
- Gy. Török — IAEA JRC-1575
— JRC-NET
- B. Újfalussy — Secretary of the Materials Science Group of Roland Eötvös Physical society
— Executive Board of the Roland Eötvös Physical Society
— Secretary of the HAS Solid State Physics Committee
- G. Vankó — Secretary of the Hungarian Synchrotron Committee, HAS
— EU COST Action MP1203 Advanced X-ray spatial and temporal metrology, MC member
- D. Varga — Particle Physics Scientific Committee of the HAS
- L.K. Varga — International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM)
— Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)
- S.Varró — Committee of Laser Physics of the Hungarian Academy of Sciences
— Committee of the Quantumelectronics Division of the Roland Eötvös Physical Society
- M. Vasúth — Virgo Scientific Collaboration
— Virgo Steering Committee
— NewCompStar EU COST MP1304 action, MC member

- P. Ván — Editorial board of Continuum Mechanics and Thermodynamics (Springer)
 — Editorial Advisory Board, Journal of Non-Equilibrium Thermodynamics (De Gruyter)
 — Secretary of the Society for the Unity of Science and Technology
 — International Association of Physics Students, honorary member
 — International Advisory Board, Zimányi Winter School series
 — International Advisory Board, Joint European Thermodynamics Conference series
 — Corresponding member of the Accademia Peloritana dei Pericolanti (Classe di Scienze Fisiche, Matematiche e Naturali)
- T. Vámi — CMS Young Scientist Comitee, vice-president
- P. Vecsernyés — Particle Physics Committee of the HAS.
- G. Veres — Governing Board, European Joint Undertaking for ITER and the development of Fusion Energy
- V. Veszprémi — CMS Phase 1 Pixel Upgrade Management Board
 — CMS Phase 2 Tracker Upgrade Management Board
 — CMS Tracker Institutional Board
 — CMS Tracker Management Board (ex officio)
- I. Vincze — Doctoral Council of the HAS
 — Member of the HAS
- A. Virosztek — Editorial Board of Advances in Condensed Matter Physics (Hindawi)
 — Chairman of the Solid State Physics Committee of the HAS
- G. Vizi — Board member of the MANT (Hungarian Astronautical Society)
- Gy. Wolf — President of the International Theoretical Physics Workshop (NEFIM), Hungary
 — President of the of the Nuclear Physics Board, Roland Eötvös Physical Society
 — Leader of the Public Awareness of Nuclear Science (PANS)
 — Secretary of the Nuclear Physics Board of the HAS
 — Hungarian representative of the NuPECC EU FP7 HadronPhysics2, HadronPhysics3, HadronPhysicsHorizon, GSI FAIR, CBM, JRA Thuric, Toric, and Meson-Net projects.
 — Representative in Physics Department of the HAS
 — Nuclotron-based Ion Collider Facility (NICA)
- Z. Zimborás — Editorial Board of Frontiers in Quantum Computing (Nature PG)
- S. Zoletnik — Eurofusion General Assembly
 — Eurofusion General Assembly Bureau
 — Eurofusion Ad Hoc Group on JET technical status
 — International Board of Advisors of the Institute of Plasma Physics, Prague

— EURATOM Scientific and Technical Committee (STC)

Conferences

Fusion Plasma Physics Winter School, Budapest, 10-12 February 2017 (about 100 students)

A fusion winter school was organized by the BES research group in collaboration with the Hungarian Association of Physics Students and the Eötvös Loránd University in February 2017. Lectures were given on the history of fusion research, the basic plasma physics phenomena and fusion technology. We had the privilege to invite Hartmut Zohm, who had received the Hannes Alfvén Prize of the European Physical Society in 2016 to give a talk on the future of fusion reactors. <http://tisk.mafihe.hu/2017-fuzios-plazmafizika-teli-iskola/>

Workshops Lithium niobate nanoarchitectures: From quantum level to cross-disciplinary applications” 25 February and 27 May 2017 (5-5 participants)

The workshops were organized as preparatory meetings for the submission of the LN2020 proposal (Lithium niobate nanoarchitectures: From quantum level to cross-disciplinary applications) to the EU COST program. Both workshops were organized by L. Kovács

E-MINDS Training course event of the COST MP 1407 program, Schwäbisch Gmünd, Germany, 2-6 April 2017 (68 students)

The e-MINDS (Electrochemical processing methodologies and corrosion protection for device and systems miniaturization) training course is a unique training opportunity for young researchers from across Europe to get a complex insight into the interdisciplinary field comprising galvanotechnology, electrochemistry, corrosion and nanotechnology and materials science. The course event was organized to highlight 3 major topics: (i) Codeposition, (ii) Structural and morphological studies related to deposition, and (iii) Laboratory techniques in electrodeposition research. The main organizer was L. Péter who serves the COST MP 1407 program as the training course coordinator.

