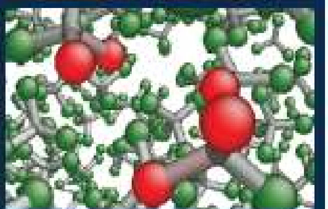
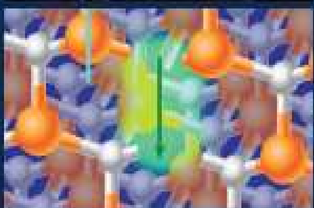
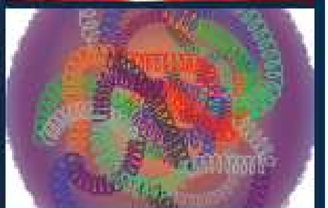
Wigner 2015

Annual Report







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

Wigner RCP 2015

Annual Report

Wigner Research Centre for Physics
Hungarian Academy of Sciences
Budapest, Hungary
2016

Wigner Research Centre for Physics

Hungarian Academy of Sciences

Budapest, Hungary

2016

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Wigner RCP 2015 – Annual Report

Edited by TS. Bíró, V. Kozma-Blázsik, A. Kmety, B. Selmeci

Proofreaders: I. Bakonyi, D. Horváth, P. Kovács

Closed on 15. April, 2016

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A. Balázs

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V. Gogokhia: Rustaveli and Georgian National prize
K. Krajczár, CMS Achievement Award
M. Dósa: Amelia Earhart Fellowship
Philae team members: Award of International Academy of Astronautics
L. Bencs: Cup/Award of Highly Cited Paper, Web of Science
L. Bencs: Outstanding Reviewer for the peer review journal, Analytica Chimica Acta.
L. Bencs: Recognized Reviewer for the peer-review journal, Atmospheric Environment.
L. Bencs: Recognized Reviewer for the peer-review journal, Microchemical Journal.
D.I. Réfy: ECPD 2015, Best Student Poster Price

N. Kroó

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I. Hagymási: National Excellence Award, 2015
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N. Kroó, József Petzval Prize of the Optical-, Accoustic-, Film- and Theatre-technical Scientific Association
T. Börzsönyi: Gyulai Zoltán Prize of the Roland Eötvös Physical Society
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G. Thiering: Publication Prize of the Department of Atomic Physics, BME
D. Beke: Best lecturer award (György Oláh Conference for PhD students)
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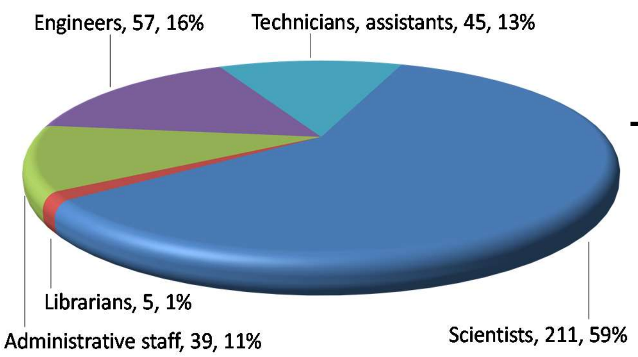
Bolyai János Scholarship of the H.A.S. granted in 2015

K. Lengyel, 2015-2018
O. Kálmán, 2015-2018
D. Nagy, 2015-2018

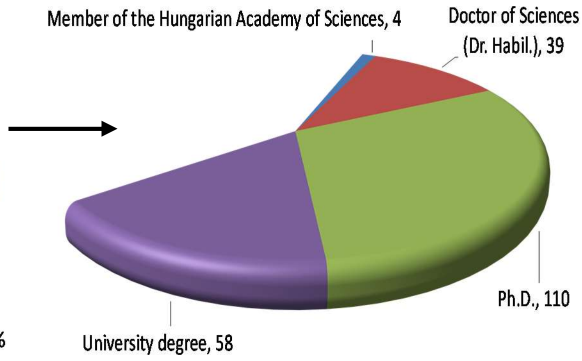
Permanent staff by profession

Total: 357

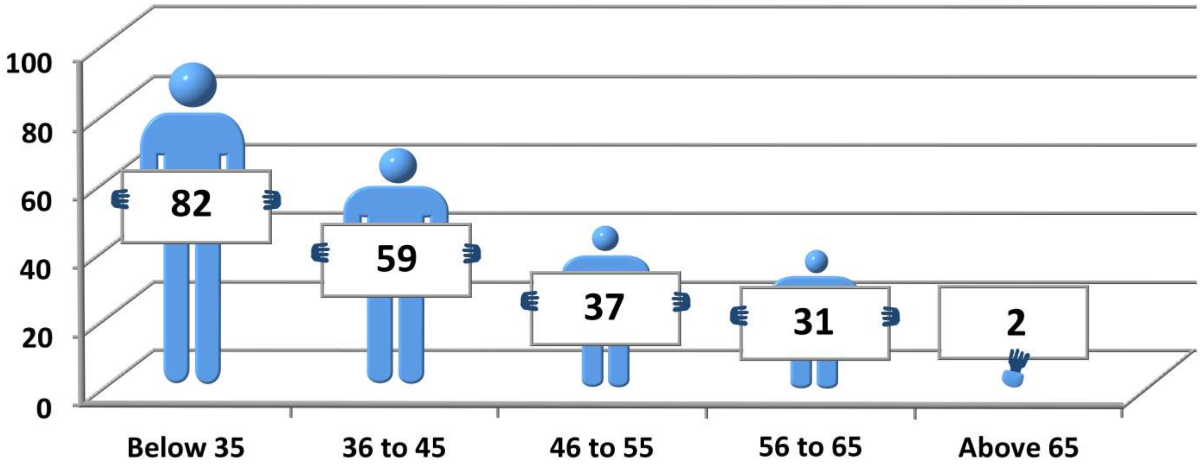


Scientists by degree/title

Total: 211

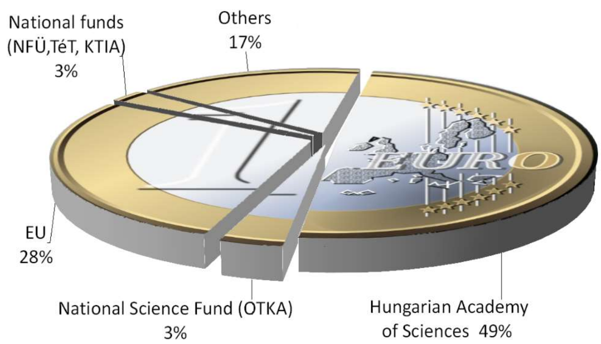


Scientists by age group

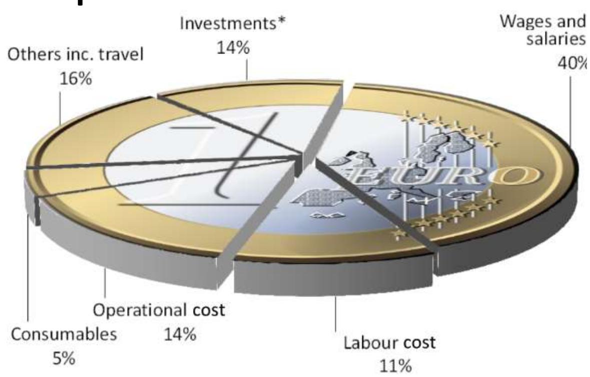


Total: 211

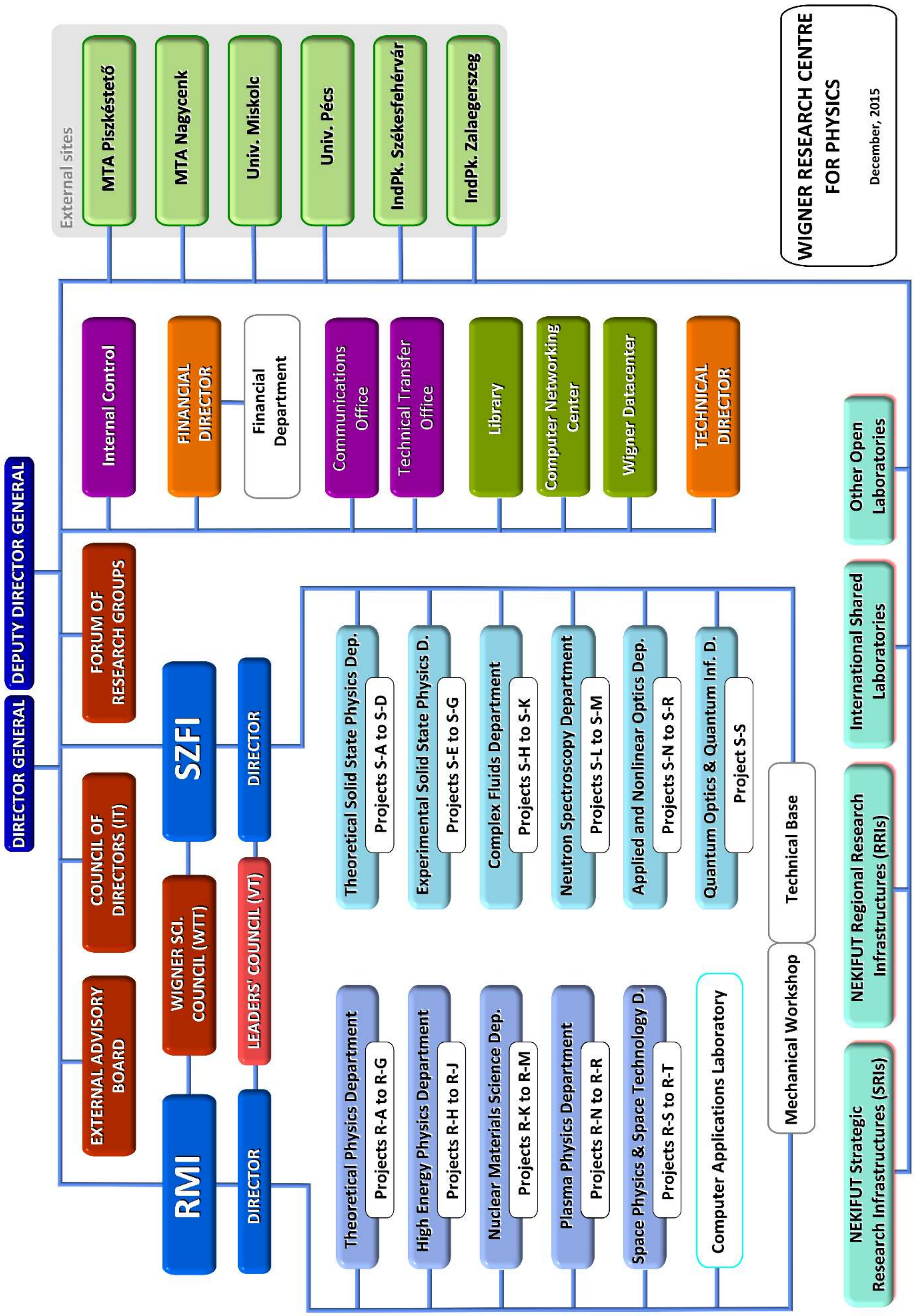
Income*



Expenditure*



*V.A.T not included.


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

MOST IMPORTANT EVENTS OF THE YEAR 2015

Csilla Péntek, communication secretary

There are a great number of accomplishments achieved year by year at Wigner RCP which deserves to take notice of. Results are published in different articles and in 2015 even a 50 minutes documentary film in two parts was shot about CERN and the involvement of the Hungarian CERN groups. It was mainly shot in our research centre.

Our colleagues play an important role in disseminating their results every year. They are frequently invited to give lectures in secondary schools, at universities and in other scientific and cultural institutions.

Pál Vizi introduces the Rosetta project during the Night of Museums in the Planetarium and Péter Lévai is at the Virtual Worlds program at the Hungarian Academy of Sciences

All Colors of Physics Roadshow. — In 2015 we continued the very successful “All Colors of Physics Roadshow” which is an interactive program for students to popularize sciences, mainly physics and engineering. Last year we visited 40 secondary- and elementary schools in different locations of Hungary and we took part in the „Road of Sciences” Festival for the first time in Serbia. The roadshow was part of the “International Year of Light” Project.

Open days. — Our three Open Days are traditional outreach programs with a long history. They are focusing on different age groups. Like every year, in 2015 we also organised Wigner Open Days for secondary school students in November. This event was part of the Celebration of the Hungarian Sciences Program series organised by the Hungarian Academy of Sciences. Another very popular one is the Girl’s Day, which is an interactive tour at the laboratories of our institutes only for secondary school girls. This is part of an international program with the goal to draw girls’ attention to natural sciences and engineering during their career planning, which is coordinated by the Association of Hungarian Women in Sciences in Hungary.

The CERN-Wigner Open Days are our longest and most significant one, which accommodated approximately 330 people during the 2 days program series. Like every year, we presented an open air poster exhibition where visitors could meet our researchers and get answers to their questions. After listening to some interesting presentations there was a opportunity to visit the Wigner Datacenter. On both days two Hungarian physicists introduced CERN online from Geneva and two teachers gave accounts of their experiences at the CERN Teacher Program.

Girl’s Day at Wigner RCP

CERN-Wigner Open Days 2015

Student Programs. — In addition to the above mentioned programs about ten secondary school groups visited our research centre and we organised a very successful two-day Nuclear Physics Students Workshop too.

We started two mentoring programs for universities and secondary school students. Young people - who participated in these programs – could win some prestigious international awards with their researches conducted in our laboratories.

Students in the Wigner RCP

In 2015 the European Physical Society pronounced the Budapest-Fasori Lutheran Secondary School - the old secondary school of Eugene P. Wigner – as an EPS Historic site. On this occasion the Hungarian Academy of Sciences, the Wigner RCP, the Eötvös Loránd Physical Society, the Hungarian Chemical Society and the Budapest-Fasori Lutheran Secondary School organised an inauguration celebration of a commemorative plaque at the school.

The inauguration of a commemorative plaque

Festivals. — Our colleagues from the Plasmaphysics Department took part in two important summer festivals (VOLT, Sziget) in order to popularize sciences among young people.

2015 – THE INTERNATIONAL YEAR OF LIGHT AND THE WIGNER RESEARCH CENTRE FOR PHYSICS

Norbert Kroó, chairman of the Hungarian Year of Light Program Committee

The idea of celebrating the International Year of Light was conceived by the European Physical Society three years ago from the realization that light plays a decisive role in not only scientific research but beyond, in light related modern technologies, our relationship to nature, and even has significant impact on our cultural fabric. Scientists were able to gain the support of UNESCO's decision makers for this important initiative and through their help convince the United Nations of its significance as well. The year 2015 immediately became a natural choice for the festivities as it is the anniversary a number of light related scientific breakthroughs that changed the course of our world.

The program series during the International Year of Light was inaugurated by an outstanding large-scale conference in mid-January at the UNESCO headquarters in Paris. Nobel Prize Laureate scientists, high-ranking politicians, members of the clergy, and other representatives of public life shared their views on the role of light in contemporary society.

The Paris inauguration was quickly followed by many other celebrations around the world. As part of this series, the Hungarian Academy of Sciences also organized an opening press conference in February 2015, took leadership to act as coordinator of the event, and set up a Program Committee. Tasks were divided into 5 sections according to scientific, educational, industrial and business oriented topics, as well as those of artistic and international interest. The primary goal was to awaken and inspire scientific interest in students by immersing them in regional and national scale programs. 'Physics for everybody' (A fizika mindenkié) was a one day event series held across the county in which 52 institutions in 45 municipalities took part, primarily secondary schools. A "beam of light" originating in Szeged ran across the country and local and national competitions were organized along its path. The 'All Colors of Physics Bus' hosted a roadshow in about 30 communities, with presentations and lectures related to optics. At research institutes and universities 'Open Days' were organized showcasing research aimed at light and optics. At another successful event astronomers helped students' navigate the sky with telescopes to investigate the partial eclipse of the sun, in front of the building of the Hungarian Academy of Sciences.

The Hungarian Academy of Sciences organized a further lecture series where distinguished speakers, the majority of whom were researchers of our institute, gave presentations aimed at students on the topic of light. Participants filled in the Main Hall of the Academy.

Light and science in the city of lights – scientific lecture series held at the Hungarian Academy of Sciences. Photo: H.A.S.

Events related to the Year of Light were also emphasized in the program of the World Science Forum in November. The internationality of the programs emphasized by the additional conferences organized by our researchers with both international and significant Hungarian participation.

The Hungarian business sector also contributed to light related events; for example TUNGSRAM, the lighting technology company, donated 13 valuable light source units of various types (incandescent lamps, luminescent lamps, LEDs) to the Year of Light Program for use by schools so students could perform relevant experiments on optimizing lighting, energy efficiency, carry out measurements investigating different parameters, and to learn about the optimal usage of light sources.

The above-described activities are only a brief account of the programs made possible through key contributions of our research centre. The success of these programs raises the question: what brought about the enormous interest and enthusiasm for the events of the International Year of Light both at home and abroad?

I think we are all astonished to see evidence of the state of crisis prevalent in our world today. Traditional industries are on the verge of collapse, their places are being taken over by new emerging technologies. The role of the production of steel is being replaced by that of computer chips, science is becoming the most important source of economic growth, and its integration into the economy is becoming faster and faster. At the same time, the efficiency of the educational system is in decline, causing a shortage of professionals hindering further economic development.

Under such circumstances came the invigorating burst from the optics of lasers, optical fibres, and a host of other revolutionary inventions, to the field of informatics-communication, biotechnology, medical and other disciplines. Today it would be difficult to name an area of life where optical technology does not play an important role. I am convinced that the significance of optical technology in the modern economy will continue to grow and research will provide us with many more surprises to come. This is why I consider it crucial to train future engineers, medical doctors, researchers, and teachers, while still in their young pliable years, to be able to optimally navigate the economic promises of the future. The goal of the International Year of Light was to serve this purpose. The primary objective was that our youth can better appreciate opportunities opened up by the developing light technology, appreciate the beauty of research, appreciate the art of light, and finally appreciate the behaviour of light in nature. This latter is especially important; the most promising and successful technologies, in my view, are those that mimic nature and the processes surrounding us.

RESEARCH GRANTS AND INTERNATIONAL SCIENTIFIC COOPERATION

Valéria Kozma-Blázsik, scientific secretary

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

As government funding accounts for only about 49% of financial revenue at Wigner RCP, the role of additional sources of income is becoming exceedingly important. Such additional funds come from a variety of sources; the National Fund for Basic Research (OTKA) makes up about 3% (2% less than in 2014), EU cofounded national grants 3% (instead of 17% of the previous year), EU FP grants complemented by other foreign grants grew to 28% from 18%, and the remaining 17% come from other scientific contracts.

Thanks to currently funded grants, there was still an increase in overall revenue secured during 2015 compared to the previous year. As we can see in the data above, the year 2015 required great flexibility in adapting to the changes in revenue sources. Hard work was expected as Wigner RCP had to balance its budget by topping up its basic government support using additional grant sources. In spite of a sharp decline in the number of newly awarded grants, the overall monetary value of grants in the different categories listed in the previous paragraph still increased, with the notable exception of OTKA grants that of the Hungarian National Fund dedicated to basic research.

Concerning OTKA and EU cofounded national grants, a significant decline occurred both in the number and the monetary value of funding received. Although the number of OTKA projects running in 2015 remained unchanged, the sharp decrease both in the number of successful new proposals, only 9 in 2015 and in overall grant amounts received as compared to the previous two years raises strong concerns for the future. As it was mentioned new EU cofounded grants were almost missing with the exception of 5 smaller mobility grants, due to the geographical location of our institute in the central Hungarian region where Structural Funds were not available. Fortunately the 36 bilateral academic projects helped common international research, though their timespan is only for maximum 12 months,

The significance of international funding lines cannot be overstated, and it is notable that the safety net that they provide is highly valued and desired by the researchers. During the previous EU framework program, Wigner RCP was among the leading research organisations among the 10 new EU countries in the Central Eastern European region in terms of attracting EU FP7 funds. The international scientific relations grew increasingly significant.

2015 was the second year of the new Horizon 2020 program period, which required a lot of preparation. Thanks to the MTA EU preparation support that was offered to research institutes, researchers could actively participate in consortium building events and conferences. In 2015 scientists worked on 15 EU projects, of which 10 still belong to FP7, 5 are H2020 projects, from the latter 4 are research infrastructure projects. To summarize these results, the scientists working on large-scale infrastructure projects are the most successful in becoming partners in various consortiums.

In 2015 altogether 41 proposals were submitted. Fortunately, one FET Open project (NEURAM) is part of the winning team. Final paperwork on NEURAM is in progress, while another eleven proposals are currently in the process of evaluation. Most of the proposals submitted are in the Excellent Science pillar. At least five researchers worked on ERC Starting and Consolidator grant projects, Marie Curie Sklodowska Actions.

WIGNER RESEARCH INFRASTRUCTURES

Wigner Research Centre for Physics has spent a lot of time and energy to develop unique research infrastructures (RI)[1] that could be offered to carry out collaborative research. Wigner's RIs have been organized into laboratories. Most of the laboratories are of open access or are members of open-access networks so that they can be used by non-local researchers and companies. Wigner RIs have about 300 external users. Five Wigner RIs, three networks coordinated by the Wigner RCP and three further networks with Wigner RI's participation were ranked as "research infrastructures of strategic importance" (SRI) [2] title in the Hungarian National register (NEKIFUT).

Research infrastructure of strategic importance of the Wigner RCP include:
- Innovative Gaseous Detector Development Laboratory
- Ion beam laboratory of Wigner Research Centre for Physics
- Non-equilibrium and Nanostructured Magnetic Materials Laboratory
- Preparation and complex study of optical single crystals
- Wigner Femtosecond Laser Laboratory

SRI networks coordinated by the Wigner RCP are:

- Hungarian CERN Grid Consortium (BNC)
- Network of Hungarian Mössbauer Laboratories
- Optical spectroscopy network

Wigner RIs participate in the following SRI networks:

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

During the last couple of years our colleagues applied to more RI calls in the Excellent Science pillar of H2020. In 2015 less H2020 proposal were published compared to the previous year and applications became more competitive, and as a result success rate was still very low. For this reason the four successful H2020 research infrastructure proposals, won by our researchers, have even more significance for our research centre.

One of them is **BrightnESS** (No. 676548), Building partnerships and promoting synergies for the highest scientific impact on ESS. In this project, where our institute is participating from

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

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

the beginning, countries have joined together to construct the world's most powerful neutron source, the European Spallation Source (ESS) in Lund. With a timeline of 36 month, involving 18 Consortium Partners from 11 countries, the BrightnESS proposal will ensure that the extensive knowledge and skills of European companies, and institutes are best deployed, that technology transfer both to, and from the ESS to European institutions and companies is optimised. Wigner is contributing to this project with methodical developments in neutron instrumentation, construction and operations of neutron moderators, neutron transport systems. Furthermore the detector developing team joined to the BrightnESS project, together with the SPOI by development work on detectors and neutron optical devices for increasing the neutron intensity at the ESS. Budget of Wigner RCP for the 3 years is 464.8 million HUF (1.478.687 EUR).

The other important project, IPERION CH aims to establish the unique pan-European research infrastructure in Heritage Science by integrating national world-class facilities at research centres, universities and museums. The cross-disciplinary consortium of 24 partners (from 13 Member States and the US) offers access to instruments, methodologies and data for advancing knowledge and innovation in the conservation and restoration of cultural heritage. BNC-WIGNER laboratories offer access to users to various non-destructive tools for investigation of Cultural Heritage objects, utilizing basically neutrons produced at the Budapest Research Reactor. The ensemble of instruments offered by BNC-WIGNER is a unique opportunity in Europe for non-invasive investigation of artefacts by neutrons complemented by other techniques within the same campus of a large infrastructure environment. The budget of Wigner RCP for the 4 years is 116.6 million HUF (370.000 EUR).

In the H2020 framework researchers of the PNPI obtained support from two large infrastructural calls. One is the AIDA 2020 (No. 654168) realized with the participation of 38 organizations from 19 countries and coordinated by CERN. This projects aims at the creation and harmonization of good conditions for detector developing technologies in Europe for particle physics research as well as ensures the necessary transnational access. The Wigner RCP joins this program by developing detectors and equipment's. The budget part for the Wigner RCP for a 4-year period amounts to 15.6 Million HUF (49 500 EUR).

Another important infrastructure support is EPN2020-RI (No. 654208) which enables an open access to the freshest research results, models, data bases and facilities necessary for the investigation of questions in since and technology related to space research. The budget part for the Wigner RCP for the total 4-year period approaches 61.4 Million HUF (195 000 EUR). Altogether 34 institutions from 18 countries participate in this project.

All of the above mentioned grants are the result of the successful participation of both institutes in Wigner RCP in predecessor FP7 projects, the European Spallation Source (ESS) Charisma, AIDA and space research projects during the last decade.

INNOVATION ACTIVITIES OF WIGNER RCP

Zsuzsanna Tandi, innovation adviser

Wigner RCP is continuously searching for the possibilities of practical utilization and commercialization of the results obtained by the researchers of the institute. The implementation of our new innovation strategy was in focus of our activities last year.

In 2015, the activities of the Research Centre related to innovation included the establishment of new business relationships, the stimulation of the protection and commercialization of the intellectual property rights created by the researchers of the Centre, the increase of our participation in market oriented research programs and the facilitation of collaborations with other institutions, companies and organizations in technology transfer and innovation management.

A number of new industrial relationships were established with businesses being interested in cooperation with us and in utilization of the research and development infrastructure of the Research Centre and marketing of our results. In frames of these collaborations several grants were submitted and awarded by the Centre. In addition to relationships with potential domestic and international investors were established.

Several channels were used to propagate our services and capabilities and to increase the visibility of the Centre. In order to be effective in the new grant environment novel services and partnerships were offered to small and medium enterprises and other institutions in forms of subcontracting, leasing of R&D infrastructure and competence etc. The Wigner RCP established new sites in different regions of Hungary, (Piszkéstető, Pécs, Miskolc, Nagycenk, Székesfehérvár, Zalaegerszeg) in order to strengthen the collaboration with research organizations and businesses in these areas and to facilitate R&D and tendering activities. As a result, more than 40 proposals were submitted under the different Economic Development and Innovation Operative Programmes and Scientific and Technological Collaboration calls. In addition, near 30 subcontractor agreements were signed with domestic and international companies.

According the Intellectual Property Rights Policy of the Wigner RCP, the IPR Committee was formed, with the main responsibilities to include assessment of newly created and potentially patentable intellectual property, its patenting, further utilization and commercialization, the possibilities of finding appropriate business partners and the protection of interests of the Research Centre in these matters. From the total of 6 patent applications several R&D results and novelties related to medical instruments and methods, sensors, material sciences were classified as important for the institute. In addition to the initiation of patent application active partner search was started, too.

Strategic partnership agreements were prepared with several institutions and companies, including the Bay Zoltán Nonprofit Ltd., MNKH Hungarian National Trading House Cls., BHE

Bonn Hungary Electronics Ltd., Scientific Council of the Police, Semmelweis University. These cooperations will further strengthen the R&D potential of the Centre.

Efforts were made to accelerate the establishment of the Technology Transfer Office of the Research Centre. In order to gather detailed information and expertise our colleagues were visiting several similar organizations, including CERN KTN (Switzerland), ESA (European Space Agency) TTO (The Netherlands), University of Cambridge, University of Oxford, Imperial College (England) and attended the summer school organized by the Joint Research Centre of the European Commission (Summer school on IP Commercialization and Technology Transfer – Belgrade and Budapest). Relationship with ESA was strengthened and Wigner RCP joined the ESA Technology Transfer Brokers' Network (Technology Transfer Initiative) and, furthermore, a BIC (Business Incubation Centre) were prepared.

The Institute became an active member of the CERN-supported organization, HepTech – Leading HEP technologies for industry Technology Transfer.

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

R-A. Field theory

Wigner research group

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

One of our main activities in 2015 dealt with multiplier bialgebras in braided monoidal categories and their 'weak' generalization.

The setting. — The initial datum in the algebraic approach to quantum field theories is the algebra of locally observable physical quantities. The equivalence classes of its suitable representations are the so-called *superselection sectors*. To each such sector there is an associated number - known as the *quantum dimension.* These numbers are unique with the property that the quantum dimension of a direct sum representation is the sum of the quantum dimensions of the summands, and for tensor product representations the quantum dimensions get multiplied. The quantum dimensions can be computed from the physical data. While in 3+1 space-time dimensional models they can be proven to take only integer values, there are known examples of lower dimension where they are irrational (e.g. the golden ratio occurs in the Lee-Yang model).

The internal, or superselection *symmetry* of a physical model is an algebraic structure – a group or something more general – whose representation theory is equivalent (in an appropriate well-defined sense) to the representation theory of the above algebra of physical observables. This means, first of all, a bijection between the equivalence classes of its irreducible representations and the superselection sectors. This bijection can be used to associate quantum dimensions to the representations of the symmetry. Further requirements are that for taking direct sums and tensor products of representations of the symmetry, the quantum dimensions get added and multiplied, respectively.

In the case of groups, direct sum representations act on the direct sums of the representation spaces and tensor product representations act on their tensor products. Consequently, the dimensions of the underlying vector spaces (which are always integers!) obey the conditions on the unique quantum dimensions. This immediately implies that in physical models admitting non-integer quantum dimensions, no group can describe the symmetry. A more general mathematical structure is needed.

In the last twenty years intensive research has been performed worldwide seeking for appropriate algebraic structures, investigating their mathematical properties and their application to the description of symmetries in physical models.

Preliminaries. — Although at the moment no mathematical structure is known yet which would fulfill all expectations in all applications, there are some very successful and promising candidates. One of them is *weak Hopf algebra,* introduced and analyzed by Böhm, Nill and Szlachányi. This is a generalization of the classical notion of Hopf algebra, the tensor product

[A] Associate fellow

of whose representation acts on a canonical subspace of the tensor product of the representation spaces (instead of the tensor product itself). This feature makes them compatible with non-integer valued quantum dimensions.

A classical example of Hopf algebra is the vector space spanned by the elements of an arbitrary group. Dually, whenever the group is finite, functions (with values in the base field) on the group also constitute a Hopf algebra. However, for this latter construction it is essential the group to be finite. In the case of arbitrary, possibly infinite, groups one can regard the functions of finite support. Their algebra (with respect to the pointwise multiplication) admits no unit thus it can not be a Hopf algebra. This situation was axiomatized by Van Daele under the name *multiplier Hopf algebra*. It was generalized recently in his collaboration with Wang to *weak multiplier Hopf algebra*, which simultaneously generalizes weak Hopf algebra and multiplier Hopf algebra. The motivating examples are the algebras of functions of finite support on groupoids (rather than on groups).

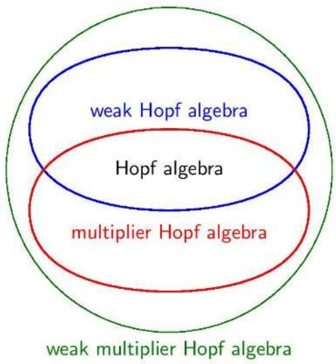

Figure 1. *Generalizations of Hopf algebra*

The logical relation between these generalizations of Hopf algebra is depicted in Figure 1.

In the definition of (weak) multiplier Hopf algebra due to Van Daele et. al., a crucial role is played by the *antipode*. In contrast to (weak) Hopf algebra, it is not built up from the more general structure of (weak) multiplier bialgebra by equipping it with the additional structure of the antipode. The missing notion of *(weak) multiplier bialgebra* was proposed by Böhm, López-Centella and Gómez-Torrecillas. They worked out the theory of (weak) multiplier bialgebras *over fields*.

In some applications however a more general setting is needed: instead of vector spaces, one should work with modules over rings, on topological vector spaces or graded vector spaces (cf. supersymmetry). All of these and many other cases can be simultaneously treated by working with *arbitrary braided monoidal categories*. The first step in this direction was made by Böhm and Lack by defining and studying *multiplier bialgebras in arbitrary braided monoidal categories*. The axioms are presented in Figure 2. The definition was based on the use of *counital fusion morphisms* (see the first two and the second two diagrams of Figure 2).

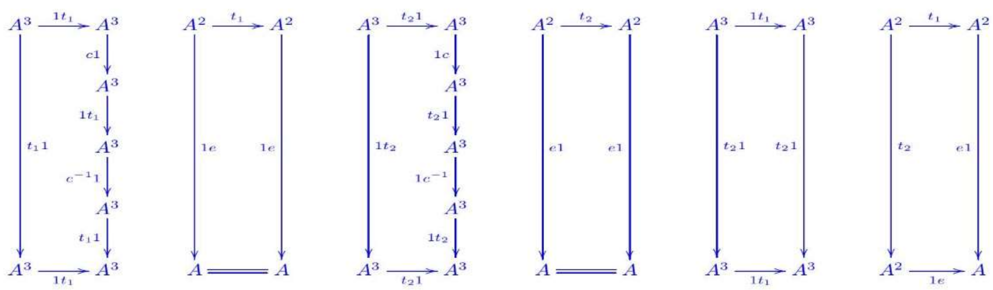

Figure 2. *Axioms of multiplier bialgebra in terms of commutative diagrams*

Results achieved in 2015. — We analyzed various aspects of multiplier bialgebras, multiplier Hopf algebras and weak multiplier bialgebras in braided monoidal categories:

A category of multiplier bimonoids. — Classical bialgebras (in any braided monoidal category) can be defined as comonoids in the monoidal category of monoids. This is no longer true for multiplier bialgebras. In this project, Böhm and Lack constructed a category of appropriate semigroups and - under mild assumptions - they characterized multiplier bialgebras as certain comonoids therein. This gave them a tool to define morphisms between multiplier bialgebras.

Multiplier Hopf monoids. — Böhm and Lack proved that multiplier bialgebras in braided monoidal categories possess monoidal categories of modules (and gave a conceptual explanation of this fact by analyzing the structure of their induced functors). Hence this symmetry structure is capable to describe the multiplication of superselection sectors; that is, the addition of charges. In the absence of an antipode, however, it can not be used to describe anti-charges. So as a next necessary step, in this project Böhm and Lack characterized multiplier Hopf algebras among multiplier bialgebras in braided monoidal categories by showing that the invertibility of the underlying fusion morphisms is equivalent to the existence of the antipode. They proved that in the category of modules over a multiplier Hopf algebra those objects which are finite in an appropriate sense admit duals. Physically this corresponds to superselection sectors with opposite charges.