Symposium ED1 Silicon-Carbide, Diamond and Related Materials for Quantum Technologies, MRS Spring Meeting 2017, Phoenix, USA, 17-21 April, 2017 (~100 attendees)

At ED1 symposium; MRS Meetings serve as an international stage for the examination and dissemination of current and emerging materials research. This symposium aims to address recent progress in solid state quantum technologies that are driven by materials preparation and the associated color center or defect characterization. The topics that will be addressed will include defect formation and characterization including scenarios on managing the effects of level crossing when appropriate, quantum photonics, entanglement, and addressing/read-out of quantum states. External materials issues that affect applications are also of interest. Ádám Gali was one of the four symposium organizers.

21st Topical Meeting of the International Society of Electrochemistry (ISE): Photoelectrochemistry of semiconductors at the nanoscale: from fundamental aspects to practical applications, Szeged, Hungary, 23-26 April 2017 (~150 participants)

The ISE topical meetings make a platform for scientists worldwide to gather for discussing a particular field of electrochemistry. The organization of the meeting was preceded by a 3-year-long preparation with the participation of L. Péter as the former national representative of Hungary in the ISE. L. Péter served as the co-chairman of the meeting.

8th Hungarian Plasma Physics and Fusion Technology Workshop, Esztergom, 26-28 April 2017 (~50 participants)

This workshop was organized as the usual biannual meeting of the Hungarian high temperature plasma physics physicists and engineers, providing an excellent forum for exchanging information between Hungarian researchers and their international colleagues working in different fields. A panel of four respected European researchers is invited to participate in the workshop, allowing them to evaluate the results of the Hungarian research organization. The three-days meeting provides an excellent basis for the next two year's research aims.

5th Work Meeting on Quantum Optics & Information, MTA PAB, Pécs, Hungary, 28-29 April 2017 (50 participants)

11th Central European Training School on Neutron Techniques, Budapest, Hungary, 8-12 May 2017 (29 participants)

The 11th Central European Training School on Neutron Techniques was held by the Budapest Neutron Centre (consortium of MTA Wigner Research Centre for Physics and MTA Centre for Energy Research). The primary aim of the school was to provide insight into the neutron beam based structure analysis of the materials on theoretical, and also practical level.

The 10 hours of theoretical training was given, besides BNC staff, by the researchers from ILL-France, ESS-Sweden, JINR-Russia, and HZB-Berlin. Employing the BNC neutron facilities 15 hours of practical training were conducted focusing on scattering techniques, such as small angle neutron scattering, neutron diffraction, neutron reflectometry, prompt gamma activation analysis and neutron radiography.

On the last day of the school, the students presented their own research via short, three minutes talks and posters as well. In the end, they received their well-earned certificates. Special awards were given for the most active participants.

Joint European Thermodynamical Conference 2017 – Equilibrium and non-equilibrium thermodynamics of planar and curved interfaces, BME, Budapest, Hungary, 21-25 May 2017 (100 participants)

Methods and concepts of equilibrium and non-equilibrium thermodynamics appear in various areas of physics, engineering, sciences and humanities. This wide range of applicability is a source of inspiration, but also a cause of separation and divergence. The aim of this conference is to improve the interaction and pull together the various application areas and theoretical branches in order to develop a more powerful and more applicable discipline. JETC is a biannual conference series, this edition was co-organized by Wigner and BME.

Low-x 2017 25th Low-x Meeting, Bisceglie, Puglia, Italy, 12-18 June 2017 (61 participants)

T. Csörgő: member, IAC

The Low-x Meeting series is the annual workshop that reviews recent developments in the field of soft QCD, diffraction and elastic scattering. Our role in the organization was limited to the usual roles of members of the International Advisory Committee: discussions on the selection of section conveners, invited talks and future organizers. Note that we organized

the Low-x 2016 meeting in Gyöngyös, Hungary, that collected the merits for becoming members of the IAC of Low-x conference series.

WPCF 2017 12th Workshop on Particle Correlations and Femtoscopy, Amsterdam, The Netherlands, 12-16 June 2017 (85 participants, 68 invited talks)

T. Csörgő: member, IAC and also a Section Convener

This meeting is the annual workshop that reviews recent developments in the field of particle correlations and femtoscopy. Our contribution to the organization of this event was to participate in the selection of section conveners and actually volunteering to organize one of the sections, corresponding to invitation and scheduling about 10 speakers, together with prof. G. Verde (INFN, Catania, Italy) on the topic of Femtoscopy and correlation studies in A+A, p+p, p+A and e+e- collisions at relativistic, intermediate and low energies. We have also played an active role in selecting the organizers and locations for WPCF 2018 (Cracow, Poland) and WPCF 2019 (Dubna, Russia).

Workshop 7th GPU Day, The Future of Many-Core Computing in Science, Wigner RCP, Budapest, Hungary, 22-23 June 2017 (80 participants)

The “GPU Day” series has been organized by the Wigner GPU Laboratory for the 7th times in this year. The two-day workshop interconnects scientists, programmers, and parallel-computing experts from all over the world. Several commercial companies visited the event from Hungary and abroad.

Hungarian – Chinese Symposium on Neutron Scattering, Budapest, Hungary, 28-29 August 2017 (25 participants)

Organized by the Department of Neutron Spectroscopy of Wigner RCP and the Key Laboratory of Neutron Physics of the Institute of Nuclear Physics and Chemistry, China. The workshop was followed by discussions on the future cooperation between the two institutes and research groups.

EUROPLANET NA1 Networking (WP12) Annual Meeting, Budapest, 29-31 August (15 participants).

The Europlanet identity has emerged from collaborations established between European scientists involved in the Cassini-Huygens space mission. The current EU H2020 Europlanet Research Infrastructure (EPN2020-RI) builds on this strong heritage. The Work Package we lead is „Innovation through Science Networking”. During the Annual Meeting the WP tasks were reviewed: dissemination of EPN2020-RI’s activities to the science community, organising meetings, workshops and personnel exchanges to strengthen the community, and setting the strategy and goals for planetary science in Europe for decades to come.

International workshop on topological properties in quantum magnets, Budapest, Hungary, 30 August – 1 September 2017 (40 participants)

Academia Europaea and ALLEA Annual Conference 2017, Budapest: Inaugural presentations by new members of Academia Europaea from Section B1-3: Physics and Engineering Sciences, 4-6 September 2017 (39 participants)

T. Csörgő: Co-convener and Local Organizer, A. Ster, member of LOC

Organizing inaugural presentations by new members of Academia Europaea was initiated by T. Csörgő, based on his previous positive experiences. We hope that based on this success the Inaugural Presentations will become a new meeting series related to the annual conferences of Academia Europaea. The four new or recent Hungarian members of AE presented a written contribution of their inaugural presentations in the journal of the Roland Eötvös Physical Society, "Fizikai Szemle".

Neural sampling: computations and experimental predictions. Satellite workshop of Bernstein Conference, Gottingen Germany, 12-13 September 2017

The workshop addressed a burning issue in systems neuroscience: how probabilistic computations can be achieved in the brain. The conference featured a very diverse presenter list, including New York University (NY, US), ETH, Zurich (Schweiz), Albert Einstein College of Medicine (NY, US), University of Cambridge (UK), TU Graz, (Austria), University of Warwick (UK), University of Rochester (NY, US), MTA Wigner RCP (Budapest), CEU (Budapest). Gergő Orbán was co-organizer of the workshop.

ICOMP 2017 14th International Conference on Multiphoton Processes, Budapest, Hungary, 24-27 September 2017 (160 participants)

The first conference of the triannual ICOMP series was held in Rochester in 1977. Budapest already hosted ICOMP for the second time, after having been the venue of the conference in 1980. As professors Yamanouchi and Midorikawa have formulated the importance of the ICOMP series recently, "This conference series has been essential in deepening of our understanding of multiphoton phenomena. Indeed, it is no exaggeration to say that the scientific basis of intense laser science in recent years has been established through the exchanges of ideas fostered by the ICOMP conferences." In 2017, ICOMP had the honour of welcoming Ferenc Krausz and Paul Corkum as keynote speakers, two of the founding fathers of attosecond science. The conference was opened by Norbert Kroó, chairman of the second ICOMP in 1980.