A simplicial approach to multiplier bimonoids. — A recent pioneering result due to Buckley, Garner, Lack and Street asserts that (co)monoids in any monoidal category can be identified with simplicial maps from the Catalan simplicial set to the monoidal nerve of the category in question. This can be used to characterize as simplicial maps (from the Catalan simplicial set to a monoidal nerve) those multiplier bialgebras which correspond to comonoids in their category of semigroups. In this project Böhm and Lack went further and identified arbitrary multiplier bialgebras with simplicial maps. The domain of these more general simplicial maps is still the Catalan simplicial set. The codomain, however, is no longer a monoidal nerve but a different carefully designed simplicial set.

Weak multiplier bimonoids. — The aim of this - yet unpublished - project of Böhm, Gómez-Torrecillas and Lack was to formulate the axioms of *weak multiplier bialgebra in arbitrary braided monoidal categories*. This was challenging both at the technical and the conceptual level. Just as the definition of multiplier bialgebra is based on the use of counital fusion morphism, the definition in the weak case rests on the newly invented notion of *weakly counital fusion morphism*; whose axioms are presented in a graphical notation in Figure 3. This definition allowed for the extension from the (very particular) category of vector spaces those theorems which are most crucial in the applications: Böhm et. al. proved the coseparable coalgebra structure of the base objects. Relying on that they showed that the monoidal structure of the category of bicomodules over the base object lifts to the category of representations over the weak multiplier bialgebra.

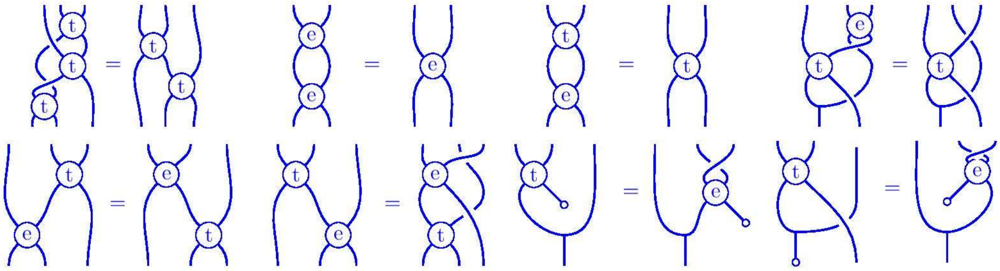

Figure 3. *Axioms of weakly counital fusion morphism in terms of string diagrams*

Figure 4 shows our most important working tool in use.

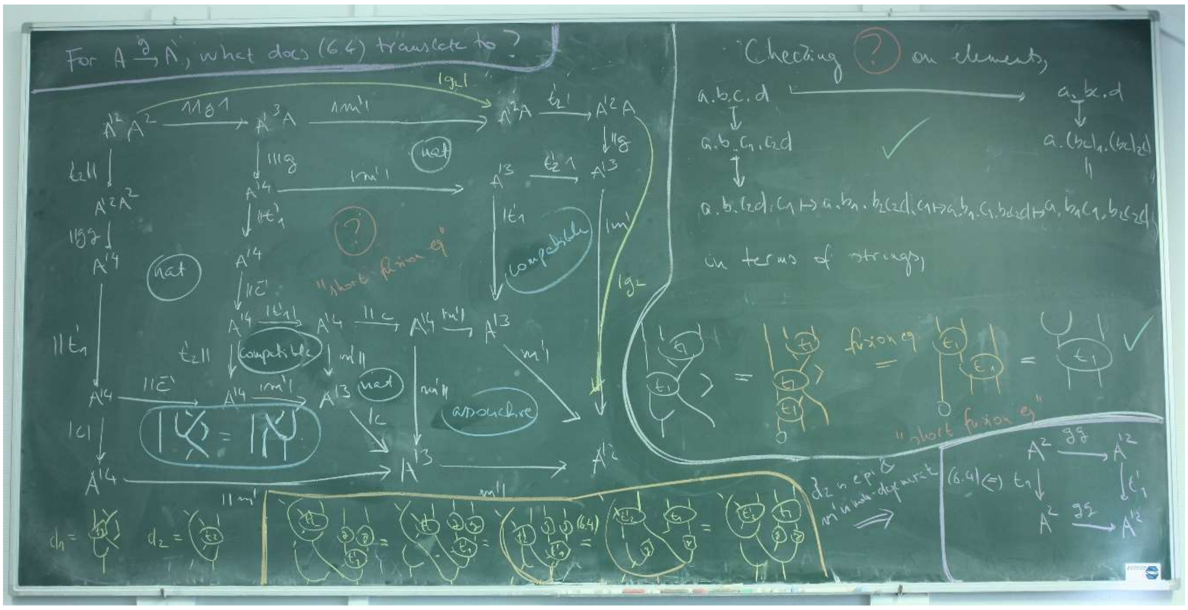

Figure 4. *After a hard-working day...*

Grants

OTKA K108384: A categorical study of quantum symmetries and their applications (G. Böhm 2013-2017)

OTKA K111697: Group-theoretic aspects of integrable systems and their dualities (L. Fehér 2014-2018)

OTKA K101709: Field theory, radiation reaction, cosmology, vortices (P. Forgács 2012-2016)

OTKA PD116892: Compact binary gravitational waves, parameter estimation (B. Mikóczi 2015- 2018)

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

International cooperation

On the particular projects described above:

Macquarie University (Sydney, Australia, S. Lack)

University of Granada (Granada, Spain, J. Gómez Torrecillas)

On other projects in 2015:

Observatoire de Paris (Meudon, France, P. Grandclément)

Universidad National de La Plata (La Plata, Argentina, F.A. Schaposnik)

Université de Tours (Tours, France)

National Research Centre, Petersburg Nuclear Physics Institute (St Petersburg, Russia, V.V.Anisovich)

The Mathematical Institute, Oxford University (Oxford, Great Britain, P. Tod)

Publications

Articles

1. Anisovich VV, Matveev MA, Nyiri J, Sarantsev AV, Semenova AN: Nonstrange and strange pentaquarks with hidden charm. ***INT J MOD PHYS A*** 30:(32) Paper 1550190. 9 p. (2015)
2. Anisovich VV, Nikonov VA, Nyiri J: Real part of scattering amplitude at ultrahigh energies. ***INT J MOD PHYS A*** 30:(30) Paper 1550188. 7 p. (2015)
3. Böhm G, Gomez-Torrecillas J, Lopez-Centella E: Weak multiplier bialgebras. ***T AM MATH SOC*** 367:(12) pp. 8681-8721. (2015)
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5. Böhm G: Yetter-Drinfeld modules over weak multiplier bialgebras. ***ISRAEL J MATH*** 209:(1) pp. 85-123. (2015)
6. Czinner VG: Black hole entropy and the zeroth law of thermodynamics. ***INT J MOD PHYS D*** 24:(9) Paper 1542015. 10 p. (2015)
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8. Fehér L, Görbe TF: On a Poisson-Lie deformation of the BCn Sutherland system. ***NUCL PHYS B*** 901: pp. 85-114. (2015)
9. Fodor Gy, Forgács P, Grandclément Ph: Self-gravitating scalar breathers with a negative cosmological constant. ***PHYS REV D*** 92:(2) Paper 025036. 19 p. (2015)
10. Forgács P, Lukács A, Schaposnik FA: Non-Abelian vortices with a twist. ***PHYS REV D*** 91:(12) Paper 125001. 12 p. (2015)
11. Frenkel A: Dependence of the Time-Reading Process of the Salecker–Wigner Quantum Clock on the Size of the Clock. ***FOUND PHYS*** 45: pp. 1561-1573. (2015)
12. Frenkel A, Rácz I: On the use of projection operators in electrodynamics. ***EUR J PHYS*** 36:(1) Paper 015022. 12 p. (2015)

13. Görbe TF, Fehér L: Equivalence of two sets of Hamiltonians associated with the rational BCn Ruijsenaars–Schneider–van Diejen system. ***PHYS LETT A*** 379:(42) pp. 2685-2689. (2015)

14. Hofer-Szabo G, Vecsernyés P: On the concept of Bell's local causality in local classical and quantum theory. ***J MATH PHYS*** 56:(3) Paper 032303. 23 p. (2015)

15. Mikóczi B, Forgács P, Vasúth M: First order post-Newtonian gravitational waveforms of binaries on eccentric orbits with Hansen coefficients. ***PHYS REV D*** 92:(4) Paper 044038. 15 p. (2015)

16. Szabados LB, Tod P: A positive Bondi-type mass in asymptotically de Sitter spacetimes. ***CLASSICAL QUANT GRAV*** 32:(20) Paper 205011. 52 p. (2015)

Others

17. Anisovich VV, Nikonov VA, Nyiri J: Hadron diffractive scattering at ultrahigh energies, real part of the amplitude and Coulomb interaction. **arXiv:1508.02140 [hep-ph]** pp. 1-5 (2015)

18. Anisovich VV, Matveev MA, Nyiri J, Sarantsev AV, Semenova AN: Pentaquarks and resonances in the pJ/ψ spectrum. **arXiv:1507.07652 [hep-ph]** pp. 1-8 (2015)

R-B. Heavy-ion physics

Wigner research group

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

High-energy heavy-ion physics is connected to a large variety of physics disciplines. Our researches probe fundamental concepts of classical and modern thermodynamics, hydrodynamics, and quantum field theory. Therefore, we have several theoretical and practical topical research directions covering a wide spectrum, such as: thermodynamics, perturbative and non-perturbative QCD, high-energy nuclear effects, hadronization, hadron phenomenology, phenomenology of compact stars, and gravity/cosmology. Our studies are strongly motivated by the needs of several recent and planned large-scale facilities, such as collaborations at the LHC (CERN, Switzerland) and RHIC (BNL, USA), and future experiments at FAIR (GSI, Germany) and NICA (JINR, Russia). We have continued our theoretical investigations of high-energy physics phenomenology related to existing and future state-of-the-art detector systems. Concerning international theoretical collaborations, we have performed joint work with the Goethe University (Germany), LBNL (USA), CCNU (China), UNAM (Mexico), and ERI (Japan). We highlight below some of our major published results in detail.

Glueballs: new particles in heavy-ion collisions. — Inspired by H. Stöcker (GSI) our group has presented the possibility that a quark-gluon plasma, temporarily produced in RHIC and LHC accelerator experiments, for a large part of its existence could be dominated by gluonic over quark effects; in particular by forming a new particle, '*glueball*' Hagedorn states before the final hadronization. This work is based on an earlier paper by T.S Biró with B. Müller in 1994, pointing out a much faster equilibration of gluon number in phase space than quark number based on QCD cross sections and zero starting numbers. This must shape the hadronization process in two ways: on the one hand it keeps the temperature higher and delays the hadron formation, on the other hand it prefers high lying resonances more easily constructed from glueball quantum numbers. Earlier results from the collaboration with A. Jakovác (ELTE) on analyzing the role of model spectral densities in the quark-gluon plasma – hadronic resonance gas-phase transition also supports this picture.

[#] Ph.D student
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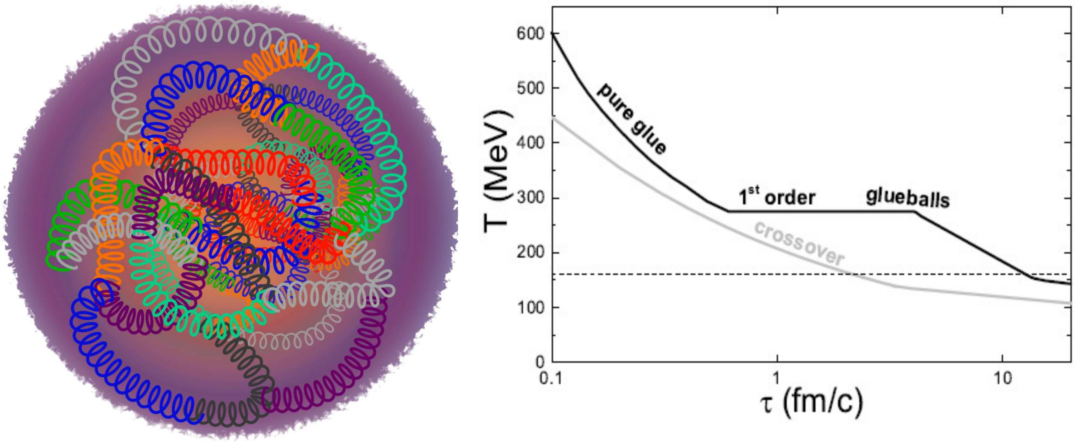

Figure 1. *Left: Artist's imagination of the gluon-formed particle, glueball by G. Bíró. Right: Schematic temperature evolution of pure-gluon matter with Yang-Mills first-order phase transition to glueballs [Astronomische Nachrichten 336 (2015) 744].*

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 Tsallis, Rényi and further non-Boltzmannian entropy formulas by T.S. Biró, P. Ván, and G.G. Barnaföldi led us to investigate the finite-reservoir effects on thermal properties. Our theoretical approach is based on the analysis of finite reservoir (finite total phase space) effects modifying the exponential one-particle energy distribution in two main ways: i) the finite heat capacity of the reservoir presses the distribution below the exponential, while ii) non-zero variance in the temperature raises it above. The Gaussian fluctuation model, standard textbook approach so far, assumes an exact balance between these two effects, equivalent to the famous one over square root of reservoir-size assumption for temperature fluctuations. We prove in our calculations that this textbook case can be realized also in small systems whenever the distribution of the fluctuating phase space dimensionality is exactly Poissonian, while for negative binomial type fluctuations – also measured experimentally – a Tsallis–Pareto type power-law tailed distribution emerges. This theory was tested by non-extensive quantum statistics as part of the Hungarian–Chinese bilateral collaboration with IoPP CCNU in Wuhan. T.S. Biró and K.M. Shen carried out a calculation about the correct handling of non-extensive quantum statistics of Bose and Fermi types. It turned out that only certain constructions with the deformed exponential function are allowed to be used in the common formulas if the particle - hole symmetry, which is a fundamental symmetry in the Nature, to be conserved. From this viewpoint the Kaniadakis kappa exponential can readily be applied, while the Tsallis formula has to be modified. Another investigation, separating soft and hard spectra components of the high-energy heavy-ion collisions was performed by G. Bíró, G.G. Barnaföldi, T.S. Biró and K. Ürmössy. In this study the soft/hard transition was found at 3.5 GeV/c transverse momentum and quantitative Tsallis parameters were also analyzed.

Phenomenological and hydrodynamical properties of Heavy-ion Collisions. — It is a hot and contemporary issue whether and why the seeming success of hydrodynamical description of heavy ion reactions is unreasonable. Our contribution with M. Horváth and Zs. Schram

(University of Debrecen) to this debate is based on semi-classical calculations of photon spectra in the electromagnetic field of decelerating charges, whose characteristics both remind one to the Unruh temperature and simulate a longitudinal flow pattern. As a new development we have established a model with collectively oriented dipole antennas in the reaction plane which delivers the observed transverse elliptic flow, too. Pair production in strong fields was modelled within inhomogeneous and time dependent electric fields by D. Berényi, P. Lévai, S. Varró, V.V. Skokov. We showed, that the particle yields and spectra can be drastically different from the predictions of the widely used homogeneous models. The transverse spectra can be used as a characteristic discriminant of homogeneous and inhomogeneous pair production processes. Work has also been started by the same authors on the investigation of models containing magnetic field besides the electric field, which can be connected to the Chiral Magnetic Effect (CME). Preliminary results show that the addition of magnetic field also increases the particle yield. Derivation of the generalized continuity-Fourier–Navier–Stokes system of equations independently of reference and flow-frames in the theory of Galilean-relativistic non-equilibrium thermodynamics has been performed by R. Kovács and P. Ván. We found this splits the source term of the Einstein equation into classical and quantum parts.

Development for heavy-ion computer simulations. — In collaboration with the University of Berkeley (USA) and IoPP CCNU (Wuhan, China), we have started the development of the HIJING heavy-ion Monte Carlo Generator. Sz.M. Harangozó, G. Papp (ELTE), G.G. Barnaföldi, G.Y. Ma (IoPP CCNU), and X.N. Wang (IoPP CCNU, LBNL), beside rewriting the 20 years old code from FORTRAN to the C++ programming languages, included new physical models and features into the codes. We included the DGLAP-evolved, QCD-scale dependent nuclear shadowing and decoherent scattering in order to describe the latest LHC results. We have also prepared the simulation framework for the inclusion of the experimental and detector simulations. In collaboration with the CERN OpenLab, G. Bíró, G.G. Barnaföldi, F. Carminati (CERN), and E. Futó took the first steps for the OpenCL version of the GeantV software. As it was presented, running GeantV on GPGPU architectures for cylindrical and cubic detector structures, the simulation became 15-30 times faster. GPGPU techniques in Boltzmann transport model were also investigated by D. Molnár (Purdue University, USA), G.G. Barnaföldi, M.F. Nagy-Egri, and D. Berényi. 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 suitable for GPGPU calculations because it mainly involves integration in two dimensions only.

Investigations of superdense matter and extra dimensions. — Cold compact stars and hot superdense matter created in high-energy heavy-ion collisions, provide the opportunity to speculate on the new states of matter. Source of the dark energy via off-shell source term in the Einstein equation was investigated by T.S. Bíró and P. Ván. We have finally published our speculative and yet interesting calculation about a possible source of dark energy, emerging from the treatment of the classical Einstein equation with a quantum source term, handled in analogy with the Madelung-transformed quantum wave function, and seeking for the optimal Jordan scheme to simplify the equations. In this model the quantum binding energy in Newtonian-gravity-bound elementary binary systems, 'gravonia' with a mass of 140 MeV each, delivers the experimentally observed extremely tiny cosmological constant. Investigations on the existence of compact stars in extra-dimensional, Kaluza–Klein space-time are also a phenomenological study by our group. In a simple extra dimensional Kaluza–Klein space-time authors Sz. Karsai, G.G. Barnaföldi, E. Forgács-Dajka and P. Pósfay reported the existence of stable solution of compact stars. The mass-radius, M(R)-relation of a degenerated, non-interacting fermion star in extra dimensional space-time was presented for the cases of large- and small-sized extra dimensions. As a result we found, there is no major effect on the size of the extra dimension. Dense matter existing in the interior of compact stars can be created in the GSI/FAIR accelerator and described by the linear sigma model. P. Kovács and Gy. Wolf presented a new equation of state, which can be tested at e.g. the planned PANDA or CBM detectors in the future. In collaboration with A. Jakovác (ELTE), G.G. Barnaföldi and P. Pósfay have constructed a framework for a politrop-like equation-of-state family using the Functional Renormalization Group Theory (FRG) for Walecka model in cold nuclear matter. Based on the first results, presented on the EPS HEP conference, the model is feasible; however the development of mathematical tools for FRG applications was required.

Identified hadron spectra with ALICE. — The Hungarian ALICE Group's main research direction is the measurements and analysis in connection with identified hadron production. We participated in the operation of the High Momentum Particle Identification Detector (HMPID) of the ALICE detector, the TPC upgrade and data analysis and the O2 DAQ upgrade projects. The HMPID aims to measure pion, kaon and proton spectra on a track-by-track basis up to 4.5 GeV/c. Besides, provided on-call shifts during 2015 for HMPID, we participated in the data analysis of the HMPID-identified spectra and the pion-to-proton ratio. On detector simulation side, the aging test of the HMPID CsI photo-cathode has been performed as well.

We also participated in the analysis of data collected by the ALICE Time Projection Chamber (TPC). TPC is able to measure the identified spectra using the relativistic-rise method. We analyzed data for proton-proton and proton-lead collisions in collaboration with the Mexican UNAM group. We signed 31 SCI referred papers, several conference proceedings and presented 5 posters.

Coordination of the ALICE upgrades. — We coordinate the Hungarian contribution to CERN's largest heavy-ion experiment ALICE. This activity is two-fold:

In addition to data analysis, our group plays an important role in the construction of the world’s largest, 80 m^3 volume, GEM TPC for ALICE. The ALICE TPC upgrade is a joint project with Wigner's Innovative Particle Detector Development “Lendület” group. Thanks to the support of the INFRA grant, we have built a new large-volume clean area dedicated to the quality assurance of the large-scale GEM foils (GEM QA). During the forthcoming 2-year project the large-scale TPC GEM foils will be scanned by an optical scanner and characterized by a Wigner-developed gain scanner. This CERN-coordinated giant project is in collaboration with the University of Helsinki (Finland), GSI Darmstadt, TU Munich (Germany) and Oak Ridge National Laboratory (USA).

Our group’s present participation and leading activity are in the ALICE Offline & Online (O2) Upgrade Project. Together with the Wigner DAQ Laboratory and Wigner GPU Laboratory, we prepare the upgrade of the ALICE data acquisition (DAQ) system for the high-luminosity (Run3) era of the Large Hadron Collider beyond 2018. We take part of the front-end and data collector development in collaboration with CERN, the University of Bergen (Norway), VECCAL (India) and the University of Marseilles (France). Our group is leading the CRU project in connection with CERN. In 2015, supported by the INFRA and KISINFRA grants we upgraded the Wigner DAQ Laboratory and equipped it with the latest technologies for development. A university-level laboratory has been created as well for MSc students from Eötvös University (ELTE) and Budapest University of Technology and Economics (BME).

Education, PR and future. — Connected to our group we had 3 BSc and 5 MSc students. Our young colleagues participated in young researcher's projects and TDK theses for competition: Sz. Karsai (Special Price, OTDK) and R. Kovács (1st place OTDK). Starting from September, these students attended to Doctoral Schools at ELTE (3) and BME (1), with them we have 6 young PhD students in the research group. Senior colleagues are members of the ELTE and BME doctoral schools. The following group members participated as guest editors: T. S. Biró as editor-in-chief in EPJ A Hadrons and Nuclei, and guest editor of the Wigner Yearbook 2015.

Group members actively participated in the organization of the following workshops, conferences and seminars: “Annual NewCompStar Conference 2015” as a member of the NewCompStar COST action MP1304; “The Future of Many-Core Computing in Science: GPU Day 2015” at Wigner RCP; “Zagreb – Budapest Meetup 2015 for ALICE” at the Wigner RCP and in Zagreb, Croatia; “CCNU – Wigner Balaton Workshop 2015”, Tihany; and the “Téridő a nyáridőben – nyáridő a téridőben” Space-time Summer School. T.S. Biró acts as the main organizer of the Wigner Colloquium series for our Institute.

Group members participated in PR activities such as the Colorful Physics Bus of the Wigner Institute, the “AtomCsill” series of the ELFT and Eötvös University, Simonyi Day (Wigner RCP), Science Day (Hungarian Academy of Sciences), and CERN and Wigner Open Days. We have regular invitations by high schools from Hungary and abroad for popular talks. Beside these activities we established a good media connection: we participated in several appearances in internet news articles, in radio programmes, in outreach films and on television.

Wigner GPU Laboratory. — The aim of the Wigner GPU Laboratory is to provide support for several fields in physics in parallel computing techniques, especially for faster numerical calculations in gravitational and high-energy physics, astronomy, astrophysics, and detector simulations. The Laboratory is working on a project basis and provides hardvare/software support for the above scientific directions. In 2015 we took part in related research projects such as: (i) Algebraic datatypes in distributed storage of structured data (B. Mórász and D. Berényi). It is known from functional programming that algebraic datatypes are well suited for storing hierarchic data widely used in numerical methods such as multi-dimensional grids and arrays. The size-dependent distributed storage of trees representing such data-structure can be automatized. A proof of concept implementation was made in C++ template metaprogramming to resolve in compile time known-sized trees. An extended demonstration will be sent to C++ developers (E. Niebler), who are also interested in such a technology. (ii) The goal of the phasespace-compression method project is to develop a massive Ordinary Differential Equation solver based on the interpolation of phase-space trajectories. The solution was demonstrated by M. Simkó and D. Berényi on simple systems, like Harmonic Oscillator and Lotka–Volterra model (implemented in Visual Basic and C++). Further studies are necessary for developing an optimal GPU compatible storage scheme. (iii) Chaotic three body problem investigated by G. Drótos (ELTE) and D. Berényi aims to perform solution of massive number of ODEs, to resolve the chaotic phase-space of the three body problem. Current code is using automatic code generation to create an OpenCL based GPU solver and the C++ host driver code. This solver can deliver 10000-100000 particle trajectories within a few tens of seconds on a consumer notebook that is more than 30 times faster than the single thread CPU solution. Currently enough data were accumulated to localize the chaotic saddle in the input and output parameter space. Further study and software developments are underway to calculate the fractal dimension, escape rate and asymptotic behaviour. (iv) We also took part in gravitational research, especially the GridRipper code development for gravitational wave simulation and detection (M.F. Nagy-Egri). We also started a joint scientific work with the international VIRGO/LIGO gravitational collaboration for investigation of the possibilities of fast, GPU-based gravitational-wave search technologies.

Grants

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

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

OTKA K109462: Theoretical investigations of the strongly interacting matter produced at FAIR (CBM, PANDA) and NICA (Dubna) (Gy. Wolf, 2012-16)

Bolyai János Scholarship of the H.A.S. (G.G. Barnaföldi, 2013-2016)

International cooperation

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

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

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

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)

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

Long term visitor

Giacomo Volpe (G.G. Barnaföldi, 2015.04.01-2015.10.31, 10 months), Dénes Molnár (G.G. Barnaföldi, 2015.11.15-2015.12.15, 1 month), Miklós Gyulassy (P. Lévai, 2 months), Guoyang Ma, Keming Shen (P. Lévai, 2 months), Ben-Wei Zhang, Daimei Zhou, Xin-Nian Wang (P. Lévai, 2 weeks)

Publications

Articles

1. Almási GA, Wolf Gy: Thermal, chemical and spectral equilibration in heavy-ion collisions. ***NUCL PHYS A*** 943: pp. 117-136. (2015)

2. Asszonyi Cs, Fülöp T, Ván P: Distinguished rheological models for solids in the framework of a thermodynamical internal variable theory. ***CONTINUUM MECH THERM*** 27:(6) pp. 971-986. (2015)

3. Barnaföldi GG, Ürmössy K, Bíró G: A 'soft+hard' model for Pion, Kaon, and Proton Spectra and v_2 measured in PbPb Collisions at √s= 2.76ATeV. ***J PHYS CONF SER*** 612:(1) Paper 012048. 5 p. (2015)

4. Berényi D, Varró S, Skokov VV, Lévai P: Pair production at the edge of the QED flux tube. ***PHYS LETT B*** 749: pp. 210-214. (2015)

5. Berényi D, Varró S, Lévai P, Skokov VV: Pair production from space- and time-dependent strong fields. ***J PHYS CONF SER*** 594:(1) Paper 012055. (2015)

6. Biro TS, Horvath M, Schram Z: Elliptic flow due to radiation in heavy-ion collisions. ***EUR PHYS J A*** 51:(7) Paper 75. 5 p. (2015)

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

ALICE Collaboration

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1. Abelev B et al. incl. Barnaföldi GG, Bencédi G, Boldizsár L, Dénes E, Hamar G, Kiss G, Lévai P, Oláh L, Pochybova S (962 authors): Charged jet cross sections and properties in proton-proton collisions at $\sqrt{s}$=7 TeV. ***PHYS REV D*** 91:(11) Paper 112012. 33 p. (2015)

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R-F. Holographic quantum field theory

"Momentum" research team

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

Richard Feynman: "*If you want to learn about nature, to appreciate n… understand the language that she speaks in.*"

According to our present knowledge the language of Nature is gauge theories: The electromagnetic, weak, strong and gravitational forces are the four fundamental interactions of Nature. The electromagnetic interaction and the weak interaction are unified by the SU(2) × U(1) electro-weak quantum gauge theory and have been tested with very high precision. The strong interaction is formulated by an SU(3) quantum gauge theory but tested analytically at high energies only. The gravitational interaction can be formulated as a classical gauge theory, but does not allow a satisfactory quantum field-theoretical formulation. Thus, although the language of Nature seems to be gauge theories, we do not have a satisfactory understanding of strongly interacting quantum gauge theories.

The primary aim of our community is to solve a strongly coupled 4D quantum gauge theory exactly. The simplest interacting 4D SU(N) gauge theory has the maximal amount of (super) symmetry and is considered to be the hydrogen atom of all gauge theories. This theory is invariant not only under scale transformations but also under conformal transformations, i.e. coordinate transformations that preserve angles. The large amount of conformal symmetry completely fixes the coordinate dependence of the two- and three-point functions in terms of the scaling dimensions of the fields. The multiplicative constant of the two-point function can be absorbed into the normalization of fields, but the three-point (3pt) coupling is a highly nontrivial dynamical quantity. Its importance lies in the fact that all higher-point correlation functions can be expressed in terms of the scaling dimensions and these three-point couplings, recursively. The unexpected opportunity to calculate the scaling dimensions and 3pt couplings of this theory came from a holographic duality.

Holographic dualities connect gauge theories with string theories including gravity. In a broad sense, holography is an equivalence between gravity in a d+1 dimensional open curved space and a strongly-coupled d-dimensional gauge theory living on the boundary of this space, in a way that is reminiscent of an optical hologram which stores a 3D image on a 2D holographic plate. Although such relations seem surprising, many holographic correspondences have been conjectured by now, the best established being the one proposed by Juan Maldacena in 1998. Maldacena's holographic correspondence relates the maximally supersymmetric 4D quantum gauge theory to superstring/gravity theory on the maximally symmetric negatively curved 5D anti de Sitter (AdS) space. Anti de Sitter space is the simplest solution of Einstein's equation with a negative cosmological constant, and is nothing but the Lorentzian analog of the Bolyai-Lobachevsky plane.

[#] Ph.D. student

The holographic correspondence is a kind of duality, as it connects strongly-coupled gauge theories to semi-classical string theory, and it relates the deeply quantum string theory (gravity) to perturbative gauge theory. This makes holography hard to prove – it remains a conjecture.

Heroic efforts have been undertaken in order to test Maldacena's conjecture. From the many case studies, the following consistent holographic dictionary has been set up: The energies of string states are related to the scaling dimensions of local gauge-invariant operators. The t' Hooft coupling of the gauge theory is proportional to the inverse of the string tension, while the number of colors is proportional to the inverse of the string coupling. In the planar (large color) limit, strings do not interact and one has to evaluate the string action on a two-dimensional cylindrically-shaped worldsheet to calculate its spectrum. The leading 1/N correction relates the 3pt couplings of the gauge theory to the amplitude of splitting a string into two other strings (see Figure 1). Due to the high number of symmetries, the effective two-dimensional field theory, namely the worldsheet string theory, turned out to be *integrable*.

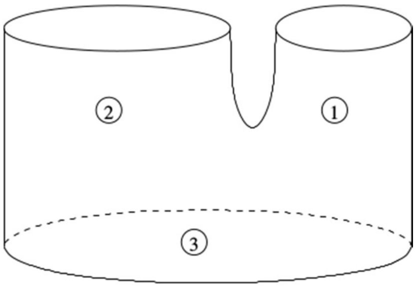

Figure 1. *Spacetime process in which a big string #3 splits into strings #1 and #2.*

Consequently, the holographic description allows us to use tools and methods that were developed for *two-dimensional* integrable quantum field theories to study the *four-dimensional* maximally symmetric gauge theory and the *ten dimensional* quantum string theory including quantum gravity.

It is instructive to recall how the two point functions were solved using the integrable S-matrix bootstrap method, since we follow a similar strategy to determine the 3pt functions. First, integrability was shown both at weak and at strong couplings and exploited in calculating systematic expansions. As these approximations didn't have any overlapping domain, bootstrap started to play the leading role. Assuming integrability for any coupling, powerful functional equations were formulated for the scattering matrix allowing the complete solution. This infinite volume S-matrix was then used to calculate the polynomially (Asymptotic Bethe Ansatz) and exponentially small (Luscher type) finite size corrections. These corrections were finally summed up by the Thermodynamic Bethe Ansatz (TBA) equations, which were nicely reformulated in a compact form via the quantum spectral curve.

The 3pt functions of the maximally supersymmetric 4D gauge theory are important for several reasons. First, they provide the missing fundamental conformal data for its complete solution. Second, they correspond, on the string theory side, to the amplitude of the process in which one big string splits into two small ones, or alternatively when two small strings join into a big one (see Figure 1). Thus it provides the exact string interactions of the theory, which is required to develop the quantum theory of strings, namely string field theory (SFT). The amplitude is called the SFT vertex, which hasn't been calculated explicitly except for the flat background. There have been already developments using integrability to calculate the 3pt functions both at weak and at strong couplings, together with their systematic expansions, but no overlapping domains have been found. Thus, just as it was the case for the spectral problem, bootstrap approach started to play a role. In our two very recent publications we advertised the adaptation of the well developed 2D integrable form factor bootstrap program to calculate the 3pt functions in the following way: We first decompactify the process in which a string of size L3 splits into two smaller strings of sizes L1 and L2 in two different ways by sending either L3 and L2 or L3 and L1 to infinity, see Figure 2. In this limit the finite size string serves as a non-local operator insertion and we derived restrictive functional relations for its matrix elements between the asymptotic states of the decompactified strings. These equations differ from the form factor equations of local operators due to the “missing space-time of the finite size string”, but reduce to them in the limit, when the small string shrinks to zero. This shrinking is a very singular limit, in which some nontrivial operator insertion can remain and the analysis requires a special care, what we started last year. In the case when both L1 and L2 are large the way that we can decompactify the problem in two alternative ways gives severe restrictions on the allowed solutions of the functional equations.