Conference High-pT Physics for the RHIC and LHC Era, Bergen, Norway, 2-5 October 2017 (60 participants)

The purpose of this workshop was to offer an opportunity for both experimentalists and theorists to get together and discuss the latest experimental results from RHIC and LHC and the latest theoretical developments. Emphasis was on discussion over a broad scope: high pT physics, jets, photons, correlations, hard scattering and hard probe phenomena. The meeting followed p+A, p+p runs at LHC in 2016 and 2017 which complement the larger statistics, we also discussed the 5 TeV LHC data. GG. Barnaföldi was a member of the International Organizing Committee.

Conference: New perspectives on Neutron Star Interiors, ICTP Trento, Italy, 9-13 October 2017 (40 participants)

This workshop will bring together high-energy and nuclear theorists, observational astronomers and gravitational physicists. We aim to overview new theoretical ideas and proposed or soon-to-be launched future facilities, bringing together results from ongoing

electromagnetic and gravitational observations and related theoretical neutron star equations of state. G.G. Barnaföldi was one of the three organizers.

NINMACH 2nd Conference on Neutron Imaging and Neutron Methods in Archaeology and Cultural Heritage, Budapest, Hungary, 11-13 October 2017 (62 participants)

The mission of the NINMACH conference series is to address neutron scientists, as well as archaeologists and conservators, by creating a stimulating environment to exchange ideas and to make a bridge between them. In 2017, the Hungarian neutron and cultural heritage communities received the honour to organize the second NINMACH. The event was organized by the Budapest Neutron Centre (BNC), the consortium of Centre for Energy Research and Wigner Research Centre for Physics, Hungarian Academy of Sciences, in cooperation with the International Atomic Energy Agency (IAEA).

Nanoscale Quantum Optics – Early Stage Researcher Workshop of the COST Action MP1403, Budapest, 26-27 October 2017 (~40 participants)

Local organizer: Department of Quantum Optics and Quantum Information; website: nqo-esr-2017.sciencesconf.org

3rd Day of Femtoscopy, Gyöngyös, 2. November 2017 (Eszterházy Károly University – ELTE - Wigner RCP of the HAS. joint organization, 18 lectures)

T. Csörgő, organizer and Chairman

This meeting collects experts in Hungary who are active in the field of femtoscopy and provides also an international environment by including talks from our direct collaborators with whom we are working on the completion of some research papers.

Symposium in Memoriam László Cser, Budapest, Hungary, 9 November 2017

An international symposium dedicated to the memory of our colleague, László Cser, was organized at the Budapest Research Centre. Co-workers from France, Russia, Austria, Hungary, friends, and colleagues, former and actual PhD students held lectures to honor his life-long scientific activity.

Workshop on the industrial use of neutrons, Budapest, Hungary, 10 November 2017

An international workshop on the industrial use of neutrons with the participation of several European experts in neutron science and the representatives of the automotive industry was held on the 10th of November, 2017. The objective of the workshop was to make a new step in the collaboration between the science and industry, to understand better the demands and needs of the industrial sector towards the scientists, and to present the different possibilities in the field of neutron scattering and imaging as potential development resource for the industry.

Conference Zimányi-THOR Winter School '17: 17th Zimányi Winter School on Heavy Ion Physics, Budapest, Hungary, 4-8 December 2017 (100 participants)

This traditional one-week international winter school used to be organized jointly between the Eötvös University and the Wigner RCP dedicated for József Zimányi, the founder-father of the

Hungarian High-energy Heavy-ion school. In this year we have organized this event for the 17th time, providing an excited platform for discussion between students and world-class experts of the high-energy heavy-ion collisions both from theoretical and experimental sides. This year the event was supported by the THOR COST action.

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 accommodation costs in Budapest for the invited speakers.