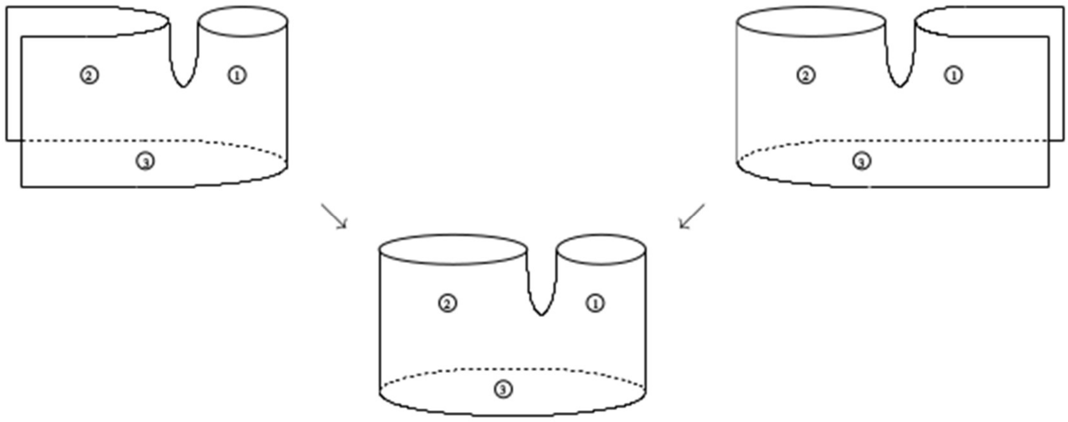

Figure 2. *The figure shows the splitting of string #3 into strings #1 and #2 and the program for obtaining the finite volume string field theory vertex via two alternative decompactifications and systematically including finite size corrections.*

Once all the amplitudes of the operator insertions are calculated in the decompactified case one has to take into account the finite size corrections. The polynomial corrections in the inverse of the sizes are related to the normalization of states and can be calculated from the Asymptotic Bethe Ansatz equations relying on the S-matrix. The exponentially small finite size corrections are not even known in the usual 2D integrable setting and we plan to advance into this direction in the future.

Grants

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

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

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

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

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

International cooperation

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

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

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

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

Long term visitors

Chaiho Rim, Seoul (Z. Bajnok, 2014.12.21-2015.02.31)

Publications

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See also: R-A.7

R-G. Computational systems neuroscience

"Momentum" research team

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Normative analysis of memory processes. — To enable learning in natural or relatively complex environments, the brain (or artificial learning agent) has to deal with the problem of model selection in a hypothesis space which grows with this environmental complexity, and which is necessarily iterative due to severe resource constraints. We hypothesize that this problem is a defining factor of the dynamics of human long term memory and its formal understanding will on the one hand lead to a normative explanation and predictions of how this system works and on the other hand allow the development of more efficient and human-like learning algorithms through abstracting away the human brain's solution.

We have investigated this problem in a probabilistic Gaussian mixture model setting, which while having the necessary complexity to require structure learning, remains tractable analytically for smaller datasets. We have developed a method that in the event of a model change lets us approximate the parameter posteriors and marginal likelihoods of the alternative models based only on the sufficient statistic for the previous model (which is the previous parameter posterior) through the predictive distribution. We have verified our hypothesis for the smaller, analytically tractable cases that selectively storing a small subset of the training set, that is by introducing an episodic memory, enables model selection. We have presented our results on a summer school and a conference during the autumn. In order to be able to generalize our argument we have developed a Sequential Monte Carlo approximation, which allowed us to scale up the problem to larger datasets that were intractable analytically - we are planning to present these results at a conference in January.

Optimal nonlinearity in the activity of visual cortical neurons. — The dynamics of the nervous system is characterized by many nonlinear effects at different levels of the computational hierarchy. From the point of view of information process, one of the most important form of nonlinearity is the firing rate nonlinearity (FRN): it has a substantial role in controlling the generation of the primary information carrier of the nervous system, the action potential. With a given neural response statistics the spiking nonlinearity is transformed into firing rate nonlinearity, which summarizes the nonlinear transformation of the integrated membrane potential response into stochastic firing rate responses. Characteristics and parametrization of the nonlinearity can differ from cell to cell and can also adapt in time.

Recent research has demonstrated that the evolution and adaptation are shaping the nervous system such that it behaves in a near optimal way. This observation is especially relevant for the early sensory cortices, including the primary visual cortex. Thus the question arises whether the firing rate nonlinearity found in the neurons of visual cortex reflects some optimality criterion posed by computations relevant to this brain area. Earlier research has

Ph.D. student

shown that the distribution of the sensitivities of visual cortical neurons reflects the statistics of natural images but the role of nonlinearity in optimal computations has not been explored before.

In the last year a general approach was adopted to the above mentioned optimality question based on a definite normative principle: the effectiveness of linear decodability from population response rates of V1 simple cells. Linear decoding is relevant because neuronal population can perform it easily. Inspiration comes from machine learning, where the role of nonlinearity in categorization and decoding is well known. We focused on decoding in the presence of so-called nuisance parameters, stimulus features other than the decoded one that still influence neural responses and that are ubiquitous in real-world tasks. We show that linear decoding of orientation from V1 simple cell membrane potentials is efficient when phase is held constant, but fails in the face of phase uncertainty.

Using simulations, the high accuracy of linear decoding based on firing rate population code is shown when phase is unknown. Importantly, this increased efficiency is relatively insensitive to the precise form of the FRN but altered membrane potential variability entails parallel changes in FRN threshold to ensure optimal decoding performance. The optimal threshold is turned out to be very close to the measured FRN threshold. Moreover, simulations based on our normative approach can predict the shift of the optimal threshold as a function of membrane potential variance, which is tested on intracellular recordings collected by our collaborators.

Since firing rate adaptation is a known phenomenon in certain situations, we examined the possibility of the alternative explanation for noise dependence of the optimal threshold based on the rate adaptation principle. We found that both normative principles lead to the same noise dependence, which indicates that a common information theoretic principle can stand behind both. This may be the subject of further investigations.

Statistical inference in the visual cortex. — To understand the mechanisms of vision in the cortex we need models that predict the measurable firing activity of neurons, and at the same time formalize computational principles that lead to object recognition and other high-level processing functions, and also lend themselves to straightforward interpretation. With this goal in mind we created a probabilistic model to predict stimulus-dependent coactivation of neurons in the visual cortex that may be described as edge detectors. We compared it to other models described in the literature from the computational point of view, and also to physiological measurements.

During the development of the visual cortex, edge detector neurons are organized according to their orientation selectivity. We demonstrated that parameter inference in a simple probabilistic model, describing learning visual regularities, is capable of explaining this organizing principle assuming local initial connectivity.

The measurable aspect of cellular activity is typically a series of action potentials, thus it is very important how the statistics of these series depend on the statistics of membrane potentials. We compared different stochastic and deterministic firing models, properties of which explain certain statistical properties of the neural response independently of the stimulus.

We used electro-physiological measurements recorded from the visual cortex of awake monkeys, collected in the Ernst Strüngmann Institute of Frankfurt, to map the dependence of the activity statistics of visual cortical neural populations on the interplay between the visual stimulus and the attentional state. By this we acquired a more complete picture of the possible implementation mechanisms of neural computation, enabling the testing of further model predictions.

Grants

"Momentum" Program of the HAS (G. Orbán, 2012-)

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

International cooperation

Central European University (József Fiser)

H.A.S. Research Institute for Experimental Physiology (Attila Gulyás)

University of Cambridge (Máté Lengyel)

UCLA (Peyman Golshani)

Ernst Strungmann Institute, Frankfurt (Wolf Singer)

Publications

See R-E.6

R-I. "Lendület" innovative particle detector development

"Momentum" research team

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The objectives of the project ran along two directions: first is the completion of the strategic infrastructure development, the other concerns research related to detector physics and specific project activities, including commitments to CERN experiments and other international communities. Considerable success was achieved to participate in H2020 projects.

The infrastructure developments led to a consolidated, flexible laboratory, which in the national "NEKIFUT" register reached the Strategic Research Infrastructure status. A key addition is a new clean room related to the re-building the Time Projection Chamber (TPC) of the ALICE detector at the Large Hadron Collider of CERN.

The single photon scanner, nicknamed "Leopard" has taken the task 13.4.4 within the AIDA-2020 project, and thus received a 45kEUR grant at a total budget of 90kEUR. This means that the "Leopard" project sustains its own financing.

Considerable results have been reached in the field of cosmic ray detection. Publications present surface and underground measurements. Two tracking detectors have been purchased abroad, which initiated research collaboration with the involved institutes (HZDR Dresden; KACST Riyadh). We have been invited to the Muographers-2015 symposium in Tokyo, where besides talks by group members, the keynote plenary talk was presented by prof. Péter Lévai, the DG of the Wigner RCP. A research collaboration agreement has been formally signed by Wigner RCP and the Earthquake Research Institute of The University of Tokyo. The main aim of the collaborative effort is to develop detectors for volcano imaging and possible eruption prediction. Muon radiography is complicated in practice: Figure 1 shows a visualization by a small size tracking system.

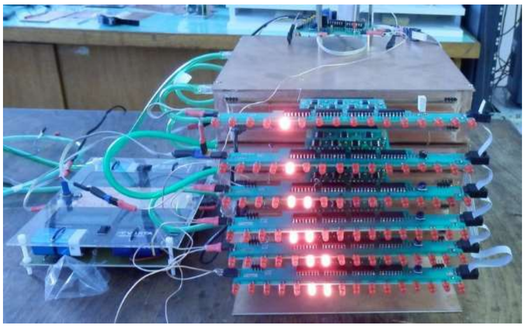

Figure 1. *Cosmic muon track visualized by an LED array, a model for the stand-alone tracking system developed by the group*

The participation of our research group has been approved in the TPC Upgrade project, which will concern the Quality Assurance of the GEM foils which will be built in. This officially means that Hungary will participate in the re-building of the ALICE TPC. The work will be performed in a newly built clean room, including optical scanning using a system developed by the Helsinki University, as well as our own system to directly measure the GEM gain map. Figure 2 shows

[#] Ph.D. student

the comparison of an optical (high resolution microscope) image of the hole sizes, with the measured amplification of the GEM layer.

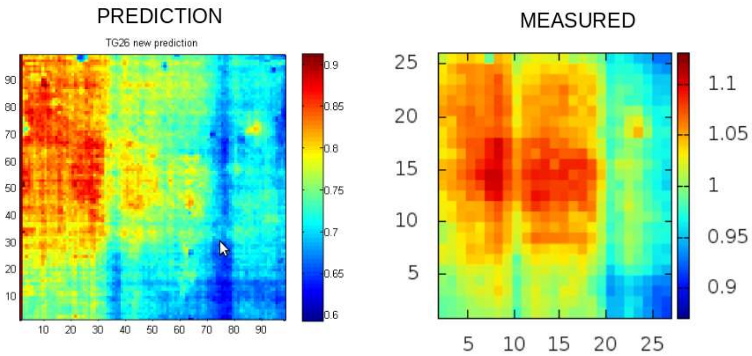

Figure 2. *Taking a GEM layer, 10 cm by 10 cm in size, the hole size distribution (left, measured at Helsinky University) correlates well with the measured amplification gain (right, our own result). The measurements are relevant to qualify GEM layers for construction in the upgraded ALICE TPC.*

The group has joined the BrightnESS project, a H2020-financed undertaking, with our aim in neutron detector development for the ESS facility in Lund. The detector concept, the so called "Multi Blade Detector", shown in Figure 3, developed by F. Piscitelli then at ILL, is based on an inclined boron layer which emits decay fragments, once it is irradiated by neutrons. Wigner RCP will contribute to construction, beam tests, simulations and electronics development.

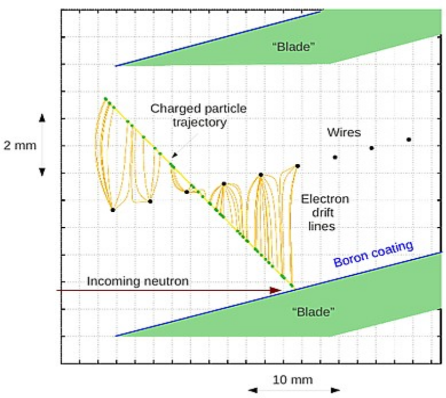

Figure 3. *The concept of a Multi-Blade neutron detector. The incident horizontal neutron arrives at grazing angle to be converted on the boron layer. The emitted charged fragment enters the sensitive volume and creates a measurable signal.*

The additional projects and assignments will progress in conjunction of availability of resources. One of the key participation is the Forward TPC construction for the NA61 Collaboration at the Super Proton Synchrotron of CERN. Along these lines, the outline for the NA61 data acquisition system has been published, led by group member András László.

Projects involving secondary school students continued with the leadership of Éva Oláh, who is a practicing teacher, and at the same time a PhD student at the Eötvös University. With the help of a successful EMET funding application, students were motivated for quality research, leading to competition results such as I. and III. Prizes at the national Innovation Competition.

Last year was particularly fruitful in defended Bachelor's and Master's theses, 4 in total, as well as presentations of TDK (undergraduate research project) activities. Notably, Gábor Galgóczi has won a I. prize at the prestigious National Scientific Students' Associations Conference competition.

Grants

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

AIDA-2020 (Advanced European Infrastructures for Detectors at Accelerators, WP13), H2020 (D. Varga, 2015-2018)

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

International cooperation

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

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

Publications

Articles

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2. Carena F, Carena W, Barroso VC, Costa F, Chapeland S, Delort C, Dénes E, Divià R, Fuchs U, Grigore A, Ionita C, Kiss T, Simonetti G, Soós C, Telesca A, Vyvre PV, Haller BV DDL, the ALICE data transmission protocol and its evolution from 2 to 6 Gb/s ***J INSTRUM*** 10:(4) Paper C04008. 6 p. (2015)

3. László A, Dénes E, Fodor Z, Kiss T, Kleinfelder S, Soós Cs, Tefelski D, Tölyhi T, Vesztergombi Gy, Wyszyński O: Design and Performance of the Data Acquisition System for the NA61/SHINE Experiment at CERN. ***NUCL INSTRUM METH A*** 798: pp. 1-11. (2015)

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Conference proceedings

7. Bencédi Gy, Barnaföldi GG, Molnár L: Identified Two-particle Correlations and Quantum Number Conservations in p-p and Pb-Pb Collisions at LHC Energies. In: *10th International Workshop on High-p_T Physics in the RHIC/LHC era . Nantes, France, 09.09.2014 – 09.12.2014* Paper B2. 11 p.

8. László A: A natural extension of the conformal Lorentz group in a field theory context. In: *Proc. Gribov-85 Memorial Workshop (2015): Theoretical Physics of XXI Century. Chernogolovka, Russia, 17.06.2015 – 20.06.2015*. Paper LaszloGR. 12 p.

See also: R-B.23, R-B. ALICE Collaboration, R-H. CMS Collaboration, R-H. NA49 Collaboration, R-J.16.

R-K. Femtosecond spectroscopy and X-ray spectroscopy

“Momentum” research team

György Vankó, Éva Bajnóczi, Csilla Bogdán, Zoltán Németh, Mátyás Pápai#, Emese Rozsályi, Dorottya Szemes#

Molecular transformations are essential for the functioning of molecular storage or switching devices, many light-harvesting systems, catalyzers, enzymes, to name a few. Such transformations take place at time scales ranging from femtoseconds to nanoseconds at the atomic or molecular level. In order to address the elementary physical steps and the intermediates of such processes, we need tools that can probe the dynamics of the electrons and the nuclei on these time scales. Pump-probe experiments are powerful tools that 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 shall promote the design of more efficient functional molecules. Here we report on experimental results and technical developments using X-ray probes in time-resolved investigations.

The performance of time-resolved X-ray spectroscopy in characterizing intermediates of photoswitching. — Photoswitchable molecular compounds have great potential in IT as molecular switches or storage systems. The usual description of the switching in Fe(II) complexes depicts changes along a single configuration coordinate (SCC), a breathing-mode-like combined stretching of the Fe–N bonds. While this gives a satisfactory description for most switchable Fe(II) complexes, several with tridentate ligands exhibit unusual and unexpected behavior when compared to predictions from the SCC model. Understanding their anomalous behavior can provide us with guidelines to design new ligands for applications. In a tridentate ligand, which has 3 atoms binding to the iron, the geometrical constraints of these atoms stemming from the molecular structure, and the interplay of the structural variations caused by the variation in the population of the 3d orbitals of Fe result in the failure of the SCC model. Moreover, due to the reduction in symmetry, the high-spin state, which is a $^5T_2$ state in octahedral symmetry, splits into two quintet states of different symmetry with terms ^5E and $^5B_2$ in this D_{2h} molecule, which raises an important question: which one is populated at the photoswitching? Quantum chemical calculations show that the answer depends on the populations of the Fe $3d_{xy}$, $3d_{xz}$ és $3d_{yz}$ non-bonding orbitals. The differences in the structure and molecular properties of these ^5E and $^5B_2$ quintet states are extremely small, presenting a significant challenge to any experiments to distinguish them. Nevertheless, it is vital for the photophysical description of the system to understand which is being populated, as this might lead to the theoretical design novel molecules with enhanced functionality that better suit applications. In order to achieve this goal theoretical and synchrotron studies of the excited state properties of the complex have been performed.

Ph.D. student

The quintet state of $[Fe(terpy)_2]^{2+}$ has been prepared with 10 ps-long 532 nm laser pulses in aqueous solution, and the changes of its molecular and electronic structure were characterized at 80 ps delay after light excitation with synchrotron probes. High-quality X-ray absorption, nonresonant and resonant X-ray emission spectra as well as X-ray diffuse scattering data (obtained at APS, Argonne) clearly reflect the formation of the quintet state. Besides, extended X-ray absorption fine structure spectroscopy resolves the Fe-N bond-length variations with extraordinary bond-length accuracy in time-resolved experiments. By ab initio calculations we have determined why one configurational coordinate is insufficient for description of the low-spin (LS) - high-spin (HS) transitions. We have identified the electronic structure origin of the differences between the two possible quintet modes, and unambiguously characterized the formed quintet state as ^5E. This exhaustive study also demonstrates the high performance of the X-ray spectroscopic and scattering techniques available in studying transient states on ultrafast time scales (Figure 1).

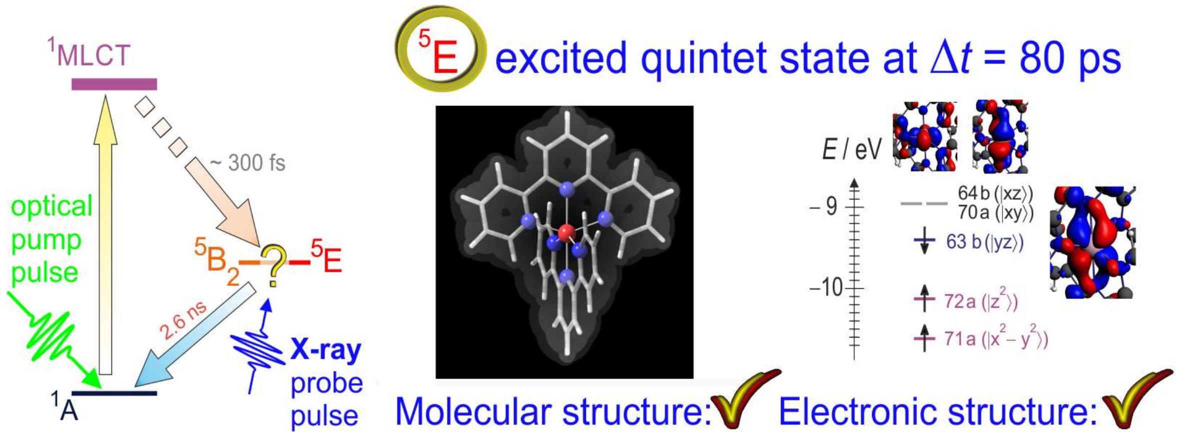

Figure 1. *Visual summary of our published paper providing a detailed characterization of the $[Fe(terpy)2]^{2+}$ system.*
(The full article can be accessed at http://dx.doi.org/10.1021/acs.jpcc.5b00557.)

Light-harvesting systems. — In our most remarkable experimental result published this year we successfully took advantage of the shorter-than-ps time resolution of the X-ray free electron lasers (XFEL), the element specificity as well as the spin momentum sensitivity of X-ray emission spectroscopy (XES), to study a model system of light-harvesting molecules. The efficiency of the widely spread multi-component photocatalytic systems is reduced by several diffusion controlled steps and cross section factors during their operation. In order to get rid of these disadvantages, it is possible to integrate both the photosensitive and the catalytic function into a single molecule. During the excitation of such a molecular system containing Ru and Co metallic centers, an electron, stemming from the absorbing Ru ion, is transported through the bridging ligand to the Co center and activates that. However, only the absorption bands belonging to the Ru ion and the electron on the bridging ligand can be identified by ultrafast optical spectroscopy, as neither the ground, nor the excited state of the Co ion has absorption in the visible range. However, with the help of different X-ray techniques the electron and structural dynamics of the Co can be investigated selectively, thus the details of the mechanism related to the Co centre can be revealed in XFEL studies. Figure 2 shows the molecule investigated at the SACLA hard X-ray free-electron laser and the steps of the light-induced transformation. X-ray emission spectroscopy revealed that the Co ion undergoes a consecutive charge and spin state change. The Co–N antibonding molecular orbitals are also populated with the spin state change, which causes a 0.2 Å bond length elongation, determined by X-ray diffuse scattering (XDS). This method also showed that the thermalization of the excited molecule happens with a 12 ps characteristic time. The details of the mechanism are listed on Figure 2.

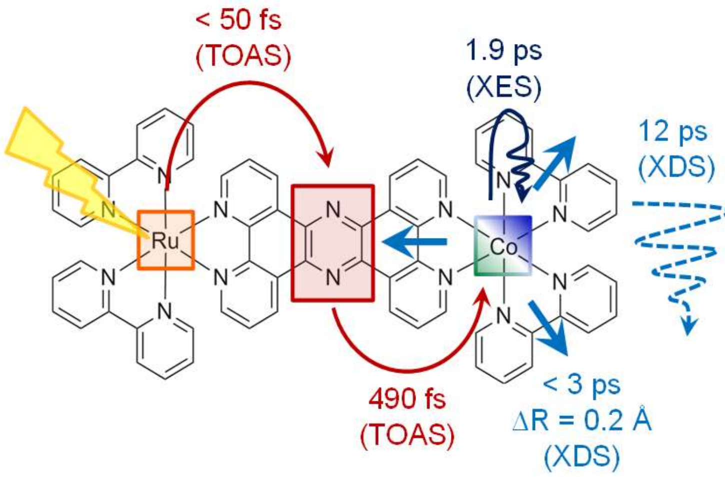

Figure 2. *The mechanism of the light-excitation triggered electron transfer process in the investigated photocatalytic model system, with the relevant characteristic times. The abbreviations of the techniques revealing the sequential steps are what follows. TOAS: transient optical absorption spectroscopy, XES: X-ray emission spectroscopy, XDS: X-ray diffuse scattering. (The article can be reached at the URL: http://dx.doi.org/10.1038/ncomms7359.)*

Valence-to-core X-ray emission spectroscopy as an ultrafast probe. — In the valence-to-core (vtc) X-ray emission, the electron hole created by the ionization of a core electron is filled by a valence electron. The final state of the process is equivalent to that in photoelectron spectroscopy; therefore, the chemical sensitivity of vtc XES is the highest among the XES techniques. It would be advantageous to apply this method as a probe during ultrafast experiments because of this sensitivity combined with the large penetration and element selectivity of the hard X-rays. However, the cross section for this emission process is quite low, three orders of magnitude lower than for the Kα emission.

The potential of the usage and development of vtc XES as an ultrafast probe were investigated in a photoionization process. The $[Fe(II)(CN)_6]^{4-}$ complex emits an electron as an effect of UV radiation, which process is used to produce solvated electrons frequently. Based on our density function theory (DFT) calculations this phenomena can be monitored via vtc XES, since the energy of the molecular orbitals shifts significantly with the change of the charge. The $[Fe(III)(CN)_6]^{3-}$ complex, the product of the ionization, is stable and can be prepared chemically, thus the expected spectral changes can be verified by static measurements. On the upper part of Figure 3 the static spectra of the above mentioned complexes are shown with blue and red line, respectively, while the difference of them is drawn with a green line (of which thickness corresponds to the experimental uncertainty). The lower part of the figure demonstrates the result of the DFT calculation, and for the Fe(II) complex it is also marked at the main transitions from which molecular orbital the electron comes from when the 1s electron hole is filled. During the first time-dependent experiment at the APS synchrotron the data acquisition was limited to only one delay time and four equidistant energy points due to the limited machine time (8 hours). The result of this experiment is shown on the upper part of Figure 3 with red dots. As it is clearly seen, the experimental transient matches the calculated one quite well. Although the intensity of the X-rays and the frequency of the data acquisition was not optimal during this experiment, the feasibility of vtc XES as a probe were successfully demonstrated, and the required experimental conditions were determined. This technique can prove particularly fruitful at the X-ray free-electron lasers and synchrotron beamlines with pink beam. Based on this experiment, and with the help of quantum chemical calculations, the feasibility of a specific experiment can be predicted with confidence.

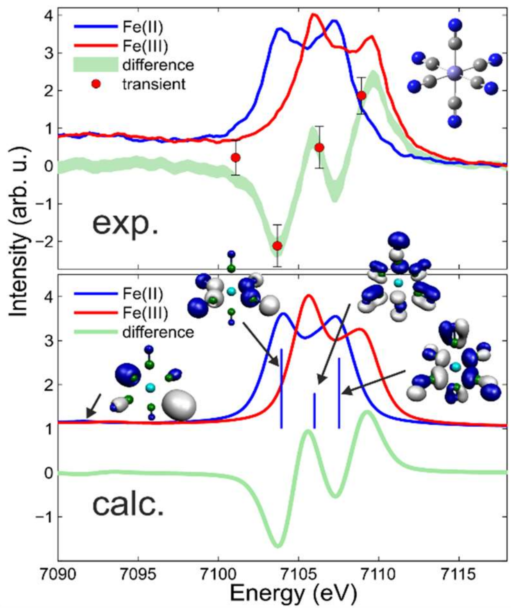

Figure 3. *The valence to core X-ray emission spectra of the $[Fe(II)(CN)_6]^{4-}$ (blue) and $[Fe(III)(CN)_6]^{3-}$ (red) complexes, and their difference (green). The experimental spectra are shown in the upper, while the DFT-calculated ones in the lower part of the figure. For $[Fe(II)(CN)_6]^{4-}$, the molecular orbitals giving rise to the transitions are also plotted. The red dots stand for the difference of the laser excited and the ground state (excitation wavelength is 266 nm, and the delay time was 120 ps after the excitation). The paper can be downloaded from* http://dx.doi.org/10.1021/jp511838q.

Grants

ERC Starting Grant, ERC-StG 259709, X-cited! : Electronic transitions and bistability: states, switches, transitions and dynamics studied with high-resolution X-ray spectroscopy (G. Vankó, 2010–2015)

"Momentum" Program of the HAS (G. Vankó, 2013 – 2018)

International cooperation

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

Publications

Articles

1. Canton SE et al. incl. Vankó G, Németh Z, Pápai M (33 authors): Visualizing the Nonequilibrium Dynamics of Photoinduced Intramolecular Electron Transfer with Femtosecond X-ray Pulses. ***NAT COMMUN*** 6: Paper 6359. 9 p. (2015)

2. Canton SE, Zhang X, Liu Y, Zhang J, Pápai M, Corani A, Smeigh AL, Smolentsev G, Attenkofer K, Jennings G, Kurtz CA, Li F, Harlang T, Vithanage D, Chabera P, Bordage A, Sun L, Ott S, Wärnmark K, Sundström V: Watching the dynamics of electrons and atoms at work in solar energy conversion. ***FARADAY DISCUSS*** 185: pp. 51-68. (2015)

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See also: R-M.5

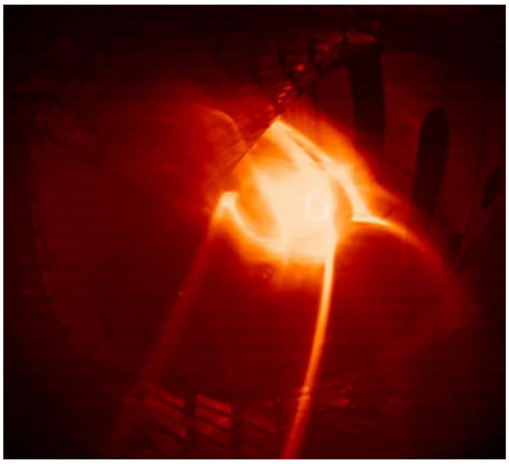
R-R. Pellet and video diagnostics

Wigner research group

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

Video diagnostics system at the Wendelstein 7-X stellarator (W7-X) — Our group has developed a 10-channel overview video diagnostic system for W7-X (based on self-developed EDICAM cameras), with the aim to monitor almost the entire inner wall, and detect dangerous events. In 2015 all ten channels were delivered, three of them in a modified set-up: two channels are using PCO Pixelfly cameras to detect low-light events, while the third channel was changed due to a leak in the housing AEQ port. In this third channel an image guide was installed, which was used to set up an ultra-fast video observation channel (camera: Photron SA5) with a frame rate up to 1 million fps. This fast observation is used to monitor rapidly changing or short-lived phenomena.

A special software "VIDACS" was developed for the simultaneous control of the multiple camera channels. The first version of VIDACS was delivered to W7-X, and it was able to operate the EDICAMs when W7-X started up. The EDICAM system recorded the first plasma discharge and displayed the images real-time for the audience in the control room. These images have been published by many newspapers and TV-channels (e.g. BBC, ZDF, Süddeutsche Zeitung, Die Welt and National Geographic Hungary).



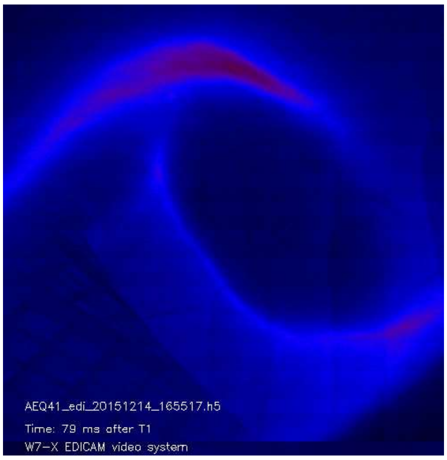


Figure 1. *Images of the first plasma discharges of Wendelstein 7-X.*

The EDICAM system was the first diagnostic tool to confirm that the plasma volume in W7-X has reached its achievable maximum. At this point, the plasma touches the limiter structures; however, no other diagnostics, including IR cameras monitoring limiter temperatures, have confirmed this. The reason for this is that a strongly radiating neutral gas mantle is formed around the plasma due to the high outgassing of the carbon plasma facing components, acting as a thermic insulating layer between the plasma and the limiter. Refined analysis of full temperature range IR cameras have shown that the EDICAM measurements were correct,

Ph.D. student

and the plasma reaches the limiter, however the temperature rise of the limiter structures is below 100°C, whereas the monitoring IR cameras' operating range starts above 300°C.

To be able to effectively analyze multiple movies simultaneously, the "EDVIS" software was developed, and the Beta version was used to display and compare plasma sequences. The EDVIS is capable to handle ten different video streams of various (file) formats, therefore, it is not only suitable to compare EDICAM movies, but also recordings from other imaging devices. The image processing toolbox of EDIVIS has the following functionality: displaying movie frames in various artificial color schemes, zooming; it is possible to select an area within a movie frame and integrate the light intensity for all frames within this area, then display the result as a time trace; the integration of the selected area can take place both in 1D and 2D, the result being a heat map or a single trace, respectively; the produced time traces can be compared to time traces from other diagnostics (read from the archive system); it is possible to load spatial calibration for the EDICAM views, allowing the user to overplot structural elements and/or plasma surfaces onto the displayed image.

Reliability study of pellet ELM pace making — The injection of cryogenic solid hydrogen isotope pellets turned out to become a potentially powerful tool for ELM pace making in devices where at least parts of the plasma facing components had carbon surfaces. In modern, more reactor relevant all-metal wall machines - due to the wall material - significant changes of the pedestal conditions and the ELM dynamics were observed. This implies that the reliability of pellet ELM pace making technique should be reconsidered as well. In the last campaigns of all-metal wall ASDEX Upgrade and JET special emphasis was put to investigate the reliability of pellet ELM triggering, with remarkable contributions of HAS scientists. The experiments revealed that - in spite of similar pellet caused perturbation - the pellet ELM triggering potential was reduced in certain plasma scenarios. In general, the probability of a pellet triggering an ELM is dependent on the time elapsed since the previous ELM. Even lag times were observed where this probability drops to zero. It was found when using Nitrogen seeding for confinement improvement also some of the pellet trigger potential was recovered.