The concept of this series is to offer to our researchers a possibility to meet colleagues from external institutions who work on hot topics and able to present their favorite research to a wide audience of physicists, working both in experiment and theory in fields ranging from high energy particle physics via nuclear and plasma physics to material and life science related problems. We restrict our invitations in number to a few per semiannual blocks.

Wigner Colloquia in 2017

<https://indico.kfki.hu/category/42/>

28-03-2017	Simon Ruijsenaars, "Sine-Gordon field theory vs relativistic Calogero-Moser N-particle systems: an overview"
04-04-2017	Stefan Thurner, "Complexity: physics beyond physics"
30-05-2017	Constantino Tsallis, "Nonadditive entropy: small price to satisfy thermodynamics -- Theory and experiments"
20-06-2017	Joachim Krenn, "Probing plasmons with photons and electrons"
05-09-2017	Hans-Jörg Kull, "Quantum plasma dynamics"
10-10-2017	Vladimir Kekelidze, "Challenges of the NICA project at JINR"

Seminars

Weekly meetings of the Budapest and Debrecen Compact Muon Solenoid (CMS) groups:
<http://www.grid.kfki.hu/twiki/bin/view/CMS/WeeklyBudapestDebrecenMeetings>

Talks for the annual Zimányi School:
<https://indico.cern.ch/event/464154/other-view>

Wigner RCP RMI Seminars

Theoretical physics seminars
<http://indico.kfki.hu/category/28/>

20-01-2017	E. Elsen (Deputy Director General, CERN): The High Luminosity Phase of the LHC – Scientific and Computing Challenges
27-01-2017	M. Jan Homor (ELTE): Thermalisation properties of various field theories
17-02-2017	A. Tilloy (Max Planck Institute of Quantum Optics, Garching): Relativistic state vector collapse as an interpretation of QFT
24-02-2017	G. Etesi (BME): Strong cosmic censor hypothesis and four dimensional exotic differentiable structures
17-03-2017	P.G. LeFloch (University of Paris 6 and CNRS): The nonlinear stability of Minkowski spacetime for self-gravitating massive fields
24-03-2017	Dr. M. Scholtz (Charles University, Prague): Meissner effect for black holes
13-04-2017	L. Dobos (ELTE): Concordance cosmology without dark energy
28-04-2017	G. Etesi (BME): Generic counter-example for strong cosmic censor hypothesis ---technical details
05-05-2017	M. Oszmaniec (ICFO, Barcelona): Universal extensions of restricted classes of quantum operations - a group theoretical approach
12-05-2017	A. Telcs (BME-Wigner): In seek of causality
19-05-2017	N. Dadhich (IUCAA, Pune, India): Understanding General Relativity after 100 years: a matter of perspective
26-05-2017	P. Kovács (Wigner RMI): Chiral phase transformation and thermodynamic properties of strongly correlating material from PQM model
29-05-2017	G.Zs. Tóth (Wigner RMI): The weak cosmic censure conjecture and an extension of the Noether theorem
02-06-2017	M.C. Abbott (University of Cape Town): On the necessity of massless modes in AdS ₃ integrability
16-06-2017	R. Zeier (Technische Universität München): Controllability and symmetries of coupled quantum systems
23-06-2017	L. Völgyesi (BME): Significance of the Eötvös-pendulum today
29-06-2017	A. Ortiz Velasquez (ALICE, UNAM, Mexico): Isolation of new physics in small collision systems
30-06-2017	M. Bejger (Nicolaus Copernicus Astronomical Center of the Polish Academy of Sciences): Testing general relativity with gravitational waves
07-07-2017	J.P.S. Lemos (University of Lisbon): Black hole entropy from matter entropy
11-08-2017	Y. Mao (ALICE, CCNU, Wuhan, China): Probe QGP properties using jet observables at LHC

01-09-2017	P. Vecsernyés (Wigner RMI): An effective toy model in $M_n(C)$ for selective measurements in quantum mechanics
07-09-2017	A. Mischke (University of Utrecht): Quest for the dynamical properties of the Quark-Gluon Plasma
06-10-2017	H. Siahhaan (Wigner RMI): Some Aspects of Magnetized Black Holes
13-10-2017	G. Rupp (Lisbon University): Modern Meson Spectroscopy - Models & Lattice vs. Experiment
27-10-2017	G. Almási: Modeling chiral criticality and its consequences for heavy-ion collisions
01-12-2017	B. Gyeniss (Institute for Philosophy, HAS): Striving towards equilibrium and the interpretation of probability
15-12-2017	T. Görbe (SZTE): Compactified trigonometric Ruijsenaars-Schneider systems