Pellet cloud database analysis with a synthetic diagnostic — Cryogenic pellet injection is one of the most successful ways to fuel fusion plasmas. The goal at pellet fueling is that the pellet material penetrates into the plasma as deep as possible. The penetration depth is determined by the process of ablation, a complex interaction of the incident energy with the dense pellet cloud and the pellet itself. The characteristics of the pellet cloud (e.g. density and temperature) play a key role in the ablation process, however, they cannot be measured due to the extremely short lifetime (several microseconds) – only the light emitted by the cloud can be detected using ultra-fast imaging. Using spatially calibrated images of fast visible cameras, a database was established containing pellet cloud images and the related pellet- and plasma parameters. Using this pellet cloud database, four main cloud types were identified, based on the number of detected radiation maxima. A synthetic diagnostic, simulating the observation system and producing a synthetic pellet cloud image based on the output of pellet cloud simulations, was developed. The aim of this synthetic diagnostic is to reveal the underlying density and temperature distributions of the observed pellet clouds, by matching light emission distributions of simulated and measured cloud images. Our goal is to derive a scaling law for the toroidal extension of the pellet cloud at

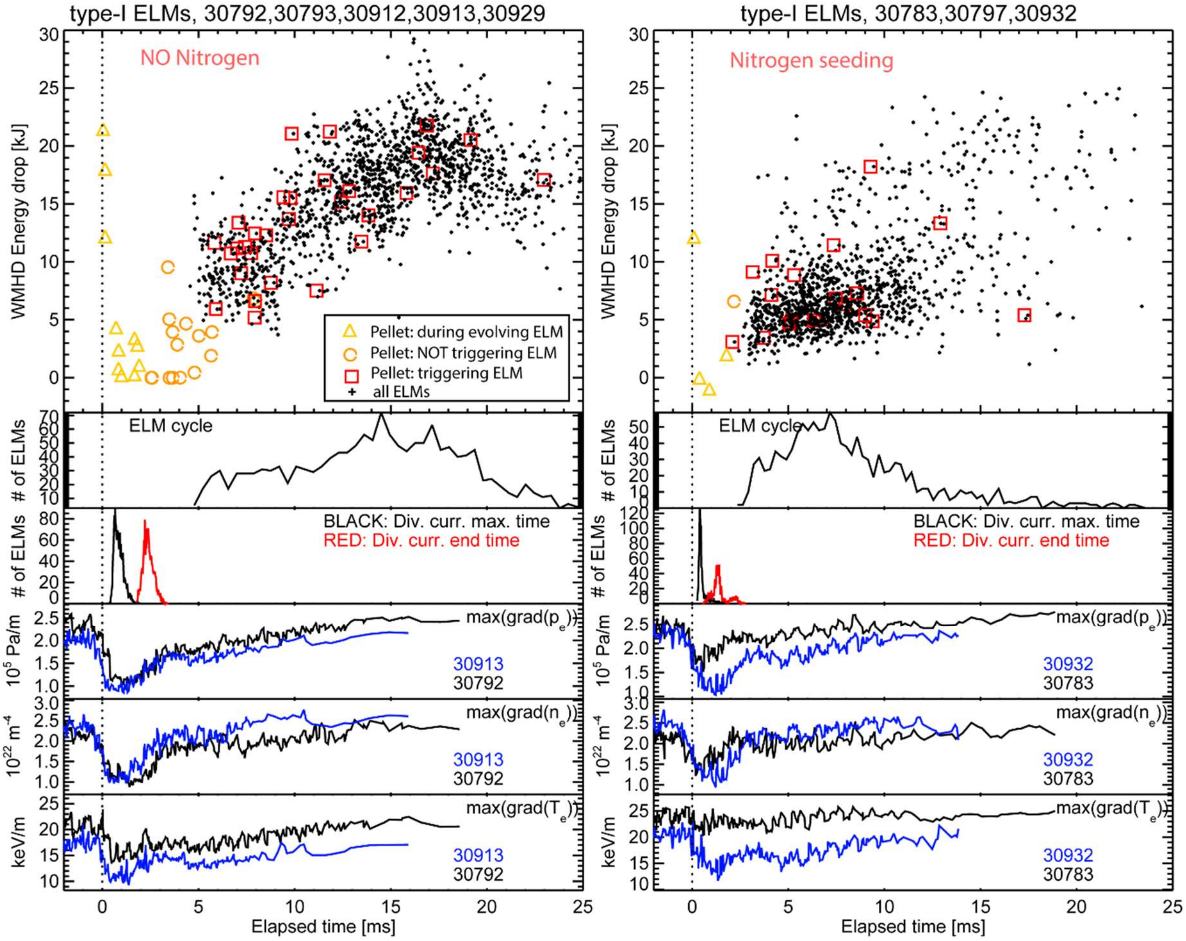


Figure 2. *The ELM provoked plasma energy drop as a function of the time elapsed after the previous ELM both for spontaneous and pellet triggered ELMs. The right column shows the Nitrogen seeded case (Nitrogen puff rate is about 2.5*10*^{21} *s*$^{-1}$*), while the left column is for similar discharges without Nitrogen puffing. The evolution of the pedestal gradients and statistics about the ELM dynamics (cycle, crash dynamics characterised by the divertor current measurements) are also plotted for both cases.*

different pellet- and plasma conditions, to give a more reliable input for the pellet ELM triggering simulations and using these two results for a better understanding of the pellet-caused pressure perturbation. Running the synthetic diagnostic with density- and temperature distributions coming from a simulation, we experienced fair agreement between the calculated and the experimental two-dimensional brightness distribution. Then, using the simulation data, the electron pressure of the cloud was calculated and normalized with the background plasma electron pressure used in the simulation. The calculation shows, that there are two maxima of the pressure in the cloud, which are located at 5 cm (measured from the middle of the cloud), where it is 45 times the pressure of the background plasma and it stays above 10 times the background plasma value as far as 6 m along the magnetic field line. This means, that the two maxima of the pressure perturbation are at around the edge of the visible cloud - the location of these maxima can be estimated using the above mentioned scaling of the pellet cloud length - and the whole (including the fully ionized part of the) pellet cloud length can be more than 10 m at a machine similar to ASDEX Upgrade in size.

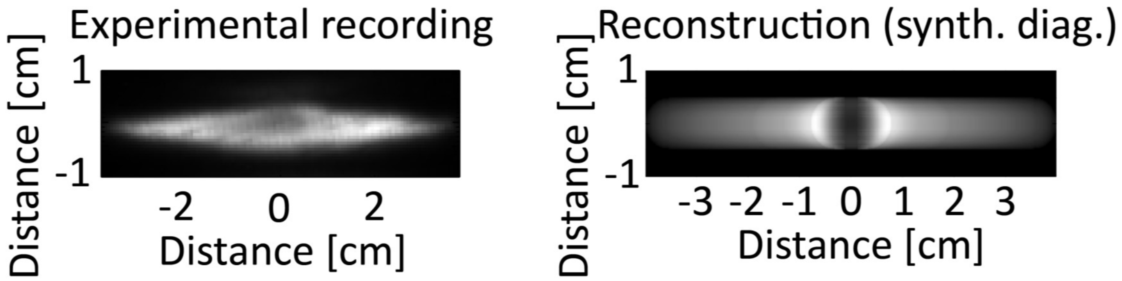


Figure 3. *Left: an original recording of the „cigar" cloud type with two radiation maxima. Right: the reconstructed cloud type with two radiation maxima.*

Table-top pellet injector (TATOP) development — In 2015 a new test with vacuum capability has been designed and constructed, in order to optimize the pellet launching mechanism as well as the collection efficiency. Several new designs were developed for the stop cylinder, addressing the problem of a large scatter in the angle of the launched pellets.

Grants

EUROfusion: WP Medium-Size Tokamak 1 (G. Kocsis, 2014-2015)
EUROfusion: WPJET1 (G. Kocsis, 2014-2015)
EUROfusion: WPS1 (T. Szepesi, 2014-2015)
EUROfusion: WP SA (T. Szepesi, 2014-2015)

International cooperation

Max-Planck-Institut für Plasmaphysik, Garching, Germany (G. Kocsis)
Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald, Germany (T. Szepesi)
Culham Centre for Fusion Energy, Oxfordshire, UK (G. Kocsis)
Japan Atomic Energy Agency, Naka, Japan (T. Szepesi)

Publications

Articles

1. Dibon M, Baldzuhn J, Beck M, Cardella A, Köchl F, Kocsis G, Lang PT, Macian-Juan R, Ploeckl B, Szepesi T, Weisbart W: Blower Gun pellet injection system for W7-X. ***FUSION ENG DES*** 98-99: pp. 1759-1762. (2015)

2. Kocsis G, Baross T, Biedermann C, Bodnár G, Cseh G, Ilkei T, König R, Otte M, Szabolics T, Szepesi T, Zoletnik S: Overview video diagnostics for the W7-X stellarator. Proceedings of the 28th Symposium On Fusion Technology (SOFT-28). ***FUSION ENG DES*** 96-97: pp. 808-811. (2015)

3. Szabolics T, Cseh G, Kocsis G, Szepesi T, Zoletnik S: Event Detection Intelligent Camera: Demonstration of flexible, real-time data taking and processing. Proceedings of the 28th Symposium On Fusion Technology (SOFT-28). ***FUSION ENG DES*** 96-97: pp. 980-984. (2015)

ASDEX Upgrade Team

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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See also: R-Q: JET EFDA Contributions

R-S. Space Physics

Wigner research group

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Solar System Bodies and Magnetospheres

Cometary physics. — The Rosetta spacecraft of ESA performed the first ever orbital insertion and landing on a comet in 2014. Since August 2014 the orbiter is continuously measuring the properties of the induced magnetosphere – the environment surrounding the nucleus of the comet. It followed the variation of the activity from its very beginning to its maximum, and observed the properties and interactions of the gas, dust, plasma and electromagnetic fields in the coma. Thanks to these measurements our knowledge about comets has grown enormously.

At the beginning of the year we observed a low activity comet with a tenuous neutral atmosphere and relatively few dust grains around it. The solar wind still reached the spacecraft orbiting in the inner regions of the induced magnetosphere, and probably also reached the nucleus. The interaction of the solar wind with the cometary matter caused solar wind deflection, acceleration of cometary ions and electrons as well as some instabilities generating persistent low frequency waves near the comet. The Rosetta Plasma Consortium (including researchers from Wigner RCP) presented their findings about this unique environment in several scientific papers.

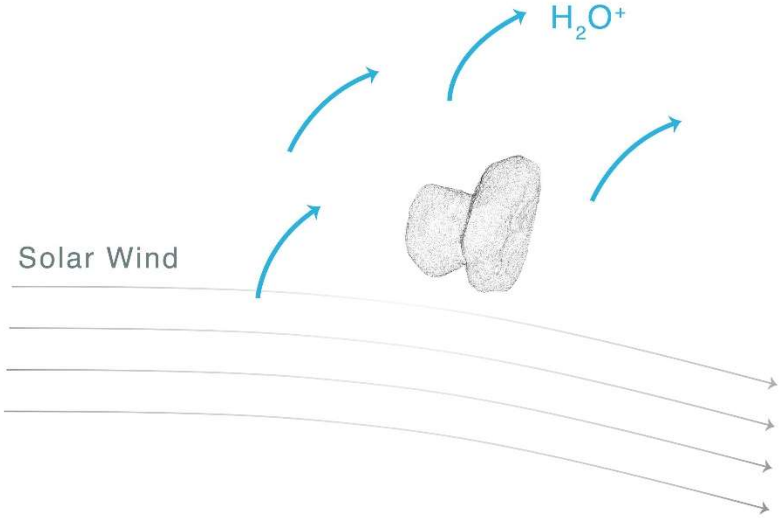

Figure 1. An illustration of the simultaneous processes of solar wind deflection and cometary ion acceleration (credit: RPC ICA).

In the spring and early summer the plasma environment changed drastically. The density of the cometary plasma increased and this plasma expelled the solar wind out of the inner

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magnetosphere. Strange ion events occurred frequently during this period, in which the measured ion energy first increased then decreased. Near the perihelion of comet 67P/Churyumov-Gerasimenko in August 2015 the cometary activity reached its maximum. Most accelerated ion events disappeared and the spacecraft observed a calmer inner region in that time. During this period Rosetta has discovered the diamagnetic cavity of the comet and explored its properties. Most of the papers describing this phase of the mission will be published in 2016. In the autumn of last year the comet moved away from the Sun, the activity decreased and the accelerated ion events reappeared. We now have enough information about the plasma environment to separate temporal and spatial effects, and we can start to build a model of the structure of the magnetosphere. Also we are beginning to understand the physical processes governing this unique environment.

The Grain Impact Analyzer and Dust Accumulator (GIADA) instrument on board Rosetta was able to constrain the origin of the dust particles detected within the coma of comet 67P/Churyumov–Gerasimenko. The collected particles belong to two families: (i) compact particles (ranging in size from 0.03 to 1 mm), witnessing the presence of materials that underwent processing within the solar nebula and (ii) fluffy aggregates (ranging in size from 0.2 to 2.5 mm) of sub-micron grains that may be a record of a primitive component, probably linked to interstellar dust. The dynamics of the fluffy aggregates constrain their equivalent bulk density to <1 kg/m^3. These aggregates are charged, fragmented, and decelerated by the spacecraft negative potential and enter GIADA in showers of fragments at speeds <1 m/s. The density of such optically thick aggregates is consistent with the low bulk density of the nucleus. The mass contribution of the fluffy aggregates to the refractory component of the nucleus is negligible and their coma brightness contribution is less than 15%.

The magnetosphere and moons of Saturn. — The Cassini spacecraft detected rock nanograin dust particles in the Kronian system. Our extensive, four-year analysis of data from the spacecraft, combined with our computer simulations and laboratory experiments led us to conclude that the tiny dust particles most likely form when hot water containing dissolved minerals from the moon's rocky interior travels upward, coming into contact with cooler water. It is exciting that we can use these tiny grains of rock, spewed into space by geysers on Enceladus, to tell us about conditions on -and beneath- the ocean floor of an icy moon in the Kronian system. These results were reported in Nature.

We used numerical ion velocity moments derived from the measurements of the Cassini Plasma Spectrometer to reveal the latitudinal structure of the nightside outer magnetosphere of Saturn. It turns out that the magnetosphere consists of shells rotating with different velocities; the innermost shell is rotating with the highest speed and the speed is decreasing as moving outward.

We were taking a leading part in a review of the magnetodiscs of giant planets. The magnetodisc is a complex magnetized plasma phenomenon, which influences almost every property of the magnetospheres of Jupiter and Saturn.

Space Weather. — The Sun, the planets and other solar system objects are connected by charged particles and fields, which fill the interplanetary space. The details of this complex plasma interaction are the subject of space weather studies. It includes questions about how particles and fields of solar origin interact with solar system objects. In this year we investigated several aspects of space weather, including the “prediction” of space weather by propagating effects measured by several spacecraft to other interesting sites of the Solar System; its effects on the magnetospheres of Solar System bodies; and also suprathermal ion and electron events.

Space weather propagation. — Propagation of measured solar wind parameters to other distances from the Sun is a key to predict space weather. The ambient solar wind and transient events have to be handled separately. Our team develops a new, problem-tailored propagation tool that takes into account these differences and concentrates on the exact location where the prediction should be the most accurate. Based on our expertise in these propagation methods, we participate in the EU financed Europlanet2020-RI project, where we work on the improvement of such planetary space weather services. This work is performed in the work package of joint research activity for planetary space weather services.

Space weather effects on Solar System bodies. — Interplanetary coronal mass ejections (ICMEs) bombard the induced magnetosphere of Venus frequently. Their influence on the position and size of the bow shock, on the plasma properties of the magnetic barrier, and on the position of the ion composition boundary (ICB) was explored by our group.

Other solar wind disturbances, the so-called corotating interaction regions (CIRs) cause abrupt changes in cometary magnetospheres according to our findings. Strong ion, electron, and magnetic field disturbances follow the arrival of CIRs, which also influence the interaction of the solar wind with the cometary plasma.

Suprathermal ions

The energy spectra and abundance ratios of 0.04-2 MeV/nucleon ^{3}He, ^{4}He, Fe, C, and O ions were studied using ULEIS/ACE data during the recent solar minimum. The ratio of suprathermal C/O and Fe/O arising from coronal holes were found to correlate with their bulk solar wind ratios from coronal holes (SWICS/ACE data) whereas 40-80 keV/nucleon ^{4}He/O ratios were about two times higher than their bulk wind values. The ion spectra obtained were fitted by power-law functions or combined power-law/exponential and they suggest different mechanisms of acceleration.

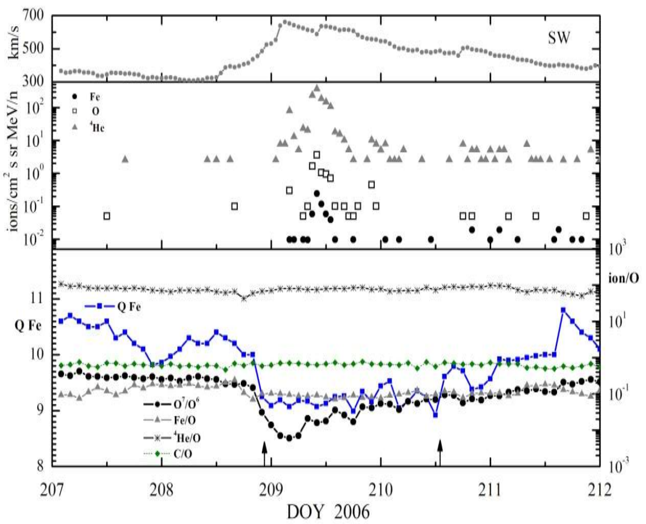

Figure 2. Solar wind speed (top panel), suprathermal ion intensities (middle panel) and bulk wind ion abundance ratios (bottom panel) in the fast solar wind stream from a near-equatorial coronal hole in 2006.

Jovian electrons. — Simultaneously with 27-day variations of MeV Jovian electrons, observed during the deep solar minimum in 2007-2008 in 14 consequent solar rotations, short duration

(2-3 days) enhancements of the fluxes of 0.1-1 MeV electrons and protons were also registered. We explained the observations hypothesizing that a magnetic trap with trapped Jovian electrons, corotating with the Sun, had some specific regions – «ridges» - with enhanced level of turbulence inside capable of accelerating electrons and protons up to 1 MeV. These ridges appear to be rather stable, surviving a few solar rotations. According to our model, confirmed by numerical simulations, the electrons registered have two components: (a) periodic 27-day gradual Jovian-originated variations; (b) quasi-periodic short (2-3 days) increases of low-energy electrons and protons, accelerated directly inside the magnetic trap.

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S-A. Strongly correlated systems

"Momentum" research team

Örs Legeza, Gergely Barcza, Imre Hagymási, Jenő Sólyom[E], Szilárd Szalay, Máté Tímár[#], Libor Veis[A]

In this year we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG) and *Tree Tensor Network State* algorithm (TTNS) resulting in thirteen accepted articles. Another three manuscripts are under referee procedure. We have also given thirty-one talks on different conferences and seminars, and we have presented fourteen posters. 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 molecular quantum chemistry, or for the quantum simulation of the information technology itself. Major algorithmic developments have also been carried out concerning the quantum chemistry TTNS algorithm. The TTNS code has become Hamiltonian-independent, such as the QC-DMRG code, and several parts of the code have been converted to C++. We have developed an improved version of the relativistic 4c-DMRG based on local C^4 tensor space representation. We have also developed a UHF version of the DMRG code. 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 ultra cold atomic systems, and determined the correlation and entanglement patterns in molecules playing important role in chemical reactions.

Method of Increments (MoI). — We have employed the Method of Increments (MoI) using a multireference approach to calculate the dissociation curve of beryllium ring-shaped clusters of different sizes. Benchmarks obtained through different single- and multireference methods, including the ab-initio DMRG, have been used to verify the validity of the MoI truncation, which showed a reliable behaviour for the whole dissociation curve. Moreover, we have investigated the size dependence of the correlation energy at different distances in order to extrapolate the values for the periodic chain and to discuss the transition from a metal-like to an insulating-like behaviour of the wave function through quantum chemical considerations.

Nuclear structure theory. — We have presented an efficient implementation of the DMRG algorithm that includes an optimal ordering of the proton and neutron orbitals and an efficient expansion of the active space, utilizing various concepts of quantum information theory. First we have shown how this new DMRG methodology could solve a previous 400 keV discrepancy in the ground state energy of ^{56}Ni. We have then reported the first DMRG results in the pf+g9/2 shell model space for the ground 0+ and first 2+ states of ^{64}Ge, which are benchmarked with reference data obtained from Monte Carlo shell model. The

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corresponding correlation structure among the proton and neutron orbitals has been determined in terms of the two-orbital mutual information. Based on such correlation graphs, we have proposed several further algorithmic improvement possibilities that can be utilized in a new generation of tensor network based algorithms.

Fermionic orbital optimization in tensor network states. — Tensor network states and, specifically, matrix-product states have proven to be a powerful tool for simulating ground states of strongly correlated spin models and fermionic problems. A new freedom arising in non-local fermionic systems is the choice of orbitals, it is far from clear what choice of fermionic orbitals to make. We have proposed a way to overcome this challenge and suggested a method intertwining the optimization over MPSs with suitable fermionic Gaussian mode transformations, hence bringing the advantages of both approaches together. The described algorithm generalizes basis changes in the spirit of the Hartree-Fock methods to MPSs, and provides a black-box tool for basis optimization in TNS methods.

Treatment of high-dimensional problems. — The treatment of high-dimensional problems, such as the Schrödinger equation, can be approached by concepts of tensor product approximation. We have presented general techniques that can be used for the treatment of high-dimensional optimization tasks and time-dependent equations, and connect them to concepts already used in many-body quantum physics. Based on achievements from the past decade, entanglement-based methods developed from different perspectives for different purposes in distinct communities already matured to provide a variety of tools can be combined to attack highly challenging problems in quantum chemistry. We have given a pedagogical introduction to the theoretical background of this novel field and demonstrated the underlying benefits through numerical applications on a text book example.

Bond-formation processes in metal-driven catalysis. — We have presented a conceptionally different approach to dissect bond-formation processes in metal-driven catalysis using concepts from quantum information theory. As a proof-of-principle example, the evolution of nickel-ethene bond-formation is dissected which has allowed us to monitor the interplay of back-bonding and π-donation along the reaction coordinate. Furthermore, the reaction pathway of nickel-ethene complexation has been analyzed using quantum chemistry methods, revealing the presence of a transition state. Our study supports the crucial role of metal-to-ligand back-donation in the bond-forming process of nickel-ethene.

Bonding mechanism of ethene to a nickel or palladium center. — The bonding mechanism of ethene to a nickel or palladium center has been studied by the DMRG algorithm, the complete active space self-consistent field method, coupled cluster theory, and density functional theory. Specifically, we have focused on the interaction between the metal atom and bis-ethene ligands in perpendicular and parallel orientations. The bonding situation in these structural isomers has been further scrutinized using energy decomposition analysis and quantum information theory. Our study highlights the fact that when two ethene ligands are oriented perpendicular to each other, the complex is stabilized by the metal-to-ligand double-back-bonding mechanism. Moreover, we have demonstrated that nickel-ethene complexes feature a stronger and more covalent interaction between the ligands and the metal center than palladium-ethene compounds with similar coordination spheres.

Concept of chemical bond and aromaticity based on quantum information theory. — Quantum information theory (QIT) emerged in physics as standard technique to extract relevant information from quantum systems. It has already contributed to the development of novel fields like quantum computing, quantum cryptography, and quantum complexity. This raises the question what information is stored according to QIT in molecules which are inherently quantum systems as well. Rigorous analysis of the central quantities of QIT on systematic series of molecules offered the introduction of the concept of chemical bond and aromaticity directly from physical principles and notions. We have identified covalent bond, donor-acceptor dative bond, multiple bond, charge-shift bond, and aromaticity indicating unified picture of fundamental chemical models from ab-initio data.

Quantum phase transitions in the SU(2)⊗XY spin-orbital Kumar model. — We have added a Heisenberg interaction term λ in the one-dimensional SU(2)⊗XY spin-orbital model introduced by B. Kumar. We have shown that a finite $\lambda>0$ leads to spontaneous dimerization of the system, which in the thermodynamic limit becomes a smooth phase transition at $\lambda \to 0$, whereas it remains discontinuous within the first order perturbation approach. We have presented the behavior of the entanglement entropy, energy gap and dimerization order parameter in the limit of $\lambda \to 0$, confirming the critical behavior. We have also shown the evidence of another phase transition in the Heisenberg limit $\lambda \to \infty$.

Extended periodic Anderson model. — We have also studied the ground-state properties of an extended periodic Anderson model to understand the role of Hund's coupling between localized and itinerant electrons using the DMRG algorithm. By calculating the von Neumann entropies we have shown that two phase transitions occur and two new phases appear as the hybridization is increased in the symmetric half-filled case due to the competition between Kondo-effect and Hund's coupling. In the intermediate phase, which is bounded by two critical points, we have found a dimerized ground state, while in the other spatially homogeneous phases the ground state is Haldane-like and Kondo-singlet-like, respectively. We have also determined the entanglement spectrum and the entanglement diagram of the system by calculating the mutual information thereby clarifying the structure of each phase.

We have also studied the momentum distribution of the electrons in an extended periodic Anderson model, where the interaction, U_{cf}, between itinerant and localized electrons is taken into account. In the symmetric half-filled model, due to the increase of the interorbital interaction, the f electrons become more and more delocalized, while the itinerancy of conduction electrons decreases. Above a certain value of U_{cf}, the f electrons become again localized together with the conduction electrons. In the less than half-filled case, we have observed that U_{cf} causes strong correlations between the f electrons in the mixed-valence regime.

Ultracold atomic systems. — We have investigated the competition of various exotic superfluid states in a chain of spin-polarized ultracold fermionic atoms with hyperfine spin F=3/2 and s-wave contact interactions. We have shown that the ground state is an exotic inhomogeneous mixture in which two distinct superfluid phases - spin-carrying pairs and singlet quartets - form alternating domains in an extended region of the parameter space.

We have investigated the spin-polarized chain of ultracold fermionic 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 have been studied analytically and by DMRG simulations. We 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 was 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 which is also reflected in the static structure factor. For strong enough coupling, spatial segregation between molecular crystals and ferromagnetic liquids emerges due to the large effective mass of the composite particles.

One- and two-dimensional Hubbard models in momentum space representation. — We have studied the properties of the ground states of the one- and two-dimensional Hubbard models at half filling and moderate doping, using entanglement-based measures using the momentum-space DMRG. The distribution of various entropic quantities in momentum space gives insight into the fundamental nature of the ground state, insight that can be used to make contact with weak-coupling-based analytical approaches and to optimize numerical methods, the momentum-space DMRG in particular.

Multipartite correlations. — We have revealed the lattice-theoretic structure of the partial separability classification. Then, we have introduced the notion of multipartite monotonicity, expressing that a given set of entanglement monotones, while measuring the different kinds of entanglement, shows also the same hierarchical structure as the entanglement classes. Then, we have constructed such hierarchies of entanglement measures, and proposed some physically well-motivated ones, based on the notion of statistical distinguishability.

Trans-polyacetylenes. — Quantum chemistry calculations provide the potential energy between two carbon atoms in ethane ($H_3C{-}CH_3$), ethene ($H_2C{=}CH_2$), and ethyne ($HC{\equiv}CH$) as a function of the atomic distance. Based on the energy function for the σ-bond in ethane, $V_\sigma(r)$, we have used the Hückel model with Hubbard-Ohno interaction for the π electrons to describe the energies $V_{\sigma\pi}(r)$ and $V_{\sigma\pi\pi}(r)$ for the $\sigma\pi$ double bond in ethene and the $\sigma\pi\pi$ triple bond in ethyne, respectively. The fit of the force functions has shown that the Peierls coupling can be estimated with some precision whereas the Hubbard-Ohno parameters are insignificant at the distances under consideration. We have applied the Hückel-Hubbard-Ohno model to describe the bond lengths and the energies of elementary electronic excitations of trans-polyacetylene, $(CH)_n$, and adjust the σ-bond potential for conjugated polymers.

Graphene nanoribbons. — We have investigated the ground state properties of graphene nanoribbons with two different edge configurations. Using the numerically exact DMRG algorithm, we have determined the entanglement patterns between the electrons on a honeycomb lattice. We plan to publish our results next year.

Grants

“Momentum” Program of the HAS (Ö. Legeza, 2012-2017)
OTKA K-100908 Simulating strongly correlated systems with fermionic alkaline earth atom isotopes in optical lattices and related quantum chemistry of transition metal complexes (Ö. Legeza, 2012-2016)
European Research Area Chemistry (OTKA NN110360, DFG SCHN 530/9-1 project under Grant No. 10041620 and FWF-E1243-N19) (Ö. Legeza, R. Schneider, F. Verstraete, 2013-2016)

International cooperation

ETH Zürich, (Zürich, Switzerland), Development of the relativistic DMRG algorithm (S. Knecht, M. Reiher)
Philipps-Universität Marburg, (Marburg, Germany), Optical properties of polydiacetylenes (F. Gebhard); Entanglement scaling in momentum space DMRG (G. Ehlers, R.M. Noack)
Freie Universität, (Berlin, Germany), Basis optimization using matrix product state (MPS) based approach (C. Krumnow, R. Schneider, J. Eisert); Ab initio description of metal Insulator transitions (E. Fertitta, B. Paulus)
Universität Wien, (Vienna, Austria), Development of tree tensor network state (TTNS) algorithm (V. Murg, F. Verstraete)
Technische Universität Berlin, (Berlin, Germany), Tensor factorizations in high dimensional problems (M. Pfeffer, R. Schneider)
McMaster University, (McMaster, Canada), Bond braking and formation through entanglement (K. Boguslawski, P. Tecmer, P. Ayers)
Ustav Fyzikalni Chemie J. Heyrovskeho AV CR, (Praha, Czech Republic), Development of the quantum chemistry version of the DMRG method (L. Veis, J. Pittner)
Universidad Autonoma de Madrid, and Instituto de Estructura de la Materia, CSIC, (Madrid, Spain), Development of the nuclear shell version of the DMRG method (A. Poves, J. Dukelsky)

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S-D. Semiconductor nanostructures

"Momentum" research team

Ádám Gali, Dávid Beke[#], Zoltán Bodrog, Jyh-Pin Chou, Viktor Ivády[#], Gyula Károlyházy[#], Elisa Londero, Bálint Somogyi[#], Attila Szállás, Krisztián Szász[#], Gergő Thiering[#], Viktor Zólyomi

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. Dániel Áron Major, Klaudia Horváth, Dániel Utyi, Fanni Temesváry-Kis (BSc students in chemical engineering), András Csóré and Péter Udvarhelyi (MSc students in physics) are also active members of the group. Two laboratory assistants (István Balogh, Bence Lázár) mediate the experiments.

Diamond is a known host of solid state qubits and single-photon emitters. Our group seeks for novel potential qubit candidates in diamond, and carries out in-depth characterization by means of *ab initio* atomistic simulations. The chemical vapor deposition of diamond is known to introduce complexes of silicon, vacancy, and hydrogen. We theoretically examined several such complexes, some of which have already been observed, others which could potentially form (see Figure 1). Using hybrid density functional theory for the treatment of highly correlated orbitals, many measurable quantities are calculated. The SiV_2H negatively charged defect is found to be a promising candidate for a long-lived solid state quantum memory. The study is highlighted as Editor's suggestion in *Physical Review B*.

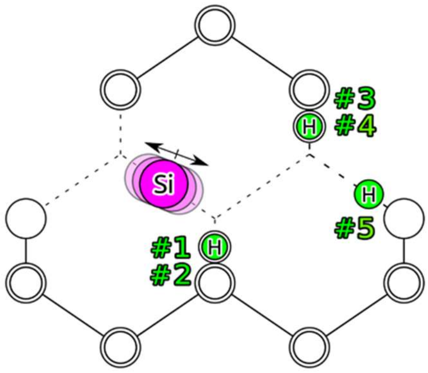

Figure 1. *Complex of vacancies, silicon and hydrogen atoms in diamond. The diamond lattice is shown in the (110) plane. The numbers label the hydrogen atoms. Typical vibrational motion of Si atom is shown.*

Significant results have been achieved in the research of solid-state quantum bits, which are the building blocks of a future implementation of the quantum computer. In collaboration with Awschalom group at Chicago University, we have shown that the nuclear spins can be effectively spin polarized near the divacancy and related defects (see Figure 2). The 99%±1% degree of polarization that we observe at room temperature corresponds to an effective nuclear temperature of 5 μK. By combining ab initio theory with the experimental identification of the optically excited states of color centers, we quantitatively model how the

[#] Ph.D student

polarization derives from hyperfine-mediated level anticrossings. These results lay a foundation for SiC-based quantum memories, nuclear gyroscopes, and hyperpolarized probes for magnetic resonance imaging. The study is featured in *Physics* as Viewpoint and highlighted as Editor's suggestion in *Physical Review Letters*. We further developed a theory about the dynamic nuclear spin polarization of defects in solids that we published in *Physical Review B*. In addition, our *ab initio* calculations predicted that the so-called carbon antisite-vacancy defect could have a high-spin ground state when it is neutral in the 4H polytype of silicon carbide. Furthermore, we proposed what conditions are needed to observe this defect and realize a new solid state qubit. The results were published in *Physical Review B* as *Rapid Communication*. We also worked together with scientists at Melbourne University: they fabricated a diode from SiC where single-photon emitters are engineered into this junction. These single-photon emitters can be driven electrically to realize a quantum light-emitting diode operating at room temperature. We developed a model by simulations for the origin of these emitters that is a combination of stacking faults with a point defect (silicon antisite). These results were published in *Nature Communications*.

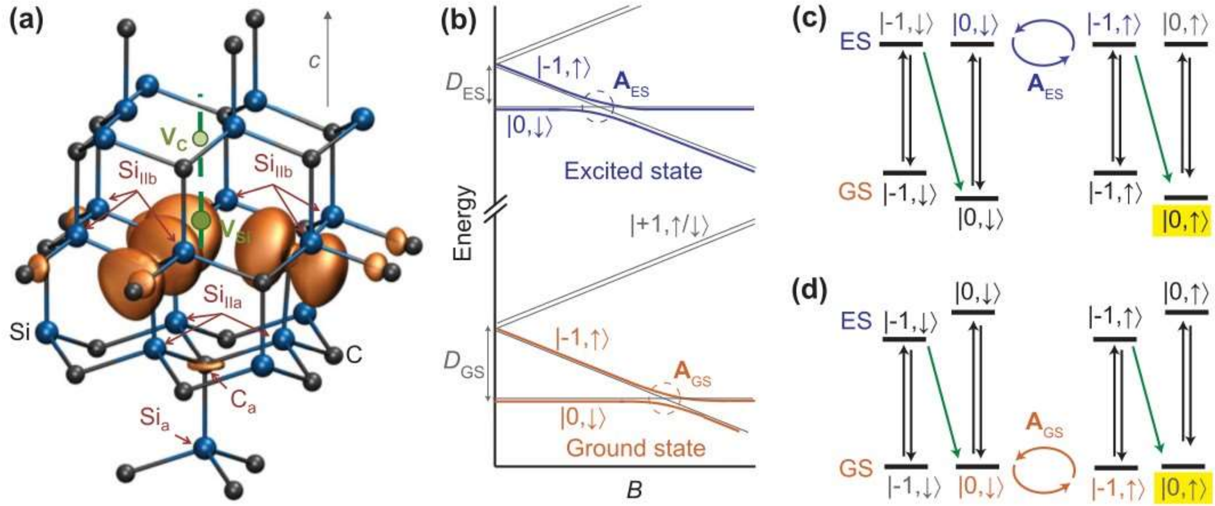

***Figure 2. (a)** Calculated spin density on a divacancy defect in 4H-SiC Ground state at so-called hh configuration. **(b)** The scheme of level anti-crossing is shown for the ground and excited states. The dynamic spin polarization of the nuclear spin represented by an arrow is shown for **(c)** excited-state branches and **(d)** ground-state branches, respectively.*

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. Although such systems have already been developed, but most of them are either unstable or toxic, thus they are not suitable for therapy. Our “Lendület” Semiconductor Nanostructures Research Group is, however, seeking 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. Furthermore, SiC nanoparticles with engineered vacancy-related emission centres may realize magneto-optical probes operating at nanoscale resolution. Understanding the nature of molecular-sized SiC nanoparticle emission is essential for further applications. Our group members at Wigner ADMIL laboratory have succeeded to develop an efficient and simple method to produce a relatively narrow size distribution of water-soluble molecular-sized SiC nanoparticles. The tight control of their size distribution makes it possible to demonstrate a switching mechanism in the luminescence correlated with particle size. We show that molecular-sized SiC nanoparticles of 1–3 nm show a relatively strong and broad surface-related luminescence whilst the larger ones exhibit a relatively weak band edge and structural defect luminescence with no evidence of quantum confinement effect (see Figure 3). These results were published in *Nanoscale*.

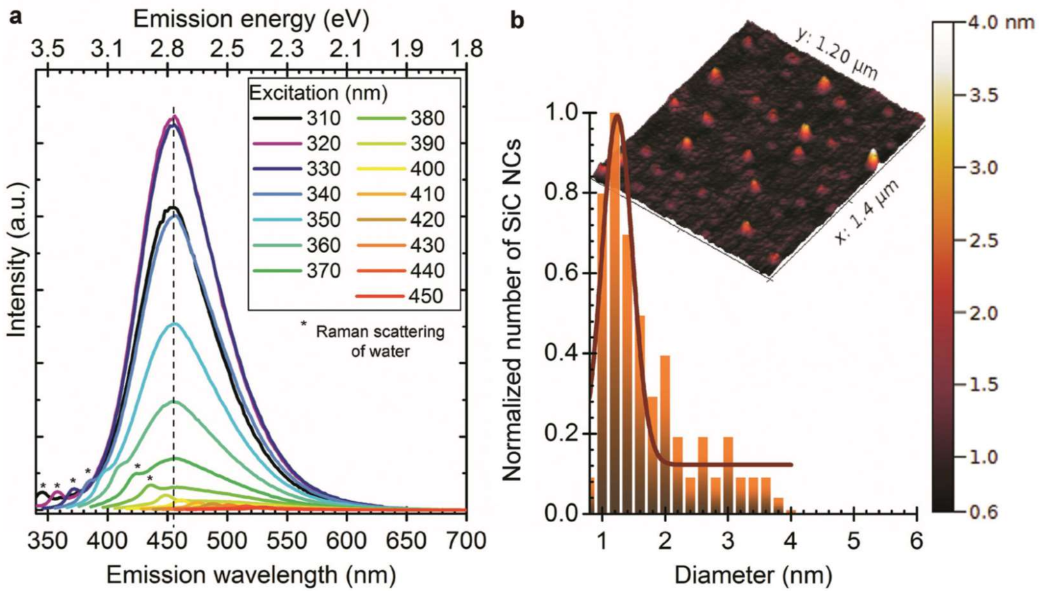

***Figure 3. (a)** PL spectra of the sample (filtrate) at different excitation wavelengths after SiC NCs were filtered through a 30 kDa centrifuge filter. After filtration, the red shoulder does not occur in the PL spectra.* ***(b)** AFM image and size distribution of the sample. The average size is about 1.5 nm and most of the particles are smaller than 4 nm.*

Understanding the fluorescence of complex systems such as small nanocrystals with various surface terminations in solution is still a scientific challenge. We showed that the combination of advanced time-resolved spectroscopy and *ab initio* simulations, aided by surface engineering, is able to identify the luminescence centers of such complex systems. Fluorescent water-soluble SiC nanocrystals have been previously identified as complex molecular systems of silicon, carbon, oxygen, and hydrogen, held together by covalent bonds that made the identification of their luminescence centers unambiguous. The aqueous solutions of molecular-sized SiC nanocrystals are exceedingly promising candidates to realize bioinert nonperturbative fluorescent nanoparticles for *in vivo* bioimaging, and thus the identification of their luminescent centers is of immediate interest. We presented identification of two emission centers of this complex system: surface groups involving carbon−oxygen bonds and a defect consisting of silicon−oxygen bonds that becomes the dominant pathway for radiative decay after total reduction of the surface. The identification of these luminescent centers reconciles previous experimental results on the surface- and pH-dependent emission of SiC nanocrystals and helps design optimized fluorophores and nanosensors for *in vivo* bioimaging (see Figure 4). The results were published in *The Journal of Physical Chemistry C*.

Finally, we mention that the Wigner ADMIL infrastructure could be significantly developed by the installation of a new induction generator and heat chamber for alloying new materials and annealing. The investment was financed by the Infrastructure program of the Hungarian Academy of Sciences.

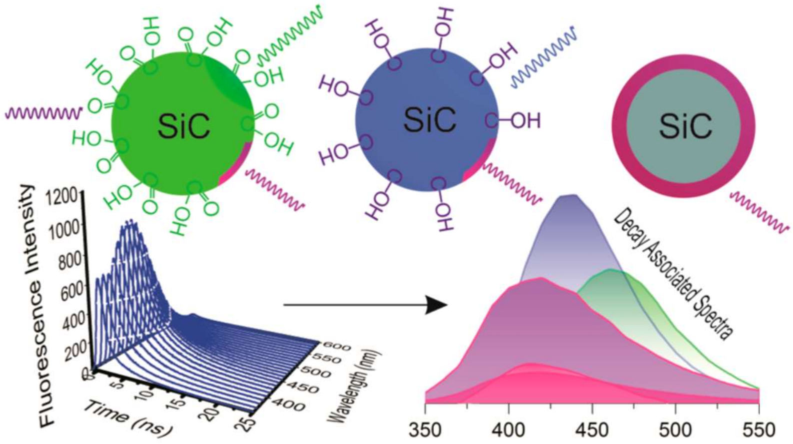

Figure 4. *Schematic diagram showing the surface- and environment-dependent luminescence of SiC nanocrystals*

Grants

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

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

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

International cooperation

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

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

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

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

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

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

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

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

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

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

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

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

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

Charles University (Czech Republic), Si nanoparticles (Prof. Jan Valenta)

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

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

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

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

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S-H. Partially ordered systems

Wigner research group

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Granular materials. — Secondary flow and heaping of a granular material consisting of shape-anisotropic grains has been detected in a split-bottom shear cell.

An assembly of elongated particles was sheared in a cylindrical geometry by rotating a disk at the bottom of the shear cell as indicated in Figure 1 (left). A secondary flow developed perpendicular to the shear flow, resulting in the formation of a heap in the middle of the setup. The full 3D structure of the grains was tracked by X-ray tomography during the shearing process. The resulting velocity map, together with the density map is presented on Figure 1 (right). We gave a symmetry argument and our experimental data show that the generation of the secondary flow is driven by the misalignment of the particles with respect to the streamlines of the primary flow.

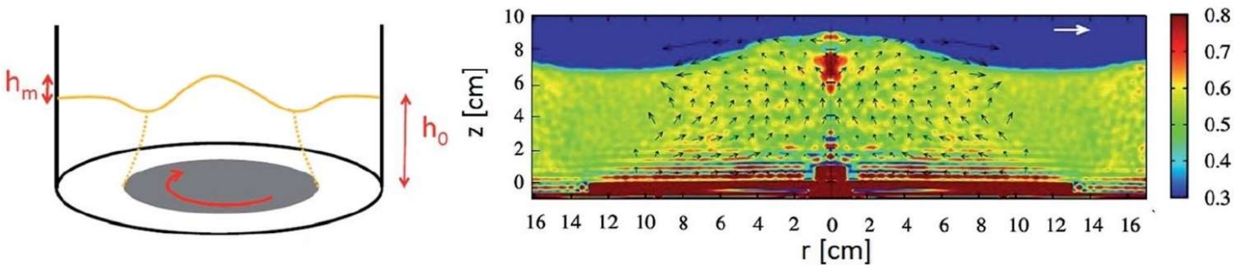

Figure 1. *Secondary flow and heaping is observed in a sheared granular material consisting of elongated grains in a cylindrical split bottom shear cell. The image shows the velocity map (perpendicular to the primary flow) and the density map, both detected by X-ray tomography.*

Pattern formation in bent-core liquid crystals. — Alternating-electric-field-induced periodic patterns have been observed and characterized in two members of the 2,5-bis(4-(difluoro(4-alkylphenyl)methoxy)phenyl)-1,3,4-oxadiazole (nP-CF2O-ODBP) bent-core nematic liquid crystal homologous series.

In 7P-CF2O-ODBP, a regular domain structure consisting of parallel stripes – flexodomains – have been induced by low frequency (subHz) electric voltage. The wavelength of the pattern is in the range of 1–10 micrometers and thus can conveniently be observed in a polarizing microscope. It also serves as an optical grating and produces a regular system of laser diffraction spots. The pattern was found to emerge and disappear consecutively in each half period of the driving, with the wavelength of the flexodomains changing periodically as the ac voltage oscillates (see Figure 2). Analyzing the polarization characteristics of the diffracted

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light, the polarization of the first-order spot was found to be perpendicular to that of the incident light, in accordance with a recent theoretical calculation.

In 9P-CF2O-ODBP, electroconvection patterns of diverse morphology have been observed over a wide frequency range. At low frequencies (up to ~25 Hz), the bent-core nematic liquid crystal exhibited unusual polarity-dependent patterns (Figure 3). When the amplitude of the ac field was enhanced, these two time-asymmetrical patterns turned into time-symmetrical prewavy-like stripes. At ac frequencies in the middle-frequency range (50–3000 Hz), zigzag patterns were detected whose obliqueness varied with the frequency. Finally, if the frequency was increased above 3 kHz, the zigzag pattern was replaced by another, prewavy-like pattern, whose threshold voltage depended on the frequency; however, the wave vector did not. For a more complete characterization, material parameters such as elastic constants, dielectric permittivities, and the anisotropy of the diamagnetic susceptibility were also determined.

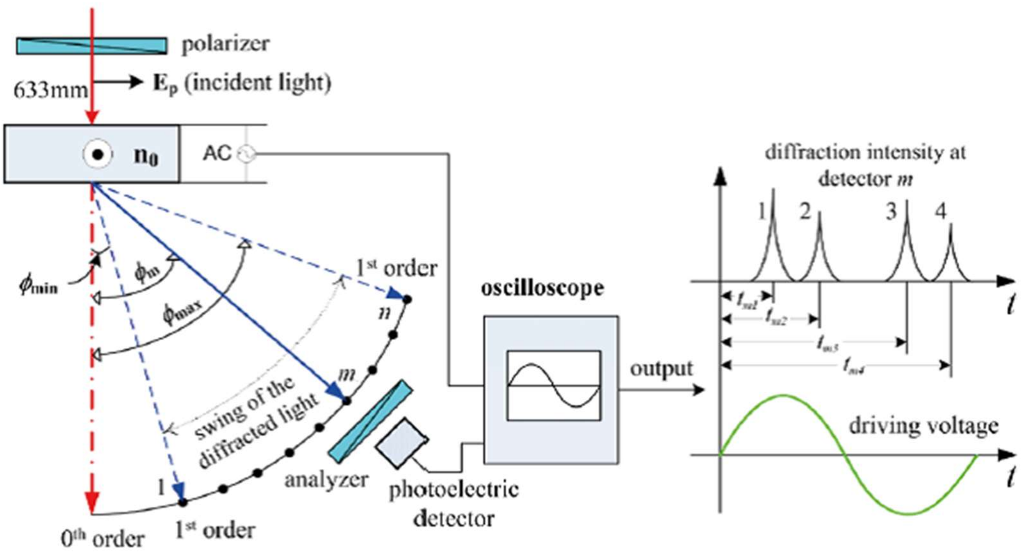

***Figure 2**. The set-up for monitoring the dynamics of the diffracted light, and an example of the time dependent intensity signal from the mth detector.*

Liquid crystal composite materials (ferronematics). — The influence of doping with spherical magnetic nanoparticles on the mixture of a bent-core (11DClPBBC) and a calamitic (6O8) liquid crystal was investigated. Magnetization curves were determined for the undoped nematic mixture as well as for the ferronematic (Figure 4), proving the superparamagnetic behaviour of the latter. A reduction of the critical field of the magnetic Fréedericksz transition by more than a factor of two was detected after the doping. Moreover, for the first time, experimental evidence was provided for the theoretically predicted magnetically induced negative shift of the isotropic-to-nematic phase transition temperature.

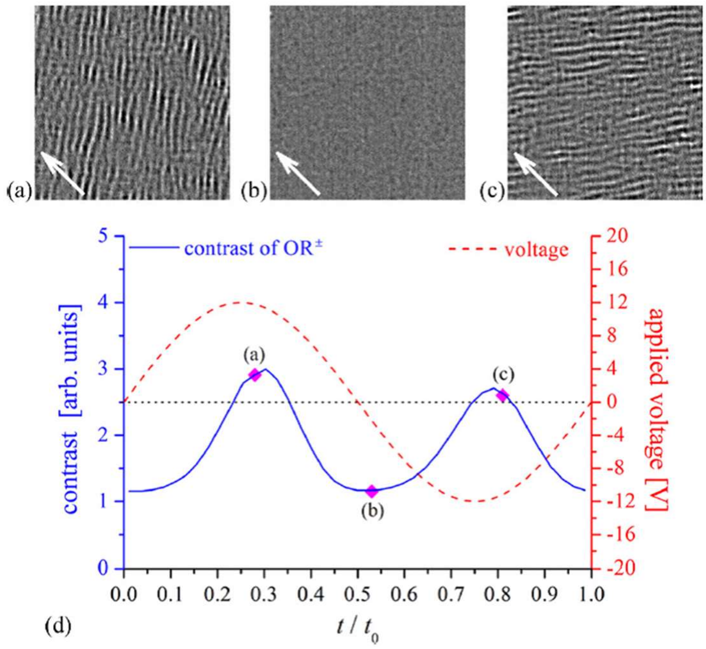

Figure 3. *Snapshots (100µm × 100µm) of the low frequency oblique roll pattern. (a) OR+ in the positive half period; (b) no pattern around the zero crossing of the voltage; (c) OR− in the negative half period. The white arrows indicate the initial director* ***n****0; the polarizer direction is vertical. (d) Temporal dependence of the pattern contrast and of the applied voltage within one full period.*

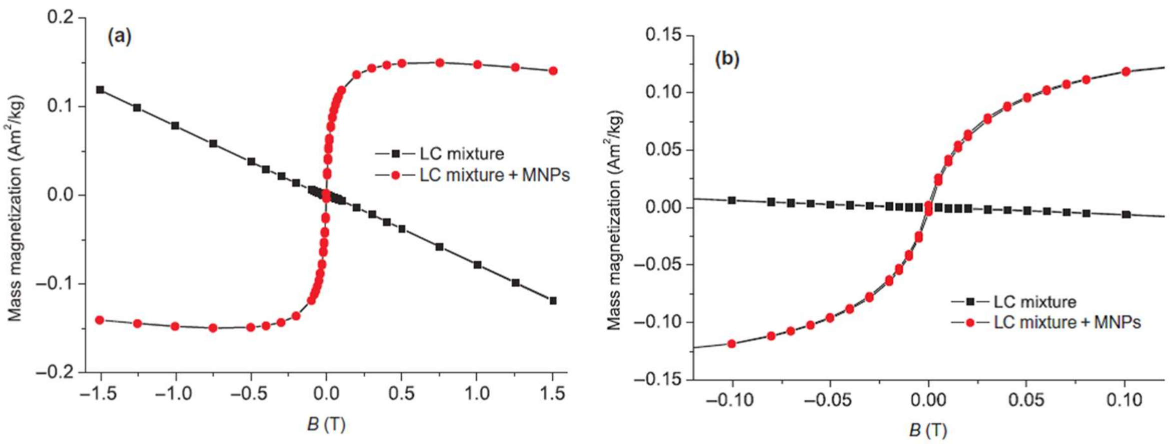

Figure 4. *(a) Magnetisation curves of the liquid crystal (LC) mixture and of the LC mixture doped with magnetic nanoparticles (MNPs), measured at T = 80°C. (b) A blow-up of the magnetisation curves around zero magnetic field.*

Phase transitions and thermal stability of binary mixtures of another bent-core (10DClPBBC) and a rod-shaped (6O8) liquid crystal were studied using differential scanning calorimetry. The binary mixture with 50:50 weight ratio of the constituents, a nematic to smectic transition below 40 °C and crystallization at sub-ambient temperature was detected. Crystallization was found to be the phase transition with the lowest apparent activation energy. The influence of doping the compounds with magnetic nanoparticles on the kinetics of observed phase transitions was also studied. The phase transition temperatures were shifted for all studied liquid crystal samples, with the degree of the shift depending on the nanoparticle type.

Synthesis of mesogenic compounds. — A new series of azo-containing bent-core liquid crystals derived from 3-hydroxybenzoic acid has been synthesized. Their mesomorphic properties have been characterized by polarizing optical microscopy, differential scanning calorimetry (see Figure 5 for a member of series), small-angle x-ray diffraction and electro-optic studies. Almost all the compounds form an enantiotropic modulated smectic (B_7 type) phase over relatively broad temperature ranges. Structural modifications, such as the type and length of the terminal chains, the rigidity of wings, and the presence of a Cl-substituent in different positions of the bent core, affect the appearance and temperature range, but not the type of the mesophase of the investigated compounds. Light-induced changes in the texture and phase transition of the mesophase, attributed to the decrease of the order parameter due to the *trans-cis* isomerization, have also been observed.

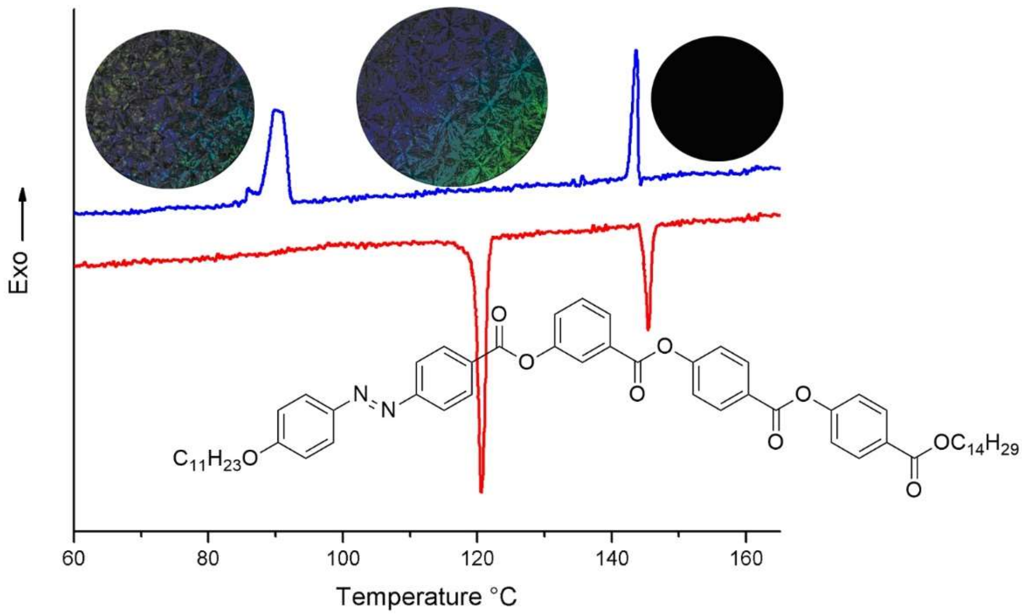

Figure 5. *DSC curves, polarizing microscopy snapshots, and the molecular structure of one of the synthetized compounds.*

Grants

OTKA NN 107737: Anisometric granular materials (T. Börzsönyi, 2013-2016)

EU M-ERA.NET FP7 (OTKA NN 110672): Magnetically active anisotropic composite systems, (T. Tóth-Katona, 2013-2016)

"Wigner research group" support

International cooperation

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

Otto Von Guericke Universität Magdeburg (Magdeburg, Germany), Flow properties of suspensions and granular materials (T. Börzsönyi, 2015-2016)

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

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

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

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

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

Institute of Experimental Physics, SAS (Košice, Slovakia), Magnetic properties of anisotropic composite nanosystems (N. Éber, 2015-2016)

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S-I. Electrodeposited nanostructures

Wigner research group

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

Electrodeposition of metals from non-aqueous solutions. — Electrodeposition experiments of Ni from alcoholic solutions were completed and published. A striking contrast was found between the results of the short-time cyclic voltammetry experiments and long-run depositions. In the cyclic voltammetry experiments completed with a quartz crystal microbalance study, metallic Ni was found to deposit in the cathodic-going sweeps and to dissolve during the anodic-going sweeps. In all cases, the deposition efficiency estimated from the cyclic voltammograms was higher than that obtained for d.c. deposits. Based on magnetic properties, deposits containing Ni were obtained from ethylene glycol, 1,2-propanediole and 1,3-propanediole. However, no metallic Ni was found in the deposits obtained from ethanol and glycerol. In the latter cases, a salt film was obtained on the substrate, which was a result of the chemical precipitation of the alcoholate anions and nickel cations. No ferromagnetic component was found in the salt film deposits. Where metallic Ni was present in the deposit, the magnetic properties of the film were comparable to those of Ni plated from a conventional aqueous bath, regarding to both squareness of the magnetization curves and coercive fields.

Electrodeposition of cobalt was achieved not only from alcoholic solutions, but also from N,N-dimethylformamide and dimethylsulfoxide. A comparative study of the cobalt deposit obtained from various solvents in underway.

Composition depth profile analysis of electrodeposited alloys. – In earlier experiments performed with stagnant solutions and upward-facing horizontal cathodes, the initial composition transient of electrodeposited Fe-Co-Ni alloys ranged to about 250 nm, and the mole fraction vs. depth functions exhibited various extrema before the stabilization of the steady-state composition. In order to clarify the origin of the unexpected trends in the composition of the near-substrate zone, a rotating disk workstation was constructed with a downward-facing cathode and easily replaceable metal-coated Si disc as working electrode. With this electrode configuration, the sample preparation for the reverse depth profile analysis could be carried out essentially in the same way as with our earlier columnar cell, by having the advantage of the controlled hydrodynamics, too.

The first step of the check of the sample preparation was the composition analysis along the radius of the rotating disc. As Figure 1 shows, there is no systematic composition deviation as a function of the distance from the disc center but all uncertainty in the composition can be ascribed to the normal experimental error of the composition analysis by EDX.

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

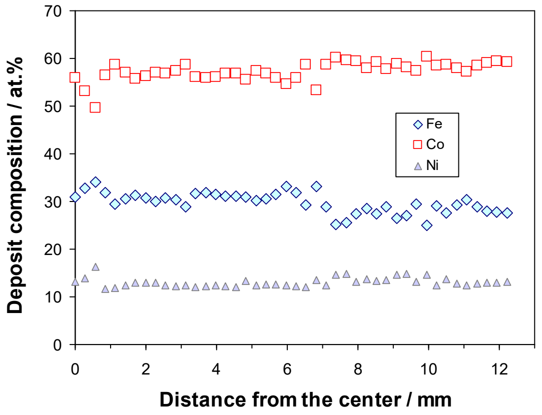

__Figure 1.__ Local composition of an electrodeposited Fe-Co-Ni sample as a function of the distance from the center of the rotating disc electrode

The composition analysis with reverse sputtering direction was carried out with secondary neutral mass spectrometry. Since the lateral homogeneity of the samples was checked previously, any part of the rotating disc could be used for the composition depth profile measurement. The composition depth profile curves revealed that the initial zone with varying composition was much thinner in the well-stirred system than in the stagnant solution. Another important difference as compared to the earlier measurement was that the decay of the mole fraction vs. depth curves was smooth and never exhibited any extreme. Also, there was no composition fluctuation after the steady-state was achieved. (The composition depth profile measurements were performed in collaboration with the Nuclear Research Institute of HAS) (Figure 2).

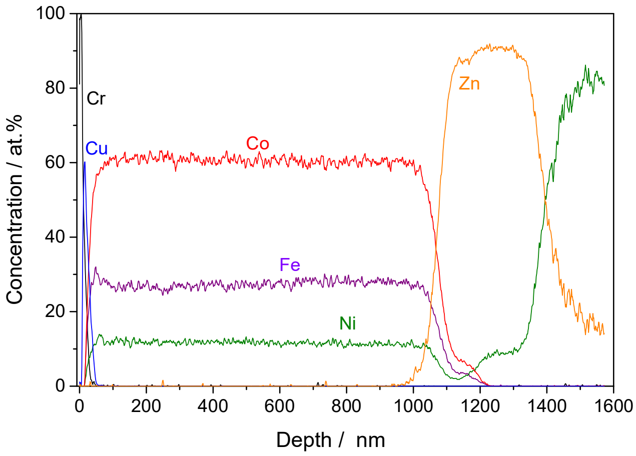

__Figure 2.__ Composition depth profile of an electrodeposited Fe-Co-Ni sample with the following layer structure: Cr(5nm)/Cu(25nm)//Fe-Co-Ni(1μm)/Zn(300nm)/Ni

Defect structure of electrodeposited nickel. — Grain and defect structure of nickel deposited with direct current from an additive-free solution was compared with those deposited from saccharine- and formic acid-containing solutions. Nickel specimens produced under various conditions proved to be an ideal model material to compare the results of various structural tests on the same samples. The columnar growth detected for the additive-free solution turned into a nearly isotropic fine-grained structure as a result of either of the additives used. The grain size trends as estimated by the transmission electron microscope and the line profile fitting of the X-ray diffractograms were in good agreement; nevertheless, the line profile analysis proved to be more sensitive to the occurrence of subgrains and, hence, it resulted in smaller crystallite sizes. Similarly, nanotwins with spacings less than 5 nm could be detected more sensitively with the line profile fitting than with transmission electron microscopy. (These results were achieved in cooperation with the Department of Materials Physics, Eötvös University and the Institute for Technical Physics and Materials Science, Centre for Energy Research, HAS.)

Fabrication of nanoporous anodic aluminum oxide (AAO) templates. — The conditions of the aluminum electropolishing and of the anodization in oxalic acid were elaborated in the previous year. It was revealed with an ellipsometric study that not only the surface roughness can be reduced during the electropolishing but the oxid layer remaining at the surface is thinner that the native oxide. While the thickness of the native oxide can be assessed as 25 nm, the electropolished surface is covered by an 8-nm-thick oxide only. (These experiments were performed in cooperation with the Institute for Technical Physics and Materials Science, Centre for Energy Research, HAS.)

The optimization of the experiments in order to establish the routine production of open porous AAO templates was continued with the pore opening tests. The removal of the aluminum could be carried out in HCl+$CuCl_2$ solution that left the barrier layer at the bottom of the nanopores intact. The removal of the barrier layer could be successfully performed with a dilute solution of phosphoric acid. An electrochemical cell with permeation geometry was adopted for the real-time control of the pore opening process, in which the step-wise rise in the current between the two sides of the AAO template indicated the opening process. In these experiments, a neutral KNO_3 solution was used at the pore side of the AAO template, while at the barrier layer side, phosphoric acid was used. With these solutions, the pore widening after the removal of the barrier layer could be avoided since the etching agent (H_3PO_4) cannot significantly penetrate into the nanopores.

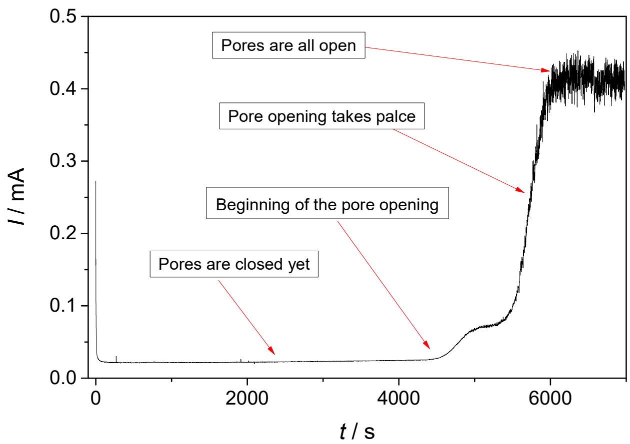

Figure 3. *Result of a typical pore opening experiment with electrochemical detection of the conductivity increase*

The permeation cell used for the pore opening experiments could also be used for the measurement of the diffusion coefficient of the solutes in the nanopores. In these experiments, the two compartments of the permeation cell was first filled with distilled water, then a concentrated salt solution was added to one of the compartment, also by compensating the level difference of the solutions by pure water in the other compartment. Hence, the only means of the salt transport between the two compartments was the diffusion. By recording the conductivity of the solutions in time and fitting the solution of the Fick equation to the result, the diffusion coefficient of the salt could be calculated (Figure 3). The results showed that the transport of the solute was by 4-8 times slower in the nanopores than expected from its diffusion coefficient (which was known from the literature). This can be an inherent feature of the salt diffusion in the 40-nm-wide nanopores. Since the experiments were carried out with a single salt (KCl) in a few experiments only, these tests must be continued in the next year to establish general trends for solutes of various polarity, cation and anion size, and also for non-ionic solutes with a detection method independent of the solution conductivity.

Laboratory tests of the acid pickling process of low-alloyed steels. – An automated laboratory-scale workstation was constructed in 2011 by the group leader to simulate the processes taking place during acid pickling of low-alloyed steels. The workstation constructed was installed in the Technical Institute of the College of Dunaújváros. The operation of this workstation was closely supervised by the design coordinator, also serving as a scientific advisor of the experimental activity. The results could be published in Steel Research International, a leading publication forum of the field that also devoted a cover page to highlight the results (see Figure 4). The outcome of this research field can be summarized as follows:

***Figure 4**. Automated laboratory-scale workstation. Cover page of Steel Research International*

The weight loss of the hot-rolled specimens during the laboratory test is a linear function of time. Since the dissolution of the several micrometer thick surface oxide (the so-called scale) is much faster than the dissolution of the base metal, the weight loss extrapolated to zero residence time yields the oxide thickness, while the slow increase of the weight loss in time refers to the metal dissolution (overpickling). The simulator device made it possible to separate the impact of the technical variables that cannot be carried out in the production line. It was revealed, among others, that the motion rate of the samples negligibly impact the weight loss, while the residence time is of primary importance. It was revealed that the weight loss measurement during the pickling simulation sensitively indicates the subtle changes in the production technology of the samples. The change of the surface roughness was also followed during the pickling experiments. The surface roughness increased by about 38±15 % after the removal of the scale by the pickling process. The scanning electron microscopic images of the cross-sectionaly polished samples showed that the roughness increase can be fully ascribed to the difference of the roughness of the oxide at the outside ("free") and the internal (metal side) surfaces, the latter being much larger. Due to the roughness difference between the inside and outside surfaces of the oxide layer, there is a necessary overpickling degree where the removal of the oxide becomes complete and the steel surface is cleaned for further treatments.

Industrial activities. — Experiments have been carried out for obtaining thick cadmium coatings on aluminum. This field of research was opened for the order of H-ION Kft., a start-up enterprise operated in the campus. Specimens of 10 cm^2 surface area were used to test whether cadmium coatings with small surface roughness and large thickness (more than 100 μm) can be produced with a good adherence and sufficient mechanical stability. The results of the successful experiments have been reported to the partner who seeks further funding to continue this joint activity.

Near-surface composition depth profile of rolled aluminum samples of different pretreatment conditions have been studied for the order of KÖFÉM-ALCOA, one of the largest light metal manufacturing company in Hungary. The composition depth profile measurements were coordinated by the Wigner Research Centre for Physics and were performed with glow-discharge optical emission spectrometry (at DUNAFERR) and secondary neutral mass spectrometry (at the Nuclear Research Institute of the Hungarian Academy of Sciences). The results of this project elucidated the metallurgical processes taking place during mechanical and thermal treatment of rolled aluminum raw materials.

Grant

OTKA K 104696: Electrodeposition of special magnetic materials from nonaqueous solutions (L. Péter, 2012-2016)

International cooperation

COST Action MP1407 (17 COST and 3 non-COST countries): Electrochemical processing methodologies and corrosion protection for device and systems miniaturization: e-MINDS (Management Committee members: I. Bakonyi and L. Péter, 2014-2018)

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

Ultrafast nanooptics Lendület research team

Péter Dombi, Viktor Ayadi, Viktória Csajbók[#], Győző Farkas[E], Norbert Kroó[E], István Márton[#], Benedek Nagy[#], Péter Rácz, Sándor Varró

High-intensity interactions and nanooptics. – We investigated nonlinear photoemission from plasmonic films with femtosecond, mid-infrared pulses at 3.1 mm wavelength. Transition between regimes of multi-photon-induced and tunneling emission was demonstrated at an unprecedentedly low intensity of around 1 GW/cm^2. Thereby, strong,- nanoscale electromagnetic fields can be accessed at extremely low laser intensities by exploiting nanometric plasmonic field confinement, enhancement and ponderomotive wavelength scaling at the same time. Results agreed well with quantum mechanical modelling. This scheme demonstrates an alternative paradigm and regime in strong-field physics.

In the framework of a collaboration with the University of Oldenburg, we reported on photoelectron emission from the apex of a sharp gold nanotaper illuminated via grating coupling at a distance of 50 µm from the emission site with few-cycle near-infrared laser pulses (Figure 1).

We found a fifty-fold increase in electron yield over that for direct apex illumination. Spatial localization of the electron emission to a nanometer-sized region is demonstrated by point-projection microscopic imaging of a silver nanowire. Our results reveal negligible plasmon-induced electron emission from the taper shaft and thus efficient nanofocusing of few-cycle plasmon wavepackets. This novel, remotely driven emission scheme offers a particularly compact source of ultrashort electron pulses of immediate interest for miniaturized electron microscopy and diffraction schemes with ultrahigh time resolution.

Femtosecond photonics. – We discovered the repetition rate dependence of femtosecond damage of optical components. Comparative measurements of dielectric high reflector, chirped mirror and metallic mirrors showed a factor of 3-5 lower femtosecond damage threshold at MHz repetition rates than at kHz. We attribute this to thermally assisted femtosecond damage mechanisms supported by complex heat transfer simulations.

Surface plasmon interactions. – Time-of-flight electron emission studies were carried out, changing the angle of polarization of the incident light, exciting surface plasmon oscillations. It was found that those parts of the electron spectrum which have been attributed to electron pairing have a significantly different angular dependence around 80 GW/cm^2 where the pairing effect has been found with respect to outside this region. These results are interpreted as the appearance of ideal or partly ideal diamagnetism, on the one hand, and as an anomaly in the magneto-optical effect (rotation) on the other hand, in the same laser intensity region where the pairing effect was found.