Wigner Space Seminar

<http://www.rmki.kfki.hu/~opitz/WignerSpaceSeminar>

19-01-2017	Zs. Bebesi: Exoplanets and extrasolar planetary systems
09-02-2017	P. Király: Directional distribution of cosmic radiation
16-02-2017	Z. Németh and A. Timár: Diamagnetic cavities of comet 67P
09-03-2017	A. Gucsik: Asteroid Itokawa by Hayabusa-1
23-03-2017	M. Dósa: ExoMars talk
20-04-2017	M. Dósa and A. Opitz: Solar wind propagation by magnetic lasso (EGU talk)
04-07-2017	K. Szabó: Space weather of Mars
05-10-2017	P. Király: 40 years of Voyager mission: scientific results and new challenges
19-10-2017	Zs. Bebesi: Exoplanet foundations
23-11-2017	K. Vida (CsFK/CsI): Flares and coronal mass ejections on cool stars
07-12-2017	Á. Kis (CsFK/GG): Ion acceleration in the area in front of Earth's quasi-parallel bow shock: Cluster results
19-12-2017	B. Forczek and A. Opitz: The mysterious planet Venus

Wigner RCP SZFI Seminars

<https://www.szfki.hu/seminar>

10-01-2017	Z. Dudás (Wigner RCP SZFI): Physicochemical characterization of hybrid silica gels obtained by sol-gel technique
17-01-2017	Z. Németh (Wigner RCP RMI): High energy resolution X-ray spectroscopy in laboratory and in X-ray lasers High energy resolution X-ray spectroscopy in the laboratory and in X-ray lasers
24-01-2017	L. Temleitner (Wigner RCP SZFI): Structural study of disordered systems by diffraction: from fluids containing hydrogen to disordered crystalline phases
31-01-2017	P. Dombi (Wigner RCP SZFI): Measuring nanooptical near-fields (field enhancement) by ultrafast photoelectrons
07-02-2017	G. Vattay (ELTE Faculty of Physics of Complex Systems): The trans-Turing machine

14-02-2017	B. Poirier (ELTE Complex Chemical Systems Research Group / Dept of Chemistry and Biochemistry, Texas Tech University): Exact Quantum Dynamical Treatment of Hydrogen-material Interactions
21-02-2017	P. Nemes-Incze (ERC-MFA): Kvantum dot in graphene: how to grab a Dirac-electron with a scanning tunneling microscope
28-02-2017	F. Araoka (RIKEN Center for Emergent Matter Science, Wako, Japan): Polarity and chirality in liquid crystals as observed by nonlinear optical imaging and spectroscopy
07-03-2017	Zs. Szaller (Wigner RCP SZFI): Growth and study of stoichiometric LiNbO ₃ single crystals
21-03-2017	D. Nagy (Wigner RCP SZFI): Nonequilibrium quantum-critical phenomena in a non-Markovian environment
28-03-2017	P. Magyar (Wigner RCP SZFI): Response functions of strongly coupled plasmas
04-04-2017	Sz. Szalay (Wigner RCP SZFI): Multipartite correlations in quantum systems and the chemical bond
11-04-2017	G. Roósz (Wigner RCP SZFI): Non-equilibrium dynamics of one-dimensional isolated quantum systems (in-house thesis defence)
11-04-2017	B. Somogyi (Wigner RCP SZFI): Study of silicon carbide nanocrystals using ab initio numerical methods (in-house thesis defence)
18-04-2017	L. Rátkai (Wigner RCP SZFI): Dendrites in a centrifuge (work summary)
18-04-2017	B. Korbuly (Wigner RCP SZFI): Polycrystalline solidification and grain coarsening in phase-field theory
25-04-2017	M. Krzystyniak (ISIS Science & Technology Facilities Council, UK): Mass-resolved neutron spectroscopy
02-05-2017	B. Nagyfalusi (Wigner RCP SZFI): Theoretical study of the magnetic anisotropy of thin films using metadynamics
09-05-2017	M. Máté (ELTE physics student): Investigation of multipartite entanglement using matrix product state approximation
09-05-2017	B. Bódi (Wigner RCP SZFI): Creation of attosecond pulses using synthesized optical waves (work summary)
16-05-2017	A. Vukics (Wigner RCP SZFI): The theory and experimental realization of photon-blockade breakthrough as a first-order dissipative quantum phase transition
25-05-2017	Á. Vibók (Institute for Physics, University of Debrecen): Natural, laser- and vacuum-induced ultrafast quantum dynamics
29-05-2017	A. Belyanin (Dept of Physics and Astronomy, Texas A&M University): Optics and plasmonics of Dirac and Weyl fermions
30-05-2017	P. Rácz (Wigner RCP SZFI): Study of the field enhancement of nanolocalized electromagnetic fields by ultrafast photoemission (work summary)
30-05-2017	B. Nagy (Wigner RCP SZFI): Ultrafast photoemission from nanostructures and measurement of the femtosecond damage threshold
06-06-2017	M. Markó (Wigner RCP SZFI): Neutron optics research for the European Spallation Neutron Source, currently under construction (work summary)