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

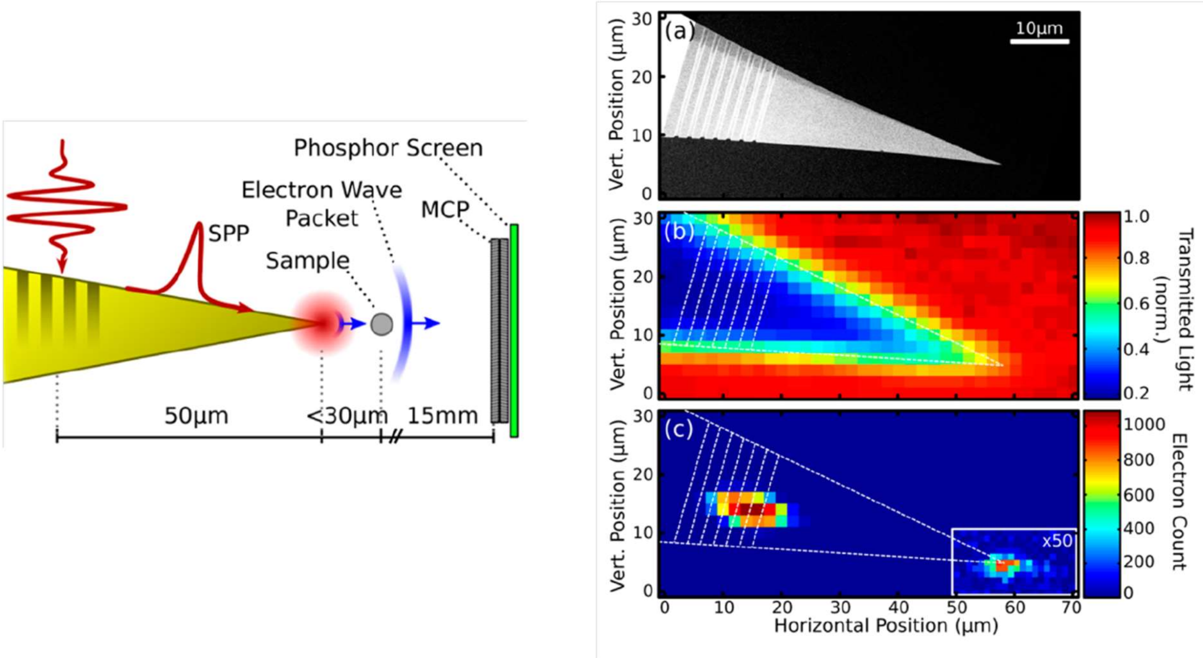

Figure 1. *Scheme of the setup for remotely driven electron emission on the left-hand-side. Few-cycle near-infrared light pulses are grating-coupled to a chemically etched gold taper. The launched surface plasmon (SPP) wavepacket propagates along the taper shaft and is nanofocused at the apex. The resulting high field concentration leads to plasmon-induced electron emission. Electrons are detected in a point-projection setup using a microchannel plate equipped with a phosphor screen. (a) SEM image of a gold nanotaper with grating coupler. (b) Shadow-image of the taper recorded by scanning the taper through the laser focus with a spot size of 6 μm. The laser light on the back side of the taper is measured with a photodiode. (c) Simultaneously recorded electron emission from a gold nanotaper illuminated with 160 pJ, 16 fs laser pulses centered at 1.6 μm. Electron emission is detected when placing the focus either on the grating or on the apex of the taper. The weak electron emission for apex illumination is magnified by a factor of 50. The contours of taper and grating are overlaid as white dashed lines.*

Theoretical quantum optics – Concerning our recent quantum optics research, by correspondence with saw-tooth function of classical Fourier analysis, we have constructed a regular phase operator, its diagonal representation in the regular phase state basis, and the associated quantum phase probability distributions. We have also introduced a new number-phase Weyl-Wigner correspondence between operators and phase-space functions, and defined new, regular number-phase Wigner functions, which stem from this description. These functions are joint quantum distributions of the integer photon number and the continuous phase variable, and may also allow a faithful reconstruction of the quantum phase properties of extreme electromagnetic signals from measured data. Figure 2 illustrates a comparison of our regular Wigner function and the so-called special Wigner function introduced earlier.

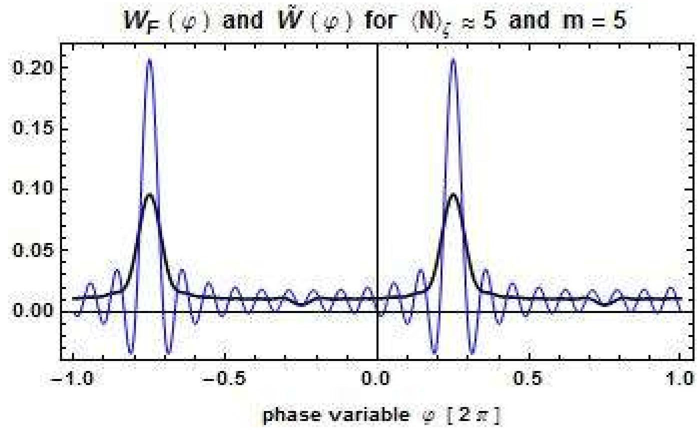

Figure 2. *Functional dependence on the phase variable ϕ (at the given photon number value m=5) of the regular Wigner function (thick black curve) and special number-phase Wigner functions (thin blue curve). The parameters of these states correspond to the photon number expectation value 5, and their phase has been taken $\pi/4$. The regular Wigner function is always positive, thus it can be considered as a true probability distribution; moreover, it is free from oscillations, which property makes the reconstruction reliable.*

Grants

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

OTKA K 104260 Particles and intense fields (T. S. Bíró and S. Varró, 2012-2016).

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

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

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

HAS Infrastructure Grant: Development of ultrafast high-resolution instrumentation (P. Dombi, Gy. Vankó, 2015)

International cooperation

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

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

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

Institute of Photonic Sciences (Barcelona, Spain) with P. Dombi.

University of Erlangen (Germany) with P. Dombi.

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Articles

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See also: R-B.4, R-B.5, R-P. 3, R-P.6

S-R. Nanostructures and applied spectroscopy

Wigner research group

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

Color centers in nanodiamonds. - In the last decades the production of highly luminescent color centers in nanometer sized diamond is one of the most interesting research fields due to the unique properties of nanocrystalline diamond, like biocompatibility, chemical stability and inertness. Metal-related impurity centers are particularly interesting because of their relatively low electron-phonon coupling resulting in a narrow (generally 5-15 meV) and highly intensive zero-phonon line (ZPL) and a weak vibronic sideband. Ni-Si related complex color center was successfully created in nanocrystalline diamond grains through chemical vapour deposition (CVD) process. This previously undocumented light-emitting system has a highly intensive ZPL at 865 nm (1.433 eV) with a narrow bandwidth of 2 nm (3 meV) FWHM (Figure 1).

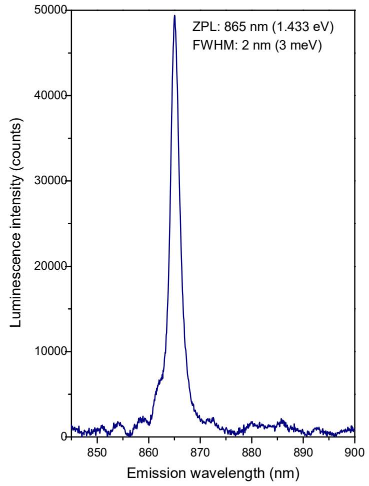

Figure 1. *Spectral feature of the 865 nm photoluminescence system excited by 488 nm at room temperature in nanodiamond grains prepared through the CVD growth process.*

The estimated Huang-Rhys factor of 0.097 indicates that a heavy impurity atom is included in the optical center. The vibronic sideband of 865 nm ZPL is dominated by quasilocal vibrations due to heavy impurity atoms that constitute the optical center. The calculation of quasilocal vibration frequencies of vibronic sideband provided information about the heavy impurity atom content of the optical center. Raman scattering study performed in the low-frequency region confirmed that the optical center contains both Ni and Si atoms.

Surface-Enhanced Raman Scattering. — Surface-Enhanced Raman Scattering (SERS) is a highly sensitive materials characterization technique. It utilizes the local enhancement of the electromagnetic field by surface plasmons of metallic nanoparticles and/or nanostructures. The method is based on Raman scattering and detects the characteristic vibrations of medium through inelastic light scattering. Here, the incident photons (one from each of 10^8 on average) change their energy during their interaction with the vibrations of the medium. In SERS, depending on the properties of the metallic particles, the interaction with surface plasmons can be used to enhance the electromagnetic field of the incident or the scattered light (or both), which results in an increase by 7-9 orders of magnitude of the Raman

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scattering efficiency. The wavelength of the surface plasmon resonance is determined by the material and the geometry of the SERS agent, and the targeted design and preparation of these structures allows the use of different excitation energies for surface-enhanced Raman scattering. Nanoparticles of specific shape could have even two or more plasmon resonance frequencies tuned for the excitation and different Raman peak wavelengths.

SERS theoretically has single-molecule sensitivity, which makes it ideal for sensing and detecting low concentrations and trace materials. It has great potential in environmental analysis, pharmaceuticals, materials science, forensics, drug detection etc. The practical application requires a cost-effective equipment, efficient and reproducible SERS agent materials and substrates, selectivity for the required materials and reliable detection algorithms. Our aim is to develop novel SERS substrates, equipment and technologies for the detection of disease markers in exhaled breath, blood and other body fluids, etc.

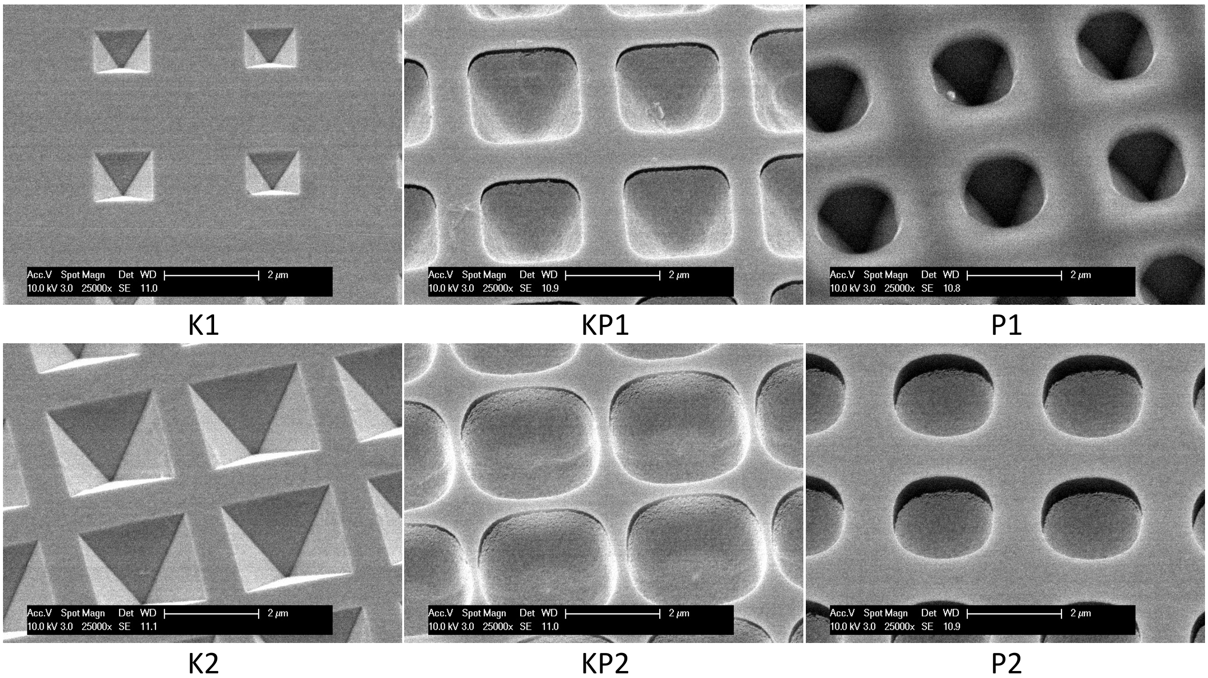

Figure 2. *Scanning electron microscopic images of gold-coated silicon SERS substrates prepared by lithography with (upper row) 1 micron and (lower row) 2 micron pattern period. K1 and K2 – samples were prepared with anisotropic etching; P1 and P2 – with isotropic etching and KP1 and KP2 – with the mixture of the two.*

Several different SERS substrates were designed and fabricated and tested for their Raman enhancement efficiency. Figure 2 shows scanning electron microscopic (SEM) images of six different surfaces produced by lithographic technique with etching and subsequent gold coating of the silicon wafer. The patterns on SERS surfaces were prepared with 1 and 2 micron periods using isotropic and anisotropic etching. The former treatment forms hemisphere-shaped voids in the substrate, while the latter inverse pyramids. A combination of the two etching techniques was also utilized resulting in inverse pyramids with rounded edges. SEM pictures show that the etching is uniform for each unit of the patterns.

The SERS efficiency of the prepared patterns was tested using a highly diluted solution of an organic benzene derivative molecule. Figure 3 compares the typical SERS spectra recorded on the different substrates as well as the normal Raman spectrum of the material. The solution was dropped onto the SERS substrates and the spectra were recorded after the evaporation of the solvent. The same excitation spot size, integration time and test solution were used on each substrate and measurement, and spectra were recorded in five different points on the samples. The normal Raman spectra were recorded on non-patterned gold surface of one of the substrates.

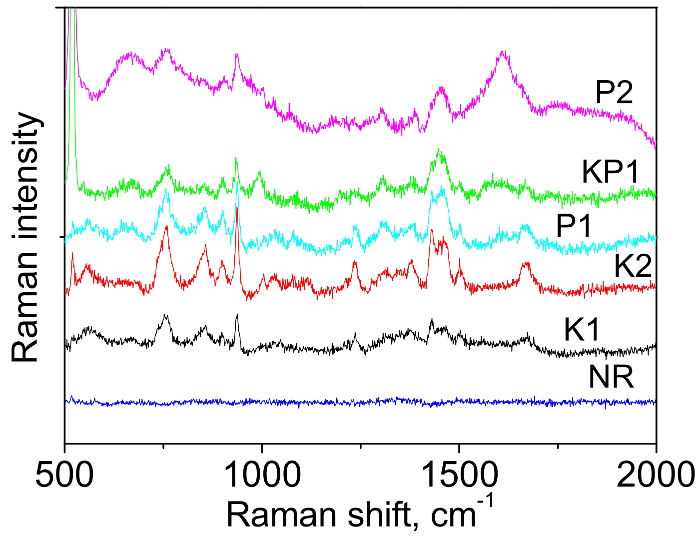

Figure 3. *Comparison of the surface-enhanced and normal Raman spectra of benzene derivative material. The SERS spectra were recorded on substrates shown in Figure 1 with 785 nm excitation wavelength, 1 micron spot size and 10 s integration time. Legend: NR – normal Raman; K1, K2, P1, KP1, P2 –see Figure 2.*

According to Figure 3, there are no Raman peaks in the normal Raman spectrum of the sample, while some narrow bands are present in all of the recorded SERS spectra. It should be noted that only an intense photoluminescence signal was recorded on the KP2 substrate, which is due to some contamination on the surface; a less intense luminescence background is present in the spectrum taken on the P2 substrate, too. Analysis of the peak intensities shows that the K2 SERS substrate has the highest Raman efficiency, followed by the P1, K1, KP1 and P2 samples.

The Raman enhancement on K2 substrate was tested also with nanodiamond powder available in form of slurry. This sample was also dropped and dried on the SERS substrate.

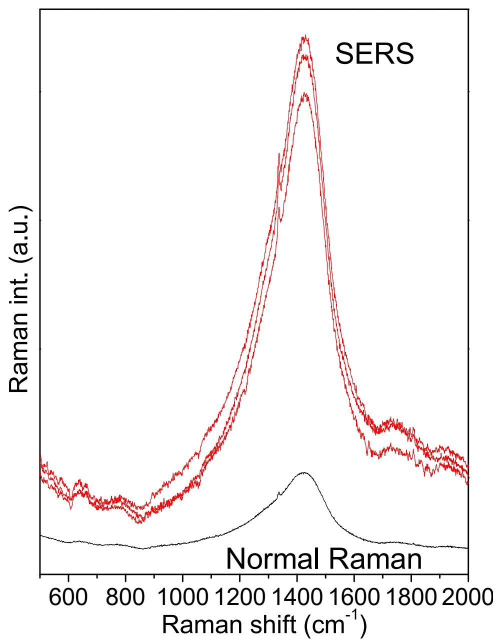

Figure 4. *Normal and surface-enhanced Raman spectra of nanodiamond slurry containing particles of 30 nm average size. The SERS spectra were recorded in three different points of the SERS substrate surface with 785 nm excitation wavelength, 1 micron spot size and 10 s integration time.*

Figure 4 shows the normal and SERS spectra of the sample. The overall Raman intensity is increased significantly, but the enhancement is less than for the test solution presented above. The characteristic nanodiamond Raman peak between 900 and 1650 cm^{-1} (consisting of a narrow diamond line at 1333 cm^{-1} and a broad band corresponding to amorphous carbon) can be seen in the normal Raman spectrum, too. Comparison of the measurements presented on Figs. 3 and 4 reveals the main feature of SERS: since the enhancement decreases rapidly with the distance from the SERS surface, this method is more suitable to study molecules or very small particles than bulk material or larger particles. In case of the latter, it will give information mainly on the surface and on subsurface structural units of the substrate.

Grants

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

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

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

Academic Excellence Program, EXMET: Development of combined LIBS-Raman equipment (M. Veres, 2015-2016)

International cooperation

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

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

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

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

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See also: S-N.1, S-N.3, S-N.5

S-S. Quantum Optics and Quantum Information

"Momentum" research team

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Cavity Quantum Electrodynamics, quantum critical phenomena. — In a recent work [Phys. Rev. Lett. 112, 073601 (2014)], we generalized the Power-Zineau-Woolley gauge to describe the electrodynamics of atoms in an arbitrary confined geometry. In the past year we complemented the theory by proposing a tractable form of the polarization field to represent atomic material with well-defined intra-atomic potential. In the constructed gauge, the direct electrostatic dipole-dipole interaction between the atoms is canceled. This theory yields a suitable framework to determine limitations on the light-matter coupling in quantum optical models with discernible atoms. We found that the superradiant criticality is at the border of covalent molecule formation and crystallization.

Quantum critical behaviour appears in driven dissipative systems when the steady state, rather than the ground state of a Hamiltonian, undergoes a non-analytic, symmetry-breaking change at a critical parameter value. The interplay of an external coherent excitation and the dissipation can lead to a steady state which is far from the ground or thermal state. Driven dissipative systems cannot be, in general, mapped onto an effective Hamiltonian system, which is the typical case, for example, in cavity QED. It is thus unclear how the critical behaviour of the open system is related to universality classes of known quantum and thermal phase transitions. We showed that the critical exponent of a quantum phase transition in a damped-driven open system is determined by the spectral density function of the reservoir. We considered the open-system variant of the Dicke model, describing the spatial self-organization of atoms in an optical cavity, where the driven boson mode and also the large N-spin couple to independent reservoirs at zero temperature. The critical exponent, which is 1, if there is no spin-bath coupling, decreases to below 1, when the spin couples to a sub-Ohmic reservoir.

Ultracold gases, Bose-Einstein condensates. — We studied the interplay between the dynamics of a Bose-Einstein condensate in a double-well potential and that of an optical cavity mode. The cavity field is superimposed to the double-well potential and affects the atomic tunneling processes. The cavity field is driven by a laser red detuned from the bare cavity resonance; the dynamically changing spatial distribution of the atoms can shift the cavity in and out of resonance (Figure 1). We found that at resonance the photon number is hugely enhanced and the atomic tunneling becomes amplified. The Josephson-junction equations were revisited and the phase diagram was calculated. We found solutions with finite imbalance and at the same time a lack of self-trapping solutions due to the emergence of a new separatrix resulting from enhanced tunneling.

[#] Ph.D student

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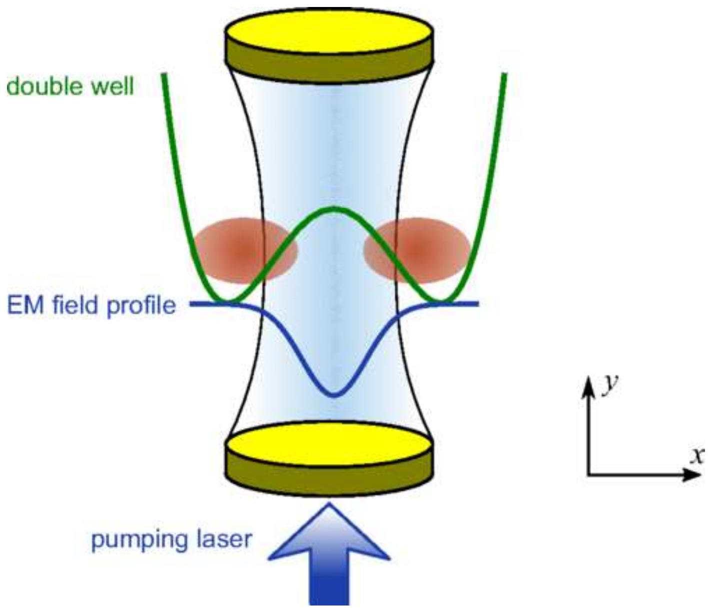

Figure 1. *The illustration of the setup. The bosonic Josephson junction is created by magnetic or optical means along the x direction. A Fabry-Pérot cavity is placed around the junction with an axis orthogonal to the junction. The resonator is operated on the TEM00 mode*

We studied the influence of photons on the dynamics and the ground state of the atoms in a bosonic Josephson junction inside an optical resonator. The system is engineered in such a way that the atomic tunneling can be tuned by changing the number of photons in the cavity. In this setup, the cavity photons are a means of control, which can be utilized both in inducing self-trapping solutions and in driving the crossover of the ground state from an atomic coherent state to a Schrödinger cat state. This is achieved, for suitable setup configurations, with interatomic interactions weaker than those required in the absence of a cavity. This is corroborated by the study of the entanglement entropy. In the presence of a laser, this quantum indicator attains its maximum value (which marks the formation of the catlike state and, at a semiclassical level, the onset of self-trapping) for attractions smaller than those of the bare junction.

Vibrational dynamics of simple molecules. — We presented a new ro-vibrational Hamiltonian operator, named gateway Hamiltonian operator, with exact kinetic energy term, T . It is in the Eckart frame and it is of the same form as Watson's normal coordinate Hamiltonian. However, the vibrational coordinates employed are not normal coordinates. The new Hamiltonian was shown to provide easy access to Eckart frame ro-vibrational Hamiltonians with exact T given in terms of any desired set of vibrational coordinates. A general expression of the Eckart frame ro-vibrational Hamiltonian operator was given and some of its properties were discussed.

Quantum information processing, quantum walks. — We showed a powerful method to compute entanglement measures based on convex roof constructions. In particular, our method is applicable to measures that, for pure states, can be written as low-order polynomials of operator expectation values. We showed how to compute the linear entropy of entanglement, the linear entanglement of assistance, and a bound on the dimension of the entanglement for bipartite systems. We discussed how to obtain the convex roof of the three-tangle for three-qubit states. We also showed how to calculate the linear entropy of entanglement and the quantum Fisher information based on partial information or device independent information. We demonstrated the usefulness of our method by concrete examples (Figure 2).

Discrete-time quantum walks (DTQWs) are nontrivial generalizations of random walks with a broad scope of applications. In particular, they can be used as computational primitives, and they are suitable tools for simulating other quantum systems. DTQWs usually spread ballistically due to their quantumness. In some cases, however, they can remain localized at their initial state (trapping). The trapping and other fundamental properties of DTQWs are determined by the choice of the coin operator. We introduce and analyze a type of walks driven by a coin class leading to strong trapping, complementing the known list of walks. This class of walks exhibits a number of exciting properties with possible applications ranging from light pulse trapping in a medium to topological effects and quantum search.

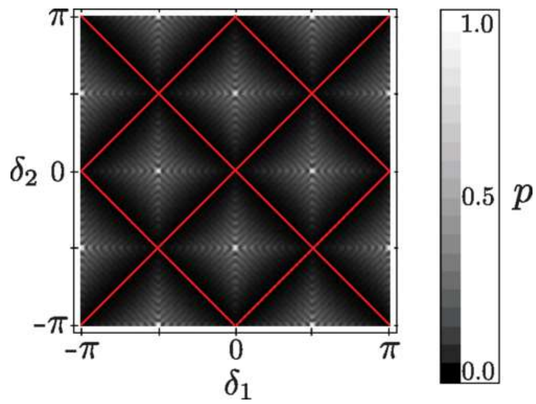

Figure 2. *Minimum probability of finding the particle at its initial position after 40 steps of a C-class coin-driven quantum walk. The probabilities are determined by numerically searching the initial states yielding the minimum probability. The red (gray) lines correspond to the condition where strong trapping disappears. On these lines, the minimum probability is naturally zero due to the appearance of the escaping state. However, where strong trapping is present, the minimum probability is larger than zero.*

Topological phases. — Quantum walks are promising for information processing tasks because in regular graphs they spread quadratically more rapidly than random walks. Static disorder, however, can turn the tables: unlike random walks, quantum walks can suffer Anderson localization, with their wave function staying within a finite region even in the infinite time limit, with a probability exponentially close to 1. It is thus important to understand when a quantum walk will be Anderson localized and when we can expect it to spread to infinity even in the presence of disorder. We analyzed the response of a one-dimensional quantum walk — the split-step walk — to different forms of static disorder (Figure 3). We found that introducing static, symmetry-preserving disorder in the parameters of the walk leads to Anderson localization. In the completely disordered limit, however, a delocalization transition occurs, and the walk spreads subdiffusively to infinity. Using an efficient numerical algorithm, we calculated the bulk topological invariants of the disordered walk and found that the disorder-induced Anderson localization and delocalization transitions are governed by the topological phases of the quantum walk.

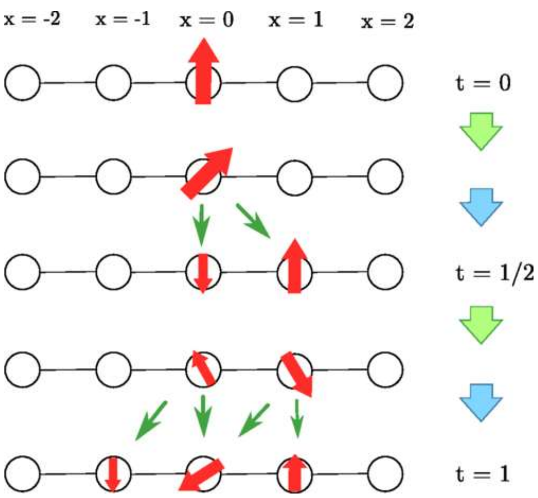

Figure 3. *A full time step of the split-step walk consisting of four operations: (1) rotation of the spin about the y axis through angle $2\vartheta_1$, (2) displacement of the s=+1 component of the wave function to the right, (3) second spin rotation through angle $2\vartheta_2$, and (4) displacement of the s=−1 component of the wave function to the left.*

We investigated time-independent disorder on several two-dimensional discrete-time quantum walks. We found numerically that, contrary to claims in the literature, random onsite phase disorder, spin-dependent or otherwise, cannot localize the Hadamard quantum walk; rather, it induces diffusive spreading of the walker. In contrast, split-step quantum walks are generically localized by phase disorder. We explained this difference by showing that the Hadamard walk is a special case of the split-step quantum walk, with parameters tuned to a critical point at a topological phase transition. We showed that the topological phase transition can also be reached by introducing strong disorder in the rotation angles. We determined the critical exponent for the divergence of the localization length at the topological phase transition, and found $\nu=2.6$ in both cases. This places the two-dimensional split-step quantum walk in the universality class of the quantum Hall effect.

Quantum walks on translation-invariant regular graphs spread quadratically faster than their classical counterparts. The same coherence that gives them this quantum speedup inhibits or even stops their spread in the presence of disorder. We asked how to create an efficient transport channel from a fixed source site (A) to fixed target site (B) in a disordered two-dimensional discrete-time quantum walk by cutting some of the links. We showed that the somewhat counterintuitive strategy of cutting links along a single line connecting A to B creates such a channel. The efficient transport along the cut is due to topologically protected chiral edge states, which exist even though the bulk Chern number in this system vanishes. We gave a realization of the walk as a periodically driven lattice Hamiltonian and identified the bulk topological invariant responsible for the edge states as the quasi-energy winding of this Hamiltonian.

Grants:

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OTKA K83858: Quantum optical and quantum information processing networks and their nonclassical properties (T. Kiss, 2011-2015)

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

OTKA PD 104652, Realization of strongly correlated matter by ultracold atoms (G. Szirmai, 2012-2015)

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Postdoctoral Fellowship of the HAS: Non-equilibrium quantum phase transitions and open-system quantum simulators (D. Nagy and P. Domokos, 2013-2015)

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International cooperation

MÖB-DAAD 65049: Dynamics and Control of Quantum Networks (T. Kiss, 2015-2016)

MÖB-DAAD 65056: Small polarons in luminescent LiNbO3: From bulk crystals to nanocrystals (Z. Kis, 2015-2016)

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Book

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See also: S-Q.6

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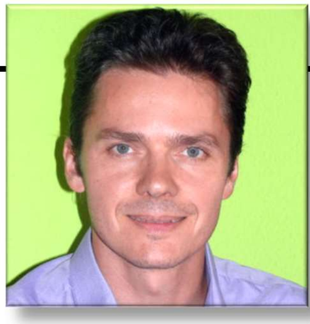
R-C. Gravitational Physics



Wigner research group

Mátyás Vasúth, Dániel Barta#, Károly Zoltán Csukás#, Gergely Debreczeni, Máté Ferenc Egri-Nagy#, István Rácz

The Gravitational Physics Research Group of the Wigner RCP is involved in various research activities including theoretical field theory, numerical and post-Newtonian general relativity calculations, experimental gravitational wave data analysis and fundamental research in algorithm optimization and many-core computer science. The main motivation of our research interest originates from gravitational wave physics as our group is involved in the Virgo Scientific Collaboration operating the Virgo detector, the European gravitational wave observatory. The progress and results of last year are summarized below.

Within the post-Newtonian framework we have computed the gravitational waveforms in the frequency domain to the first post-Newtonian order emitted by compact binary systems with arbitrary eccentricity. These systems are promising sources of the advanced gravitational wave observatories. Our results are fully analytic, ready-to-use expressions of the waveforms in terms of a suitable generalization of the Hansen coefficients known from celestial mechanics. The waveforms have a rather simple structure, greatly facilitating their use in applications.

We have analyzed Four-dimensional spacetimes foliated by a two-parameter family of two-surfaces within Einstein's theory of gravity. It was shown that, in terms of the chosen geometrically distinguished variables, the 1+3 Hamiltonian and momentum constraints can be recast into the form of a parabolic equation and a first order symmetric hyperbolic system. Moreover, we have explored a new method to solve the constraints of Einstein's equations, which does not involve elliptic equations which can be applied to provide initial data for black holes. It was shown that the sole data needed on a single large surface in the asymptotic region surrounding the system distinguishes this approach from other solutions to the constraint problem which rely on elliptic equations. Whether this feature improves the physical content and control of the initial data is a matter for further numerical investigation.

Joining to the international data analysis efforts of the gravitational wave observations started in the fall of 2015, the members of the group were involved in the use of the pycbc data analysis package of the LIGO-Virgo collaboration. With the use of this software package we are joining to the search and parameter estimation of coalescing compact binaries.

In 2015 two international scientific conferences were organized in Budapest by the members of the group. These were the Annual NewCompStar Conference 2015 and the LSC-VIRGO Collaboration Meeting 2015.

Ph.D. student

Grants

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

Bolyai János Scholarship of the H.A.S. (M. Vasúth, 2013-2016)

International cooperation

Virgo Scientific Collaboration (M. Vasúth)

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

Publications

Articles

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See also: R-A.12, R-A.15

LIGO and Virgo Collaborations

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2. Aasi J et al. incl. Debreczeni G, Nagy MF, Rácz I, Vasuth M (901 authors): Directed search for gravitational waves from Scorpius X-1 with initial LIGO data. ***PHYS REV D*** 91:(6) Paper 062008. 20 p. (2015)
3. Aasi J et al. incl. Debreczeni G, Nagy MF, Rácz I, Vasuth M (901 authors): Narrow-band search of continuous gravitational-wave signals from Crab and Vela pulsars in Virgo VSR4 data. ***PHYS REV D*** 91:(2) Paper 022004. 15 p. (2015)
4. Aasi J et al. incl. Debreczeni G, Nagy MF, Rácz I, Vasuth M (894 authors): Searches for continuous gravitational waves from nine young supernova remnants. ***ASTROPHYS J*** 813:(1) Paper 39. (2015)
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6. Acernese F et al. incl. Debreczeni G, Endrőczi G, Nagy MF, Rácz I, Vasuth M (234 authors): Advanced Virgo: A second-generation interferometric gravitational wave detector. ***CLASSICAL QUANT GRAV*** 32:(2) Paper 024001. 55 p. (2015)

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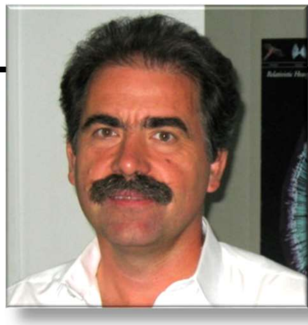
Book chapter

8. T Accadia et al. incl. Debreczeni G, Endrőczi G, Nagy MF, Rácz I, Vasuth M (195 authors): Advanced VIRGO interferometer: a second generation detector for gravitational waves observation. In: *Particle Physics at the Year of Centenary of Bruno Pontecorvo*. Ed.: Alexander I Studenikin, Singapore: World Scientific, 2015. pp. 261-270. (ISBN:978-981-4663-60-1)

R-D. Femtoscopy



Tamás Csörgő, Attila Bagoly[3], László Jenkovszky[A], Gábor Kasza[1], Dániel Kincses[1], Dávid Lucsányi[1], Frigyes Nemes[#], András Ster, András Sveiczer[1], Márton Vargyas[#], Róbert Vértesi

Exploring a new domain of QCD with elastic proton-proton scattering in the TOTEM experiment at LHC and theoretical studies in diffractive and low-x physics at LHC. — In the TOTEM experiment at CERN LHC, two special experimental studies were published with our participation. The first paper determined the pseudorapidity distribution of charged particles using a displaced interaction point at CERN LHC. Despite the inherent difficulties of measurements making use of a displaced interaction point at LHC, this measurement gave us access to a previously unforeseen pseudorapidity interval, the results made it to the cover page of the European Physical Journal C and were noted in a very positive manner by the LHC Council. In the beginning of 2015 we have received yet another recognition, our paper on the recalibration of LHC optics using measurements from the TOTEM Roman Pot detector measurements was elected, based on referee endorsement, novelty, scientific impact and broadness of appeal, to the Highlights of 2014 selection of the New Journal of Physics G. We have discovered, with significant Hungarian contribution from LHC beam optics calibration, that the shape of the differential pp cross-section in 8 TeV elastic pp collisions is not exponential. This discovery is firmed up by further results about the differential cross-sections in the very low four-momentum transfer region, corresponding to the Coulomb-Nuclear Interface (CNI) region. We have also published four theoretical contributions on diffractive physics. For the first time, we have extracted with good statistical significance the contribution of the Odderon to pp elastic scattering, solving a puzzle that created heated debates in the literature that lasted about 20 years to resolve.