06-06-2017	G. Nagy (Paul Scherrer Institute, Switzerland/Wigner RCP SZFI): Revealing the structure of photosynthetic membranes and fuel cells by neutron scattering
08-06-2017	V. Zólyomi (Wigner RCP SZFI / Quantum Technology Centre, Lancaster University): Anomalous optical response in atomically thin InSe
08-06-2017	I. Márton (Wigner RCP SZFI): Study of plasmonic photoemission and electron acceleration created by ultrashort laser pulses (in-house thesis defence)
13-06-2017	Sz. Pothoczki Szilvia (Wigner RCP SZFI): Structure of water solutions of compounds containing hydroxyl groups
13-06-2017	G. Thiering (Wigner RCP SZFI): Ab-initio computing of spin-orbit scattering rates in nitrogen vacancy centers (work summary)
05-09-2017	N. Sándor (Institut de Physique et Chimie des Materiaux, Strasbourg): Rydberg optical Feshbach resonances in cold gases
12-09-2017	P. Boross (ELTE Faculty of Materials Physics): Electric control of dopant nuclear spins in semiconductors
19-09-2017	L. Rózsa (Wigner RCP SZFI): Noncollinear spin configurations in ultrathin magnetic films
26-09-2017	T. Carrington (Queen's University, Kingston, Ontario, Canada): Calculating ro-vibrational energy levels of floppy molecules and a re-assignment of ro-vibrational energy levels of CH ₅ ⁺
10-10-2017	K. Kamarás (MTA Wigner FK SZFI): Nanocables based on boron nitride
17-10-2017	M. Droth (BME Faculty of Physics): Electron-electron attraction in graphene electromechanical systems
03-10-2017	Sz. Csonka (BME Faculty of Physics): Topologically protected ground state degeneracies in a two-spin system
24-10-2017	O. Kálmán (Wigner RCP SZFI): Measurement-induced nonlinear transformations and their application for quantum informational tasks
31-10-2017	M. Vasúth (Wigner RCP RMI): Gravitational waves - The 2017 Nobel Prize in Physics
07-11-2017	D. Datz and G. Németh (Wigner RCP SZFI): Nanoscale characterization with scattering-type scanning near-field infrared microscopy
14-11-2017	T.W. Clark (Wigner RCP SZFI): Sculpting Shadows - Structured light and the spatial shaping of fields and atoms
21-11-2017	S. Tóth (Wigner RCP SZFI): Ni-Si center with an extra-narrow emission band in nanocrystalline diamond
28-11-2017	A. Szakál (Wigner RCP SZFI): Possible applications of atomic-resolution neutron holography (in-house thesis defence)
05-12-2017	J. Andreasson (ELI Beamlines facility, Prague): The study of ultrafast phenomena in applied science at the ELI Beamlines facility
12-12-2017	A. Lindner (ESPCI, Paris, France): Transport dynamics of complex particles in simple flows
19-12-2017	R. Szipőcs (Wigner RCP SZFI): Handheld nonlinear microscope system comprising an Yb-fiber laser for in vivo biomedical imaging (Applied Research Prize 2017 of Wigner RCP SZFI)