Search for the QCD Critical Point in the BNL RHIC experiment PHENIX. — In 2015, the main result from PHENIX was the discovery of the nearly perfect fluid behaviour in 200 GeV ^{3}He+^{197}Au collisions. This result corresponds to a paradigm shift, indicating that tiny droplets of the perfectly flowing quark matter may be present in the collisions of small and large ions. It is an open question if such droplets can be created also in proton-proton collisions at RHIC or at LHC. As our group was pioneering the applications of hydrodynamics in hadron-proton and proton-proton reactions, this result was very important experimental evidence that convinced a large fraction of the research community that production of quark matter is not specific to the collisions of very large ions. PHENIX also submitted a paper on the observation of a non-monotonous behaviour in the excitation function of HBT radii in Au+Au collisions at RHIC, however, the question is still open if this is due to the vicinity of a QCD Critical Point or not, as PHENIX does not see a similarly non-monotonous pattern in the fluctuations of the multiplicity distributions. We have successfully organized (M. Csanád, chair, P. Kovács chair, T. Csörgő as honorary chair) the 2015 edition of our annual Zimányi Winter School on Heavy

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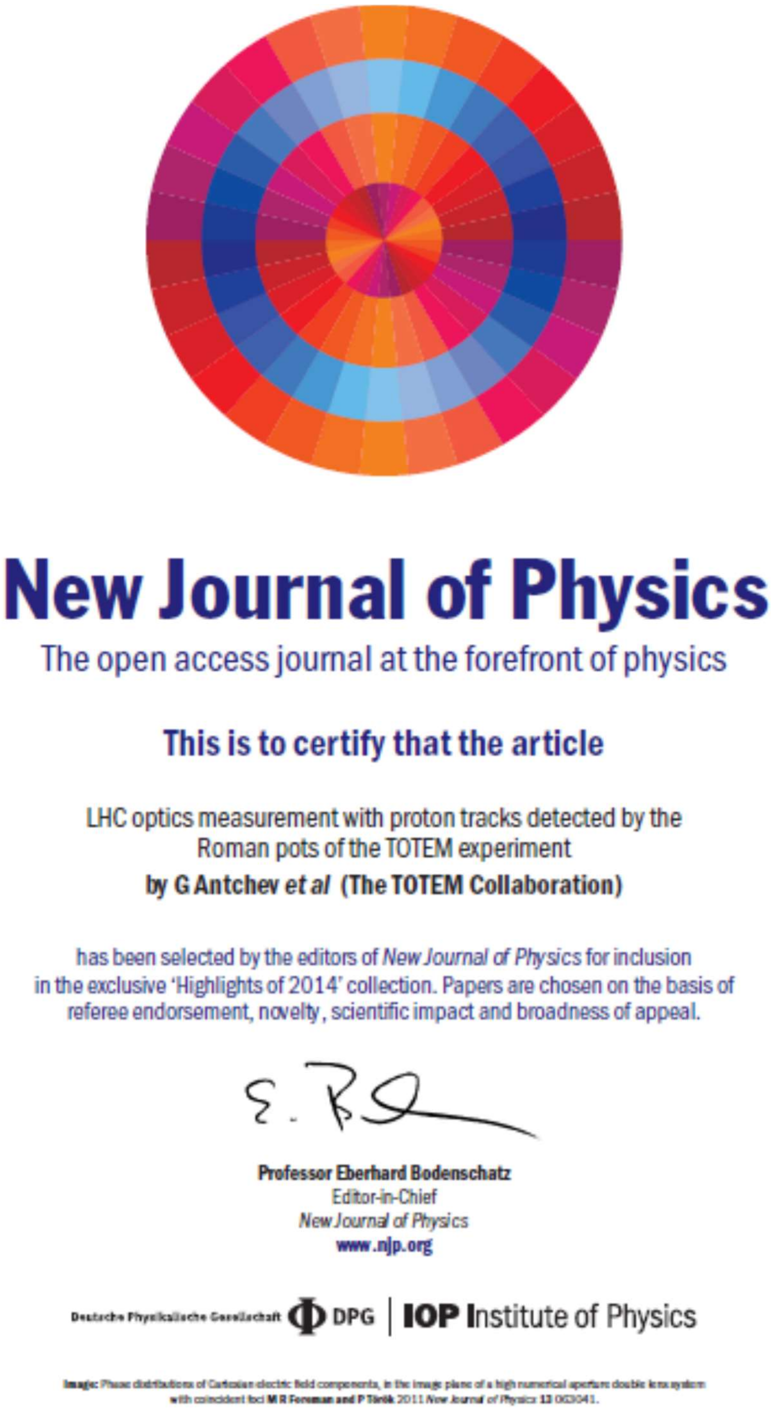
[3] Students on RMI payroll from 2015 August to 2015 December from the OTKA grant NK101438.

[A] Associate fellow

[#] Ph.D student

Ion Collisions. We hosted a 5-day meeting, with highlighted Zimányi seminars by Ch. Sasaki (Wroclaw) and T. Lappi (Jyvascyle) and a common Zimányi-Ortvay Colloqium by R. Venugopalan (BNL and Heidelberg). Zimányi'75 attracted 75 registered participants, including 38 PhD or MSc students not only from Hungary but also from the neighbouring countries, and a record number of 66 talks.



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LHC optics measurement with proton tracks detected by the Roman pots of the TOTEM experiment

by G Antchev *et al* (The TOTEM Collaboration)

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Professor Eberhard Bodenschatz
Editor-in-Chief
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Image: Phase distributions of Cartesian electric field components, in the image plane of a high numerical aperture double lens system with coincident foci M R Foreman and P Török 2011 *New Journal of Physics* 13 063041.

Figure 1. *Certificate of selection of the paper corresponding to the PhD Thesis of F. Nemes (corresponding author) and the TOTEM Collaboration, to Highlights of 2014 from the Editors of New Journal of Physics. This honor was received in February 2015. Papers that receive this recognition are selected on the basis of their referee endorsement, novelty, scientific impact and broadness of appeal.*

Grants

OTKA NK101438: (T. Csörgő et al, 2012-2015)

International cooperation

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

Brookhaven National Laboratory, USA, Memorandum of Understanding between the PHENIX Experiment and KFKI representing the PHENIX-Hungary team (Hungarian Principal Investigator: T. Csörgő, participants from Wigner: J. Sziklai, D. Kincses, M. Vargyas)

TOTEM Collaboration (CERN LHC, Svájc)

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

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

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

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

Publications

Articles

1. Gustafson G, Lönnblad L, Ster A, Csörgő T: Total, inelastic and (quasi-)elastic cross sections of high energy pA and γ⋆ A reactions with the dipole formalism. ***J HIGH ENERGY PHYS*** 2015:(10) Paper 22. 29 p. (2015)

2. Nemes F, Csörgő T, Csanád M: Excitation function of elastic pp scattering from a unitarily extended Bialas-Bzdak model. ***INT J MOD PHYS A***30: Paper 1550076. 25 p. (2015)

3. Ster A: Diffractive, inelastic and total cross sections in high energy pp, pA and γ*A reactions with the dipole formalism. ***AIP CONF PROC*** 1654:(1) Paper 100003. (2015) Primošten, Horvátország: 2014.09.10 -2014.09.16.

4. Ster A, Jenkovszky L, Csörgő T: Extracting the Odderon from *pp* and $p\bar{p}$ scattering data. ***PHYS REV D*** 91: Paper 074018. 10 p. (2015)

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5. Csörgő T, Nagy MI, Barna IF: Observables and initial conditions for rotating and expanding fireballs with spheroidal symmetry: Dedicated to L. P. Csernai on the occasion of his 65th birthday. In: *WPCF 2014 10th Workshop on Particle Correlations and Femtoscopy Gyöngyös Hungary 25.08.2014 – 29.08.2014*. Paper published online.

See also: R-B.27

Phenix collaboration

Articles

1. Adare A et al. incl. Csörgő T, Nagy MI, Ster A, Sziklai J, Vargyas M, Vértesi R (480 authors): Centrality dependence of low-momentum direct-photon production in Au plus Au collisions at$\sqrt{s_{NN}}$=200 GeV. ***PHYS REV C*** 91:(6) Paper 064904. 11 p. (2015)
2. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértesi R (382 authors): Charged-pion cross sections and double-helicity asymmetries in polarized p+p collisions at $\sqrt{s}$=200 GeV: Inclusive cross sections, charge ratio and double-helicity asymmetries for π^+ and π^- production in p+p collisions at $\sqrt{s}$=200 GeV. ***PHYS REV D*** 91: Paper 032001. 13 p. (2015)
3. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértesi R (375 authors): Cross section for $b\bar{b}$ production via dielectrons in d + Au collisions at $\sqrt{s_{NN}}$ =200 GeV. ***PHYS REV C*** 91:(1) Paper 014907. 18 p. (2015)
4. Adare A et al. incl. Csörgő T, Nagy MI, Ster A, Sziklai J, Vargyas M, Vértesi R (369 authors): Heavy-quark production and elliptic flow in Au + Au collisions at $\sqrt{s_{NN}}$=62.4 GeV. ***PHYS REV C*** 91:(4) Paper 044907. 19 p. (2015)
5. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértesi R (423 authors): Measurement of Long-Range Angular Correlation and Quadrupole Anisotropy of Pions and (Anti) Protons in Central d plus Au Collisions at $\sqrt{s_{NN}}$ =200 GeV. ***PHYS REV LETT*** 114:(19) Paper 192301. 8 p. (2015)
6. Adare A et al. incl. Csörgő T, Nagy MI, Ster A, Sziklai J, Vértesi R (480 authors): Measurement of Υ(1S+2S+3S) production in p+p and Au + Au collisions at $\sqrt{s_{NN}}$=200 GeV. ***PHYS REV C*** 91:(2) Paper 024913. (2015)
7. Adare A et al. incl. Csörgő T, Nagy MI, Novák T, Ster A, Sziklai J, Vértesi R (631 authors): Measurements of elliptic and triangular flow in high-multiplicity ^{3}He+Au collisions at $\sqrt{s_{NN}}$ =200 GeV. ***PHYS REV LETT*** 115: Paper 142301. 9 p. (2015)
8. Adare A et al. incl. Csörgő T, Ster A, Sziklai J, Vargyas M, Vértesi R (581 authors): Search for dark photons from neutral meson decays in p+p and d+ Au collisions at $\sqrt{s_{NN}}$ =200 GeV. ***PHYS REV C*** 91: Paper 031901. 17 p. (2015)
9. Adare A et al. incl. Csörgő T, Ster A, Sziklai J, Vértesi R, Zimányi J (425 authors): Systematic Study of Azimuthal Anisotropy in Cu+Cu and Au+Au Collisions at $\sqrt{s_{NN}}$ =62.4 and 200~GeV. ***PHYS REV C*** 92: Paper 034913. 20 p. (2015)
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11. Adare A et al. incl. Csörgő T, Nagy MI, Novak T, Sziklai J, Vértesi R (484 authors): ϕ meson production in d + Au collisions at $\sqrt{s_{NN}}$ =200 GeV. ***PHYS REV C*** 92:(4) Paper 044909. 14 p. (2015)

Other

12. Adare A et al. incl. Novák T, Ster A, Sziklai J, Vértesi R (476 authors): An Upgrade Proposal from the PHENIX Collaboration. http://arxiv.org/abs/1501.06197 (2015)

TOTEM Collaboration

1. Aspell P et al. incl. Csörgő T, Nemes F, Sziklai J (78 authors): Measurement of the forward charged particle pseudorapidity density in pp collisions at √s= 8 TeV using a displaced interaction point. ***EUR PHYS J C*** 75:(3) Paper 126. 9 p. (2015)

2. Aspell P et al. incl. Csörgő T, Nemes F, Sziklai J (84 authors): Evidence for non-exponential elastic proton-proton differential cross-section at low |t| and √s=8 TeV by TOTEM. ***NUCL PHYS B*** 899: pp. 527-546. (2015)

R-E. Theoretical neuroscience and complex systems

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

Within our micro-electric imaging concept, we developed a new method to reconstruct the current source density distribution from multielectrode recordings for single neurons, which includes and utilizes the known complex morphology of the cell, in the inverse solution. We showed, that the inclusion of the cell morphology improves the precision of the reconstruction and makes possible the identification of the individually activated dendritic branches in many cases.

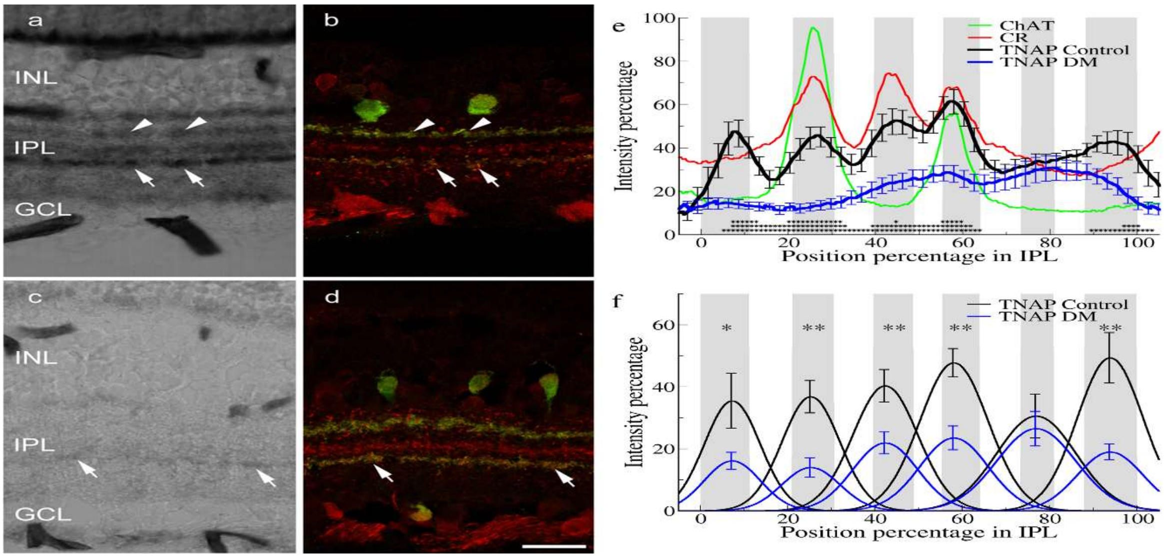

Figure 1. TNAP staining pattern of the retinal IPL layer (a-d), and it's analysis through Gaussian mixture model fitting (e-f) and the changes of the TNAP pattern due to induced diabetes mellitus.

We showed that the tissue nonspecific alkaline phosphatase (TNAP), an enzyme, which we rediscovered in the brain, plays fundamental role in the functioning and development of the central nervous system. We were able to identify more synaptic layers (11), than it was known before, by using multiple staining and large scale genetic manipulations. Moreover, our results indicate the specific role of TNAP in brain diseases especially Alzheimer's disease and diabetes by resulting specific changes in the brain TNAP patterning. A fundamental novel piece of information was added to the knowledge on Alzheimer's disease by showing that surviving neurons in tau-pathology are still functional.

Cortical neurons integrate thousands of synaptic inputs in their dendrites in highly nonlinear ways. We showed that dendritic nonlinearities are critical for the efficient integration of synaptic inputs in circuits performing analog computations with spiking neurons. Our theory

Ph.D student

accurately predicted the responses of two different types of cortical pyramidal cells to patterned stimulation by two-photon glutamate uncaging.

We built a phenomenological model to describe the synaptic plasticity changes caused by the formation of amyloid-beta protein plaques, which kept to play key role in the induction of Alzheimer disease. The model is able to capture both the normal and pathologic states via tunable parameters.

We proposed a new feedback model of the dynamics of gene expression and protein synthesis on the basis of experimental findings. We built a stochastic kinetic model to investigate and compare the “traditional” and the feed-back model of genetic expression processes.

A complete realistic dynamical simulation-model was developed, implemented, and validated which describes the real hexapod walker robot.

Grants

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

French-Hungarian Bilateral Intergovernmental S&T Cooperation TET14FR_C85E25D3_eBrain: Multiscale and multimodal analyses of brain signals using new neuro-probes. (L. Négyessy, 2015-2016)

International cooperation

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

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

Centre de Recherche Cerveau et Cognition, CNRS/Université Paul Sabatier, Toulouse, France. Neuronal Tissue-Nonspecific Alkaline Phosphatase (Caroline Fonta, Pascal Barone)

SU-Tech College of Applied Sciences, Subotica, Serbia. Model validation of a hexapod walker robot. (Péter Ódry)

Atmospheric, Oceanic and Space Sciences, College of Engineering, University of Michigan, Ann Arbor, MI, USA (Judit Szente)

Life Imaging Center, Center for Biological Signal Analysis, Albert-Ludwigs-University Freiburg (Angela Naumann, Roland Nitschke)

New York University, Langone Medical Center, NY, USA (Béla Völgyi)

Computational and Biological Learning Lab, Dept. of Engineering, University of Cambridge, Cambridge, UK (Máté Lengyel)

MRC Laboratory of Molecular Biology, Cambridge, UK, Wolfson Institute for Biomedical Research, University College London, London, UK (Tiago Branco)

HHMI Janelia Farm Research Campus, Ashburn, VA, USA (Judit Makara)

Publications

Articles

1. Érdi P: Teaching computational neuroscience. ***COGNITIVE NEURODYNAMICS*** 9: pp. 479-485. (2015)

2. Fekete Z, Pálfi E, Márton G, Handbauer M, Bérces Zs, Ulbert I, Pongrácz A, Négyessy L: In Vivo Iontophoretic BDA Injection through a Buried Microfluidic Channel of a Neural Multielectrode. ***PROCEDIA ENGINEERING*** 120: pp. 464-467. (2015)

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5. Kapitány K, Négyessy L, Fonta C, Mokso R, Szepessy Zs, Barsi Á: Automatic reconstruction of brain's micro-vascular network based on x-ray synchrotron tomography. ***BIOMECHANICA HUNGARICA*** 8:(2) pp. 15-21. (2015)

6. Négyessy L, Győrffy B, Hanics J, Bányai M, Fonta C, Bazsó F: Signal Transduction Pathways of TNAP: Molecular Network Analyses. ***SUB-CELLULAR BIOCHEMISTRY*** 76: pp. 185-205. (2015)

Book, book chapters

7. Kántor O, Cserpán D, Völgyi B, Lukáts Á, Somogyvári Z: The Retinal TNAP. In: Neuronal Tissue-Nonspecific Alkaline Phosphatase (TNAP) (Subcellular Biochemistry; 76.). Eds.: Fonta C, Négyessy L, Dordrecht: Springer Netherlands, 2015. pp. 107-123. (ISBN:978-94-017-7196-2)

8. Somogyvári Z, Érdi P: Forward and Backward Modelling: From Single Cells to Neural Population and Back. In: Cognitive Phase Transitions in the Cerebral Cortex - Enhancing the Neuron Doctrine by Modeling Neural FieldsStudies in Systems, Decision and Control. Eds.: Kozma R, Freeman WJ, New York: Springer International Publishing, 2015. pp. 135-146. (ISBN:9783319244068)

9. Fonta C, Négyessy L (eds.): Neuronal Tissue-Nonspecific Alkaline Phosphatase (TNAP) (Subcellular Biochemistry; 76.). Dordrecht: Springer Netherlands, 2015. 417 p. (ISBN:978-94-017-7196-2)

R-H. Hadron physics

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

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

Correlations of hadrons. — We have studied two-particle angular correlations between identified pions, kaons, protons and charged particles in p-Pb collisions at 5 TeV center-of-mass energy in CMS. The particles are identified via their energy loss in the silicon tracker. A long-range, near side structure appears for all particles species at high particle multiplicity. Azimuthal correlations are measured and are characterized by the second-order (elliptic flow) and third-order (triangular flow) anisotropy harmonics. They are measured as a function of transverse momentum in a wide range of particle multiplicity. The results reproduce features that are usually attributed to hydrodynamic models: mass ordering is observed at low transverse momentum at high particle multiplicities.

Hadron spectra. — We played the leading role in the analysis and publication of the measurement of pseudorapidity distribution (dN/dη) of charged hadrons in 13 TeV inelastic pp collisions in CMS. The data taking was performed without magnetic field, under special conditions. After a quick preliminary public result, based on data from the strip tracker only, we performed the analysis with a newly developed tracking algorithm. While the predictions of both Pythia8 and EPOS LHC event generators agree with the measured dN/dη value (5.49 ± 0.01(stat) ± 0.17(syst)) at mid-rapidity, the measured distribution in the full range is better described by the latter. The center-of-mass energy dependence matches well the extrapolations based on lower energy data. These results constitute the first CMS measurement of hadron production at the new center-of-mass energy frontier, in fact these were the first published results based on 13 TeV LHC data. They provide new constraints for the improvement of perturbative and nonperturbative QCD aspects of hadronic event generators.

Probes of nuclear parton distribution functions. — We have measured the Z boson production in p-Pb collisions also in the electron decay channel in CMS. The combined cross section from the muon and electron channels provides better statistical precision. The differential cross section as a function of rapidity and the forward-backward ratio shows better agreement with presence of nuclear effects. The combination of W boson, charged

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[#] Ph.D. student

particle and jet measurements in p-Pb collisions provide constraints for nuclear parton distribution functions.

Probing the hot medium with heavy flavor. — We carried out the first measurement of bottomonium production in 193 GeV U-U collisions with the STAR experiment. Bound states of heavy quarks provide a unique means for accessing the thermal properties of the quark-gluon plasma. We identified the decay electrons in order to reconstruct the ϒ(1S), ϒ(2S), and ϒ(3S) states. The production of these states is significantly suppressed in central U-U collisions compared to naive expectations from pp collisions. According to different theoretical calculations, this observation is consistent with an initial medium temperature between 330 and 442 MeV.

Differentiating jets. — We have developed a prototype machine learning classifier for differentiating between decays of quarks and gluons. The power to discriminate between these two types of particles would have a huge impact on many searches for new particles and new physics, and studies of QCD. We have devised a fast method for ranking discriminant variables. The model has been tested on Monte Carlo data with full-detector simulation and demonstrates performance that is competitive with results obtained by others in the field.

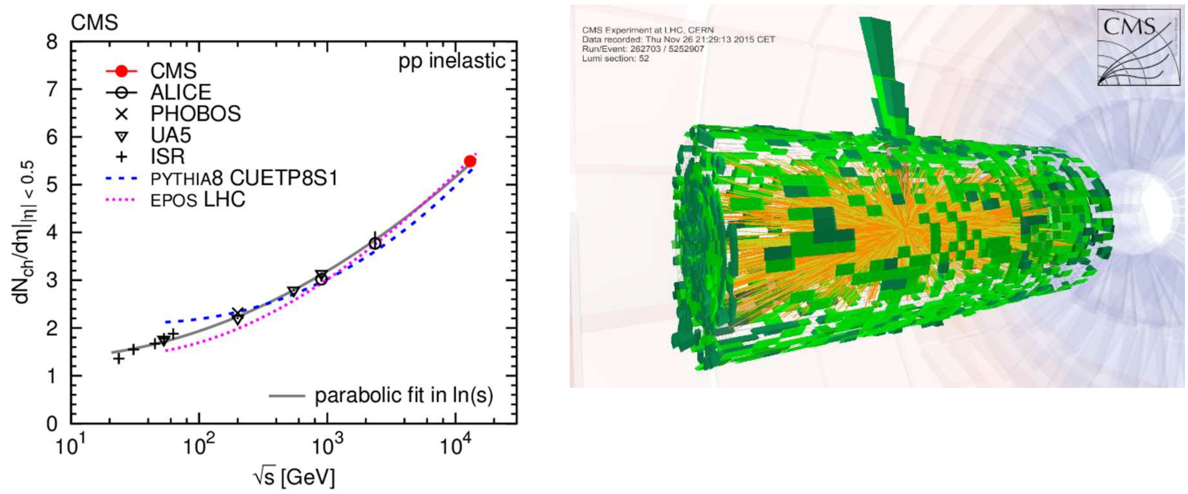

Figure 1. *Left: Center-of-mass energy dependence of* $dN_{ch}/d\eta|_{|\eta|<0.5}$ *including lower energy data. The solid curve shows a second-order polynomial fit to the data points, including the new result at 13 TeV. The dashed and dotted curves show model predictions. Right: Event display of a Pb-Pb collision taken at 5 TeV per nucleon-pair center-of-mass energy at the end of 2015. Orange curves show reconstructed trajectories of charged particles, while green towers represent energy deposits in the calorimeters.*

Grants

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

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

International cooperation

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

Publications
See: R-I.3

CMS collaboration

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

1. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2146 authors): Angular coefficients of Z bosons produced in pp collisions at √s = 8 TeV and decaying to $\mu^+\mu^-$ as a function of transverse momentum and rapidity. ***PHYS LETT B*** 750: pp. 154-175. (2015)
2. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2134 authors): Differential cross section measurements for the production of a W boson in association with jets in proton-proton collisions at √s = 7 TeV. ***PHYS LETT B*** 741: pp. 12-37. (2015)
3. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2143 authors): Long-range two-particle correlations of strange hadrons with charged particles in pPb and PbPb collisions at LHC energies. ***PHYS LETT B*** 742: pp. 200-224. (2015)
4. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2147 authors): Measurement of the cross section ratio $\sigma t\bar{t}b\bar{b}/\sigma t\bar{t}jj$ in pp collisions at √s = 8 TeV. ***PHYS LETT B*** 746: pp. 132-153. (2015)
5. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2135 authors): Measurement of the pp→ZZ production cross section and constraints on anomalous triple gauge couplings in four-lepton final states at √s = 8 TeV. ***PHYS LETT B*** 740: pp. 250-272. (2015)
6. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2147 authors): Measurement of the production cross section ratio $\sigma(\chi_{b2}(1P))/\sigma(\chi_{b1}(1P))$ in pp collisions at √s = 8 TeV. ***PHYS LETT B*** 743: pp. 383-402. (2015)
7. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2175 authors): Measurement of the Z boson differential cross section in transverse momentum and rapidity in proton-proton collisions at 8 TeV. ***PHYS LETT B*** 749: pp. 187-209. (2015)
8. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2140 authors): Measurements of the ϒ(1S), ϒ(2S), and ϒ(3S) differential cross sections in pp collisions at √s=7TeV. ***PHYS LETT B*** 749: pp. 14-34. (2015)
9. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2829 authors): Observation of the rare B_s^0 $\mu^+\mu^-$ decay from the combined analysis of CMS and LHCb data. ***NATURE*** 522:(7554) pp. 68-72. (2015)

10. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horvath D, Sikler F, Veszpremi V, Vesztergombi G, Zsigmond AJ (2309 authors)*:* Pseudorapidity distribution of charged hadrons in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS LETT B*** 751: pp. 143-163. (2015)
11. Khachatryan V, Sirunyan AM, Filipovic N, et al. incl. Bencze G, Hajdu C, Hidas P, Horvath D, Sikler F, Veszpremi V, Vesztergombi G, Zsigmond AJ (2297 authors): Search for a pseudoscalar boson decaying into a Z boson and the 125 GeV Higgs boson in $\ell^{+}\ell^{-}bb^{-}$ final states. ***PHYS LETT B*** 748: pp. 221-243. (2015)
12. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2144 authors): Search for a standard model-like Higgs boson in the $\mu^{+}\mu^{-}$ and $e^{+}e^{-}$ decay channels at the LHC. ***PHYS LETT B*** 744: pp. 184-207. (2015)
13. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2287 authors): Search for diphoton resonances in the mass range from 150 to 850 GeV in pp collisions at $\sqrt{s}$= 8 TeV. ***PHYS LETT B*** 750: pp. 494-519. (2015)
14. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2150 authors): Search for heavy Majorana neutrinos in $\mu^{\pm}\mu^{\pm}$ + jets events in proton-proton collisions at $\sqrt{s}$= 8 TeV. ***PHYS LETT B*** 748: pp. 144-166. (2015)
15. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2146 authors): Search for lepton-flavour-violating decays of the Higgs boson. ***PHYS LETT B*** 749: pp. 337-362. (2015)
16. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2149 authors): Search for narrow high-mass resonances in proton-proton collisions at $\sqrt{s}$ = 8 TeV decaying to a Z and a Higgs boson. ***PHYS LETT B*** 748: pp. 255-277. (2015)
17. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2132 authors): Search for new resonances decaying via WZ to leptons in proton-proton collisions at $\sqrt{s}$=8 TeV. ***PHYS LETT B*** 740: pp. 83-104. (2015)
18. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2133 authors): Search for pair-produced resonances decaying to jet pairs in proton-proton collisions at $\sqrt{s}$=8 TeV. ***PHYS LETT B*** 747: pp. 98-119. (2015)
19. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horvath D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2141 authors): Search for quark contact interactions and extra spatial dimensions using dijet angular distributions in proton-proton collisions at $\sqrt{s}$= 8 TeV. ***PHYS LETT B*** 746: pp. 79-99. (2015)
20. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2145 authors): Search for resonant pair production of Higgs bosons decaying to two bottom quark-antiquark pairs in proton-proton collisions at 8 TeV. ***PHYS LETT B*** 749: pp. 560-582. (2015)
21. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2132 authors): Search for stealth supersymmetry in

events with jets, either photons or leptons, and low missing transverse momentum in pp collisions at 8 TeV. ***PHYS LETT B*** 743: pp. 503-525. (2015)

22. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2140 authors): Searches for supersymmetry based on events with b jets and four W bosons in pp collisions at 8 TeV. ***PHYS LETT B*** 745: pp. 5-28. (2015)
23. Khachatryan V et al. incl. Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszprémi V, Vesztergombi G, Zsigmond AJ (2135 authors): Study of W boson production in pPb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS LETT B*** 750: pp. 565-586. (2015)

NA49 Collaboration

1. Anticic T et al. incl. Fodor Z, László A, Pálla G, Siklér F, Varga D, Vesztergombi G (66 authors): Measurement of event-by-event transverse momentum and multiplicity fluctuations using strongly intensive measures Δ[PT,N] and Σ[PT,N] in nucleus-nucleus collisions at the CERN Super Proton Synchrotron. ***PHYS REV C*** 92:(4) Paper 044905. 10 p. (2015)
2. Anticic T et al. incl. Fodor Z, László A, Pálla G, Siklér F, Varga D, Vesztergombi G (72 authors): Critical fluctuations of the proton density in A+A collisions at 158A GeV. **EUR PHYS J C** 75:(12) Paper 587. 10 p. (2015)

FOPI Collaboration

1. Piasecki K et al. incl. Fodor Z, Kecskeméti J, Seres Z (66 authors): Influence of ϕ mesons on negative kaons in Ni + Ni collisions at 1.91A GeV beam energy. ***PHYS REV C*** 91:(5) Paper 054904. 8 p. (2015)

See also: R-B. ALICE Collaboration, R-K. ATLAS Collaboration 14

R-J. Standard model and new physics

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

Physics analyses and theoretical work. — The CMS group members analyzed the discovery potential of supersymmetric processes; particularly such processes, in which top-stop pairs produced by gluino decays undergo 4-body or chargino decays. Members of the ATLAS collaboration validated the improvements of the simulation and reconstruction software packages that include the treatment of radiation-induced changes in the properties of the measurement devices and new reconstruction methods, and monitored the changes in the characteristics of the so-called topoclusters in QCD events containing top-antitop pairs and two jets with various transverse momenta. The ASACUSA group members have reached the point in the determination of the antiproton's mass with laser-spectroscopy of antiprotonic helium, where the precision is limited by the thermal movements of the helium atoms in low-pressure helium gas. The precision reached earlier with two-photon laser-spectroscopy has now been achieved with a single-photon method on a gas-target at 1.5 K temperature. The Schrödinger-Newton equation of non-relativistic quantum gravity, proposed earlier by a member of the group, continued to attract activity in 2015. His newly proposed experiment will contribute to a conclusive test of the related theory of spontaneous decoherence.

Work on instrumentation. — The CMS group has designed and produced prototypes for the control and read-out electronics of the Phase I Pixel Detector which is to be installed in CMS in 2017. The serial production has also been started. The group has organized the annual conference for the CMS detector collaboration in Visegrád hosting 70 participants from 7 countries. It has taken a leading role in starting and optimizing data-taking with the CMS tracking devices, studied the effects of radiation damage on measurement efficiency and resolution, and adjusted the simulation that is used in all physics analyses to the data recorded in 2015. The Liquid Argon Calorimeter is a basic component of the ATLAS detector. Its capabilities of detecting electrons, photons, jets and missing energy are crucial ingredients of discovering theoretically predicted new physics phenomena, like supersymmetry, and of analyzing features of the Standard Model, including detailed experimental study of the Higgs boson. The ATLAS members of our group participated in the simulation analyses targeting the upgrade of the LAr (Liquid Argon) calorimeter. The group has participated in the construction of the ELENA storage ring by performing the simulation and design of the beam line elements. The grid computing infrastructure used for analyses in the CMS and ALICE experiments was upgraded in order to fulfill the fraction of the whole CMS computing needs that is proportional to the size of the CMS group at Wigner RCP.

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

Outreach. — The group has helped organizing several events in order to promote particle physics for the public. It appeared with the "All Colors of Physics Roadshow" at several venues. It participated in the annual Particle Physics Masterclass of CERN taking place at Wigner RCP. The groups presented its activities in the CERN-Wigner Open Days at Wigner RCP. It has contributed to a week-long curricular training for high school teachers at CERN. Our group helped the media in the explanation of fascinating scientific frontiers such as quantum teleportation; as well as, the research activities performed by the group (such as on quantum-gravitation) were displayed in popular media outlets.

Grants

OTKA K 109703: Consortional main: Hungary in the CMS experiment of the Large Hadron Collider (V. Veszprémi, Cs. Hajdu, P. Hidas, D. Horváth, Gy. Vesztergombi,T. Vámi); S&T Cooperation (J. Tóth); 2013-2016

OTKA K 103917: Antimatter investigations at the CERN Antiproton-Decelerator (D. Horváth, D. Barna, L. Diósi, 2012-2016)

EU COST Action MP1006 Fundamental Problems in Quantum Physics (L. Diósi, 2011-2015);

IUPAP support for FFK-2015 conference

International cooperation

CERN: CMS Collaboration (179 institutes), ATLAS Collaboration (174 institutes)

University of Kwa-Zulu Natal, South-Africa;

University of Calgary, Canada;

Stellenbosch University, South-Africa;

University of Tokyo, Japan;

RIKEN, Wako, Japan;

Stefan-Meyer-Institut, Vienna, Austria;

MPQ, München-Garching

Publications

Articles

1. Aghai-Khozani H, Barna D, Corradini M, De Salvador D, Hayano R, Hori M, Kobayashi T, Leali M, Lodi-Rizzini E, Mascagna V, Prest M, Seiler D, Soter A, Todoroki K, Vallazza E, Venturelli L: First measurement of the antiproton-nucleus annihilation cross section at 125 keV. ***HYPERFINE INTERACTIONS*** 234: pp. 85-92. (2015)

2. Aghai-Khozani H, Barna D, Corradini M, Hayano R, Hori M, Kobayashi T, Leali Marco, Lodi-Rizzini E, Mascagna V, Prest M, Soter A, Todoroki K, Vallazza E, Venturelli L, Zurlo N: Beam Diagnostics for Measurements of In-Flight Annihilation Cross Sections of Antiprotons at 130 keV. ***JPS CONFERENCE PROCEEDINGS*** 6: Paper 030111. 4 p. (2015) Proceedings of the Conference on Advances in Radioactive Isotope Science (ARIS2014).

3. Amsbaugh JF et al, incl. Glück F (50 authors): Focal-plane detector system for the KATRIN experiment. ***NUCL INSTRUM METH A*** 778: pp. 40-60. (2015)

4. Bassa H, Goyal SK, Choudhary SK, Uys H, Diósi L, Konrad T: Process tomography via sequential measurements on a single quantum system. ***PHYS REV A*** 92:(3) Paper 032102. 6 p. (2015)

5. Diósi L: Testing spontaneous wave-function collapse models on classical mechanical oscillators ***PHYS REV LETT*** 114:(5) Paper 050403. 5 p. (2015)

6. Diósi L: Is spontaneous wave function collapse testable at all? 7th International Workshop on Decoherence, Information, Complexity andEntropy (DICE) - Spacetime - Matter - Quantum Mechanics. Castiglioncello, Italy, 15.09.2014 – 19.09.2014. ***J PHYS CONF SER*** 626: Paper 012008. 5 p. (2015).

7. Goyal SK, Konrad T, Diósi L: Unitary equivalence of quantum walks. ***PHYS LETT A*** 379:(3) pp. 100-104. (2015)

8. Hori M, Sótér A, Aghai-Khozani H, Barna D, Dax A, Hayano RS, Murakami Y, Todoroki K, Yamada H: Towards laser spectroscopy of pionic helium atoms at Paul Scherrer Institute. Technology and Instrumentation in Particle Physics 2014. Amsterdam, The Netherlands, 02.06.2014 – 06.06.2014. ***POS*** TIPP2014: Paper 342. 5 p. (2015)

9. Hori M, Sótér A, Aghai-Khozani H, Barna D, Dax A, Hayano RS, Murakami Y, Yamada H: Method for laser spectroscopy of metastable pionic helium atoms. ***HYPERFINE INTERACT*** 233:(1-3) pp. 83-87. (2015)

10. Kobayashi T, Barna D, Hayano RS, Murakami Y, Todoroki K, Yamada H, Dax A, Venturelli L, Zurlo N, Horváth D, Aghai-Khozani H, Sótér A, Hori M: Laser Spectroscopic Study on the Highly Excited States of Antiprotonic Helium. Proceedings of the Conference on Advances in Radioactive Isotope Science (ARIS2014). ***JPS CONF PROC*** 6: Paper 030073. 4 p. (2015)

11. László A, Dénes E, Fodor Z, Kiss T, Kleinfelder S, Soós Cs, Tefelski D, Tölyhi T, Vesztergombi Gy, Wyszyński O: Design and Performance of the Data Acquisition System for the NA61/SHINE Experiment at CERN. ***NUCL INSTRUM METH A*** 798: pp. 1-11. (2015)

12. Mertens S, Dolde K, Korzeczek M, Glück F, Groh S, Martin RD, Poon AWP, Steidl M Wavelet approach to search for sterile neutrinos in tritium β -decay spectra ***PHYS REV D*** 91:(4) Paper 042005. (2015)

13. Mertens S, Lasserre T, Groh S, Drexlin G, Glück F, Huber A, Poon AWP, Steidl M, Steinbrink N, Weinheimer C: Sensitivity of next-generation tritium beta-decay experiments for keV-scale sterile neutrinos. ***J COSMOL ASTROPART P*** 2015:(2) Paper 020. (2015)

14. Sótér A, Barna D, Todoroki K, Kobayashi T, Horváth D, Hori M: Segmented scintillators with SiPM readout for measuring antiproton annihilations. Technology and Instrumentation in Particle Physics 2014. Amsterdam, The Netherlands, 02.06.2014 – 06.06.2014. ***POS*** TIPP2014: Paper 286. 5 p. (2015)

Articles in Hungarian

15. Horváth D: Higgs-bozon és a világ vége vagy kezdete (Higgs boson and the start or end of the world, in Hungarian). ***FIZIKAI SZEMLE*** 95:(4) pp. 115-117. (2015)

16. Horváth D, Oláh É, Sükösd Cs, Varga D, Patkós A: Beszélgetés az elektron méretéről (Chat about the size of the electron, in Hungarian). ***FIZIKAI SZEMLE*** 65:(5) pp. 151-156. (2015)

ATLAS collaboration

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

1. Aad G et al., incl. Pásztor G, Tóth J (2890 authors): Centrality and rapidity dependence of inclusive jet production in $\sqrt{s_{NN}}$=5.02 TeV proton-lead collisions with the ATLAS detector. ***PHYS LETT B*** 748: pp. 392-413. (2015)
2. Aad G et al., incl. Pásztor G, Tóth J (2851 authors): Measurement of colour flow with the jet pull angle in $t\bar{t}$ events using the ATLAS detector at $\sqrt{s}$ =8 TeV. ***PHYS LETT B*** 750: pp. 475-493. (2015)
3. Aad G, et al., incl. Pásztor G, Tóth J (2850 authors): Measurement of exclusive $\gamma\gamma \rightarrow \ell^+ \ell^-$ production in proton–proton collisions at $\sqrt{s}$ = 7 TeV with the ATLAS detector. ***PHYS LETT B*** 749: pp. 242-261. (2015)
4. Aad G et al., incl. Pásztor G, Tóth J (2856 authors): Measurement of the branching ratio $\Gamma(\Lambda 0b \rightarrow \psi(2S)\Lambda 0)/\Gamma(\Lambda 0b \rightarrow J/\psi\Lambda 0)$ with the ATLAS detector. ***PHYS LETT B*** 751: pp. 63-80. (2015)
5. Aad G et al., incl. Pásztor G, Tóth J (2882 authors): Measurement of the production of neighbouring jets in lead-lead collisions at $\sqrt{s_{NN}}$=2.76 TeV with the ATLAS detector. ***PHYS LETT B*** 751: pp. 376-395. (2015)
6. Aad G et al., incl. Pásztor G, Tóth J (2857 authors): Measurement of transverse energy-energy correlations in multi-jet events in pp collisions at $\sqrt{s}$=7 TeV using the ATLAS detector and determination of the strong coupling constant $\alpha_s(m_Z)$. ***PHYS LETT B*** 750: pp. 427-447. (2015)
7. Aad G et al., incl. Pásztor G, Tóth J (2898 authors): Search for pair-produced long-lived neutral particles decaying to jets in the ATLAS hadronic calorimeter in pp collisions at $\sqrt{s}$=8 TeV. ***PHYS LETT B*** 743: pp. 15-34. (2015)
8. Aad G et al., incl. Pásztor G, Tóth J (2889 authors): Search for s-channel single top-quark production in proton-proton collisions at $\sqrt{s}$=8 TeV with the ATLAS detector. ***PHYS LETT B*** 740: pp. 118-136. (2015)
9. Aad G et al., incl. Pásztor G, Tóth J (2828 authors): Search for the associated production of the Higgs boson with a top quark pair in multilepton final states with the ATLAS detector. ***PHYS LETT B*** 749: pp. 519-541. (2015)
10. Aad G et al., incl. Pásztor G, Tóth J (2886 authors): Search for $W' \rightarrow tb^-$ in the lepton plus jets final state in proton-proton collisions at a centre-of-mass energy of $\sqrt{s}$=8 TeV with the ATLAS detector. ***PHYS LETT B*** 743: pp. 235-255. (2015)

11. Abbott B et al., incl. Pásztor G, Tóth J (2826 authors): Search for a CP-odd Higgs boson decaying to Zh in pp collisions at √s=8 TeV with the ATLAS detector. ***PHYS LETT B*** 744: pp. 163-183. (2015)
12. Abbott B et al., incl. Pásztor G, Tóth J (2889 authors): Search for H→γγ produced in association with top quarks and constraints on the Yukawa coupling between the top quark and the Higgs boson using data taken at 7 TeV and 8 TeV with the ATLAS detector. ***PHYS LETT B*** 740: pp. 222-242. (2015)
13. Abbott B et al., incl. Pásztor G, Tóth J: (2890 authors): Search for the X_b and other hidden-beauty states in the $\pi^+\pi^-\Upsilon(1S)$ channel at ATLAS. ***PHYS LETT B*** 740: pp. 199-217. (2015)
14. Aad G et al., incl. Pásztor G, Tóth J, Bencze G, Hajdu C, Hidas P, Horváth D, Siklér F, Veszpremi V, Vesztergombi G, Zsigmond AJ (5154 authors): Combined Measurement of the Higgs Boson Mass in pp Collisions at √s =7 and 8 TeV with the ATLAS and CMS Experiments. ***PHYS REV LETT*** 114:(19) Paper 191803. 45 p. (2015)
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25. Aad G et al., incl. Pásztor G, Tóth J (2824 authors): Search for New Phenomena in Dijet Angular Distributions in Proton-Proton Collisions at √s=8 TeV Measured with the ATLAS Detector. ***PHYS REV LETT*** 114:(22) Paper 221802. 17 p. (2015)
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See also: R-H CMS Collaboration, R-H. NA49 Collaboration

R-L. Functional nanostructures

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

A “copolymer-co-morphology” conception for shape-controlled synthesis of Prussian blue analogues and as-derived spinel oxides. — The morphologically and compositionally controlled synthesis of coordination polymers and spinel oxides is highly desirable for realizing new advanced nanomaterial functionalities. A novel and scalable strategy, containing a “copolymer-co-morphology” conception was developed for shape-controlled synthesis of Prussian blue analogues (PBAs), namely three series of $M_yFe_{1-y}[Co(CN)_6]_{0.67}\cdot nH_2O$ (M_yFe_{1-y}–Co, M = Co, Mn and Zn) with well-controlled morphology. Using Mn_yFe_{1-y}–Co PBA as a model system, by increasing the relative content of Mn, the morphology could be easily modulated. In addition, a series of porous $Mn_xFe_{1.8-x}Co_{1.2}O_4$ nano-dices with well-inherited morphologies and defined cation distribution could be obtained through a simple thermal treatment of the PBAs. All these demonstrate the good universality of this novel strategy. When evaluated as an electrocatalyst, the octahedral-site Mn^{III}/Mn^{IV} content in $Mn_xFe_{1.8-x}Co_{1.2}O_4$, as revealed by ^{57}Fe Mössbauer spectroscopy (Fig. 1) in combination with X-ray photoelectron spectroscopy, was found to directly correlate with the oxygen reduction/evolution reaction (ORR/OER) activity.

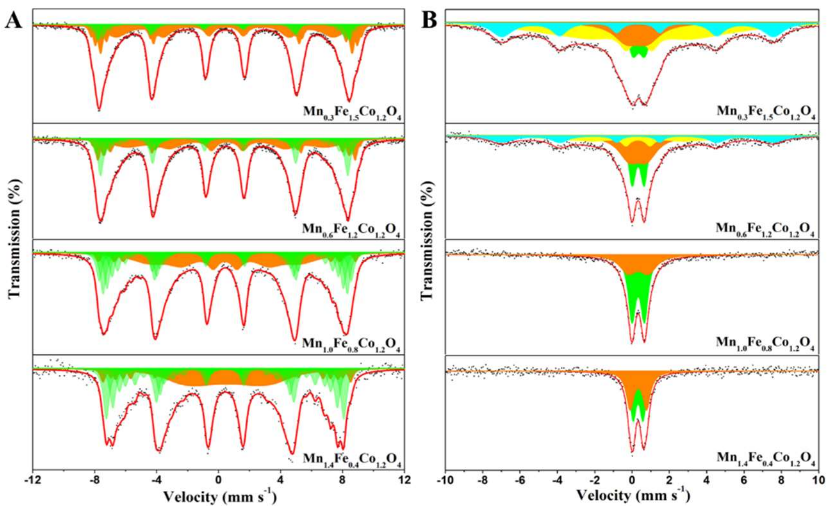

Figure 1. *(A) 77 K ^{57}Fe Mössbauer spectra of $Mn_xFe_{1.8-x}Co_{1.2}O_4$ nano-dices. The spectra were fitted with thirteen sextets. The fit model assumes binomial distribution of the iron and non-iron cations. In agreement with the fitted IS values, seven sextets (green) were assigned to the tetrahedral (A-) site Fe^{III}. The remaining six (orange) species were assigned to the octahedral-site (B-site) Fe^{III}. (B) Room temperature ^{57}Fe Mössbauer spectra of $Mn_xFe_{1.8-x}Co_{1.2}O_4$ nano-dices. The cyan sextet and green doublets were assigned to the tetrahedral (A-) site Fe^{III}, the yellow sextet and orange doublets were assigned to the octahedral (B-) site Fe^{III}.*

[#] Ph.D student

[E] Professor Emeritus

Evolution of magnetism on a curved nano-surface. — Design of custom magnetic nanostructures requires precise knowledge about the systems on the nanoscale in which the magnetism forms. Here the effect of substrate curvature on the evolution of magnetism in ultrathin iron films was investigated in details. Nominally 70 Å thick iron films were deposited in 9 steps on 3 different types of templates: (i) on a monolayer of silica spheres with 25 nm diameter (Fig. 2), (ii) on a monolayer of silica spheres with 400 nm diameter and (iii) on a flat silicon substrate for comparison. The thickness was selected close to the nonmagnetic/magnetic transition. Samples were structurally and morphologically characterized by X-ray reflectivity, atomic force and magnetic force microscopy. In situ nuclear resonant scattering experiments performed at room temperature revealed that depending on the ratio of the thickness of the evaporated iron layer to the sphere diameter, different magnetic structures develop. Such isolated, uniformly distributed (interspherical) magnetic domains, magnetic vortices and multiparticle magnetic structures could be successfully reproduced by micromagnetic simulations. The diversity of magnetic structures enables to tailor these systems to the desired applications.

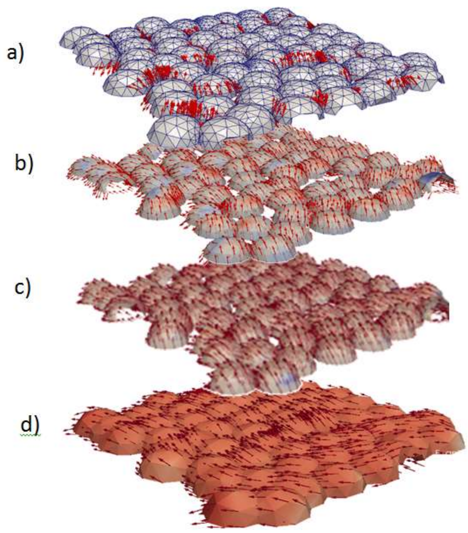

***Figure 2.** Micromagnetic simulation of magnetic moment configurations for a) 26 Å, b) 34.5 Å, c) 48.5 Å and d) 70.5Å evaporated iron thickness on 25 nm diameter spheres. The bluish color represents the magnitude of the Z component while the red stands for that of the X-Y (in-plane) component.*

International cooperation

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, (Dalian, China), Mössbauer Effect Data Center (D.L. Nagy)

Long-term visitor

Hartmut Spiering, Johannes Gutenberg-Universität Mainz, Institute of Inorganic and Analytical Chemistry, Germany, 2 to 15 November, 2015, (host: L. Deák)

Publications

Articles

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See also: R-M.7

R-M. Ion beam physics

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

Waveguide fabrication. — The refractive indices of optical materials can be modified by ion implantation. Irradiations with swift heavy ions, when the damage is caused mainly by the energy deposition of electronic stopping power, has been shown particularly effective for waveguide fabrication. In collaboration with Centre for Micro Analysis of Materials (Madrid, Spain) sillenite type ($Bi_{12}GeO_{20}$) BGO crystals were irradiated with 25 MeV C ions at an angle of incidence of 60° at relatively low fluences between 10^{13} and 10^{15} ion/cm^2. M-line spectroscopic measurements showed that planar waveguides were created when irradiating the sample with 25 MeV C ions at fluences between $2{\cdot}10^{13}$ and $1{\cdot}10^{15}$. Preliminarily results of spectroscopic ellipsometric measurements of the irradiated samples indicated that partial amorphisation of the surface layer down to the maximum of the electronic stopping power occurred at all the fluences (Figure 1).

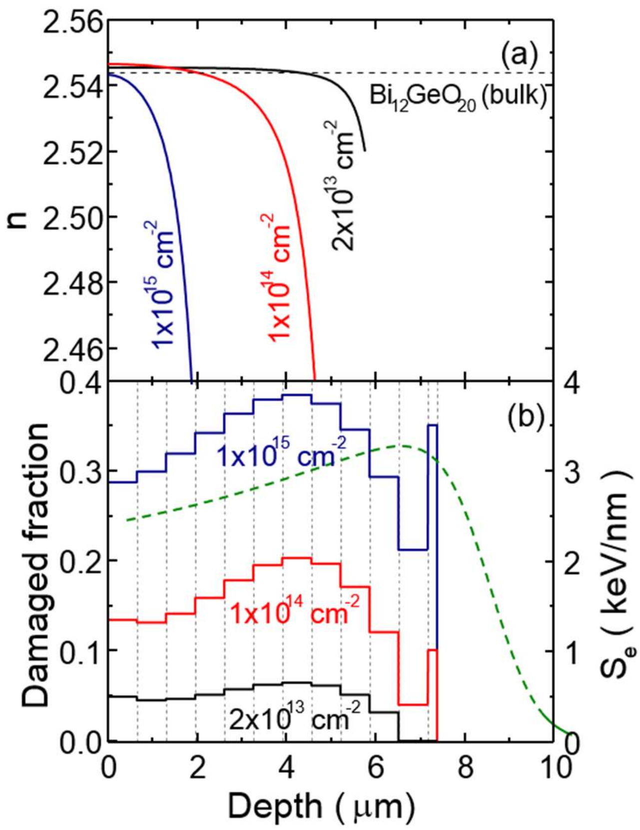

Figure 1. *(a) Refractive index profiles of the irradiated layers calculated from m-line spectra at λ = 633 nm. (b) Depth distribution of the damage obtained from spectroscopic ellipsometric measurements. Samples irradiated with 25 MeV C ions. Electronic stopping power is also shown (dashed line).*

Advanced cultural heritage research. — As a continuation of the four-year-long CHARISMA (Cultural Heritage Advanced Research Infrastructures: Synergy for a Multidisciplinary Approach to conservation/restoration) EU FP7 Program the PIXE-XRF laboratory functioning as an open infrastructure provided access to the external proton milli-beam PIXE and XRF setup developed for cultural heritage (CH) research for CH scientists. Several joint research projects were carried out in collaboration with Hungarian museums and CH institutes.

[A] Associate fellow
[E] Professor Emeritus

In collaboration with **Wosinsky Mór Megyei Múzeum** (Szekszárd, Hungary) elemental concentrations were determined in the gun fragments excavated on Béla király tér, Szekszárd in 2014. The elemental composition of the two fragments were identical, 92.0 % copper , 5,5 % tin and 2,2 % antimony, Fe, Ni, Zn, As, Ag and Pb also were detected in traces. The quantitative analyses supported and confirmed the visual archaeological survey, the fragments belong to a falcon type gun and are dated to the 16th-17th century.

Figure 2. *A gun fragment bombarded with external proton beam of 3 MeV energy for PIXE analysis.*

Grants

OTKA K 101225: Fabrication of integrated optical elements via ion beam implantation and irradiation for telecommunication applications (I. Bányász, 2012-2015)

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

Infrastructure Development of the HAS: micro-X-ray tube for XRF (Z. Szőkefalvi-Nagy 2015)

Publications

Articles

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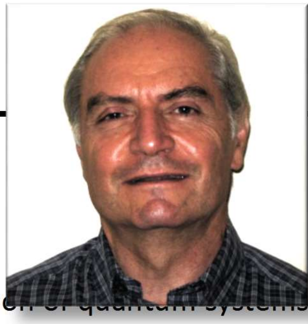
See also: S-L.22

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



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

Coherent control of atomic coherences. — The coherent manipulation of quantum systems is an important challenge in modern science and engineering, with significant applications in quantum optics and information, nuclear magnetic resonance, nonlinear optics, laser controlled chemistry and many others.We have developed a novel technique for the creation of a coherent superposition state with a controlled relative phase in a two level system using a single-shot shaped laser pulse, (see Figure 1). The robustness of the derived pulse has been analyzed in detail as a function of the imperfection of the pulse area.

The technique provides smooth and relatively simple form pulses which are in principle well implementable experimentally. In addition of their smoothness and simple form, these shaped pulses achieve a high fidelity in a controlled, robust way.

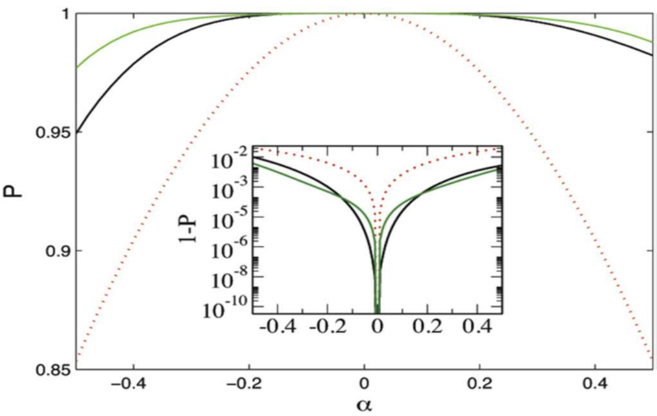


***Figure 1.** Profile P of the transfer probability to the target state as a function of the perturbation parameter α for the π/ 2 pulse (dotted line), and for the optimally shaped pulse (full lines). The inset displays the deviation from unity in a logarithm scale of the excitation profile.*

Quantum memories based on photon-echo phenomenon. — The method of composite pulses for the atomic excitation in an optically dense, inhomogeneously broadened ensemble was investigated extensively. Achieving high fidelity atomic inversion in such ensembles is very important for building optical quantum memories based on the photon echo phenomenon. Obtaining perfect inversion in an extended region (i.e. sizable frequency range and optical depth) of the ensemble is hindered by the fact that the ensemble distorts the strong control pulses that are used to invert the atoms. Single monochromatic π-pulses prove ineffective for this reason - they excite atoms in a very narrow frequency range and only to a very limited optical depth. Frequency chirped pulses that drive adiabatic transitions can excite atoms in an extended frequency range and to a sufficient optical depth, but are slow to achieve the inversion.

A possible compromise is the use of composite pulses – sequences of short pulses with a well-defined phase relationship between the constituent elementary pulses, (see Fig.2). Several such composite pulses were derived that can be used for atomic inversion in an optically dense ensemble. We have been able to derive composite sequences consisting of as few as

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

three or five elementary pulses which can excite atoms to an optical depth perfectly sufficient for an optical quantum memory to function.

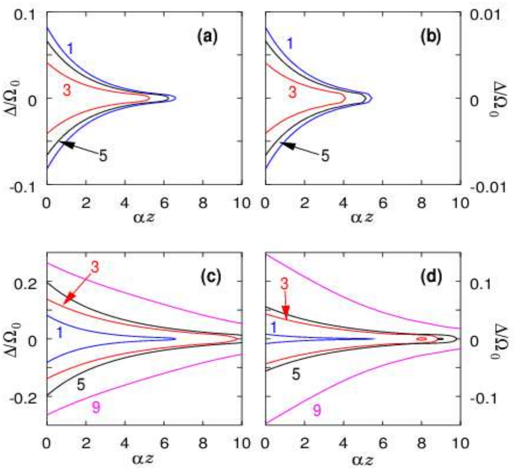
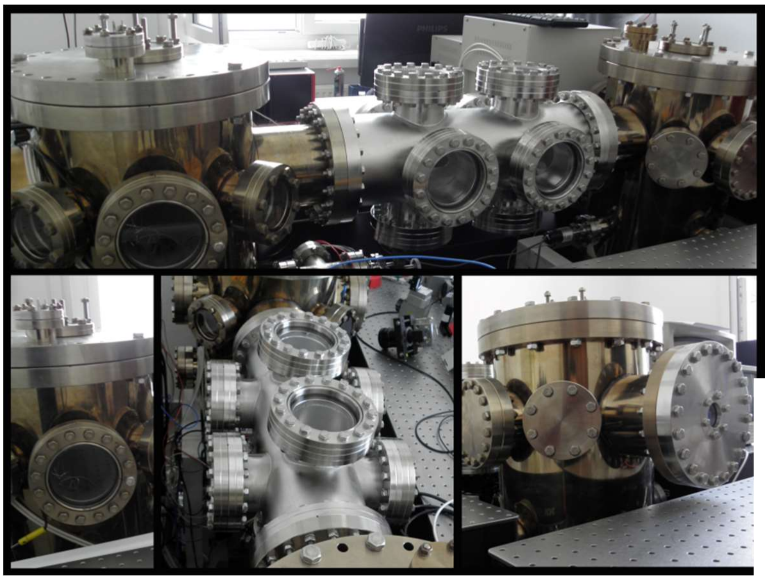


Figure 2. *Performance of composite pulses in inverting the atomic ensemble. Contour lines on the optical depth (αz) - frequency offset (Δ) plane mark the boundaries within which the probability of error is less than 1% (subfigures a) and c)) and less than 0.01% (subfigures b) and d)). The labels mark the number of elementary pulses that the composite pulse consists of.*

Generation and real-time diagnostics of homogeneous laser plasma. — This direction of our research is directly connected to the creation of novel compact accelerators of elementary particles, and namely to the AWAKE (proton-driven wake field particle acceleration in plasma) project at CERN. The novel accelerator currently under construction in CERN will utilize the proton bunch available at Large Hadron Collider (LHC) to accelerate electrons (positrons) to TeV energies in one acceleration stage. An extended volume of extremely homogeneous plasma is an indispensable part of the acceleration scheme. This plasma will be used for splitting the LHC proton bunch into micro-bunches using self-modulation instability in the plasma to provide coherent wake-field acceleration of electrons by the proton bunch.



We have built an experimental setup for generation and real-time diagnostics of Rubidium plasma, see Fig.3. The plasma is created by ultra-short (30-40 fs) laser pulses (with pulse energy about 4 mJ) from Ti:Sa laser system

Fig.3. The experimental setup.

An example of time dependence of the transmitted probe beam intensity is shown in Fig.4. We have demonstrated that a number of processes including resonantly enhanced multi-photon-, tunneling- and over-the-barrier ionization take place during interaction of different parts of the strong ionizing laser pulse with Rubidium atoms.
These processes may result in significant variation of parameters of the ionizing laser pulse propagating in the Rubidium vapor and, hence may strongly influence the homogeneity of the laser plasma volume. Results of our studies allow us to understand the physical mechanisms of generation of *extended* laser plasma in Rubidium vapors as well as to understand and describe the induced plasma instabilities.

creation and recombination of the laser plasma channel.

In this scheme, transmission of the probe laser is measur
the strong ionizing femtosecond laser pulse through the F
illuminated by the probe laser beam.

An example of time dependence of the transmitted prob
We have demonstrated that a number of processes incl

photon-, tunneling- and over-the-barrier ionization take place during interaction of different parts of the strong ionizing laser pulse with Rubidium atoms.

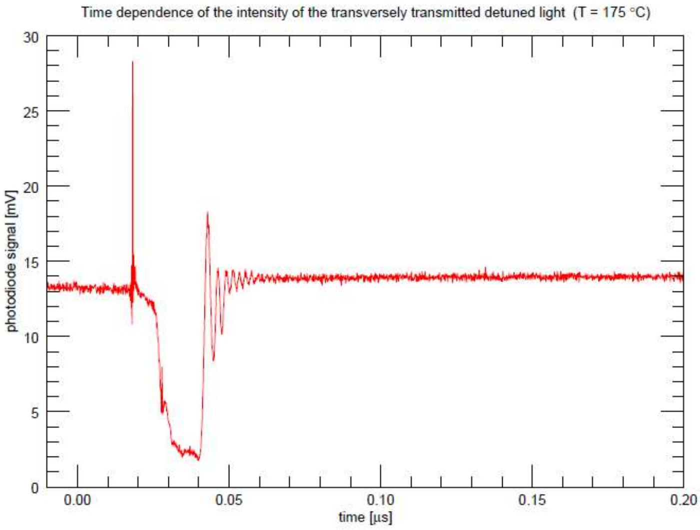


Fig.4. An example of time dependence of the transmitted signal intensity at relatively high temperature of Rb vapor.

These processes may result in significant variation of parameters of the ionizing laser pulse propagating in the Rubidium vapor and, hence may strongly influence the homogeneity of the laser plasma volume. Results of our studies allow us to understand the physical mechanisms of generation of *extended* laser plasma in Rubidium vapors as well as to understand and describe the induced plasma instabilities.

These results (in collaboration with the AWAKE team) will be used to create optimal conditions for generation of highly homogeneous plasma for application in the AWAKE project at CERN.

Grants

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

TeT_12_FR-1-2013-0019 French-Hungarian Bilateral grant with the University de Bourgogne, Dijon, France (G.P.Dzsotjan, 2013-2015)

International cooperation

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

Publications

Articles

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2. Karlewski F, Mack M, Grimmel J, Sándor N, Fortágh J: State-selective all-optical detection of Rydberg atoms. ***PHYS REV A*** 91:(4) Paper 043422. 7 p. (2015)
3. Ndong M, Djotyan G, Ruschhaupt A, Guérin S: Robust coherent superposition of states by single-shot shaped pulse. ***J PHYS B-AT MOL OPT*** 48:(17) Paper 174007. 8 p. (2015)

Conference proceeding

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See also: R-P.1

R-O. ITER and fusion diagnostic development

Tamás Ilkei, Tétény Baross, Lívia Beri, Gábor Bodnár, Fruzsina Darányi, István Gábor Kiss, Dániel Nagy, Domokos Nagy, Réka Nagy, Gábor Nádasi, József Németh, Miklós Palánkai, Ádám Pataki, Gábor Veres

In the ITER Bolometer project, which aims at the development of the whole ITER bolometry camera system, the main results of the group were:

1. the successful preparation for the next period of the Framework Partnership, where the main task of the group will be the interface definition, a comprehensive system level analysis of corresponding applicable documents to identify existing requirements, including e.g. load specifications, environmental constraints, operating conditions, safety and nuclear safety regulations;
2. Finite Element Analysis (FEA) calculations of the thermal properties (temperature and stress distribution etc.) of a general bolometer camera placed in the ITER vacuum vessel (Figure1.). The main achievement was the creation of a parametric FEA mesh for the calculations that allowed to conduct the calculations for a wide range of mechanical sizes and environmental heating conditions (neutron and gamma).

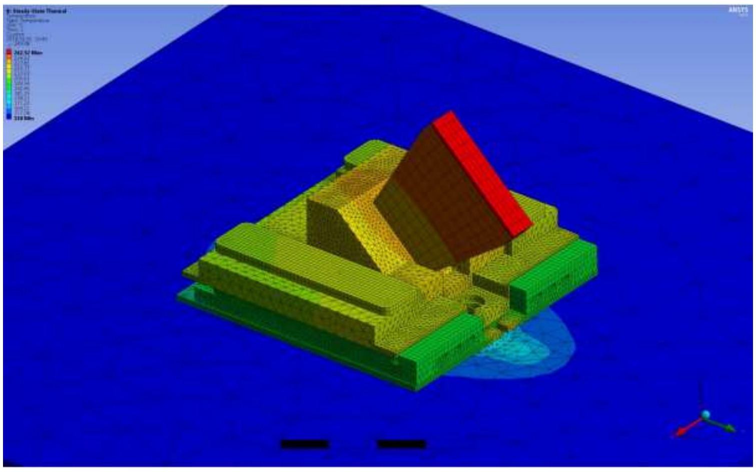

Figure 1. The result of a thermo-mechanical analysis of an ITER bolometer camera.

In the Tokamak Services for Diagnostics project the group reached a major milestone in the interface definition of various diagnostic sub-systems and services of ITER; a comprehensive system level analysis of corresponding applicable documents and as a result to successful preparation and compilation of the tendering documentation of electrical feedthrough components.

The delivery and installation of a 10 unit observation camera system to the W7X stellarator took place in this year that contributed largely to the successful start of the W7X stellarator machine at the end of the year.

Grants

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

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

International cooperation

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

Publications

Articles

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3. Mertens Ph, Castaño BDA, Baross T, Biel W, Friese S, Hawkes N, Jaspers RJE, Kotov V, Krasikov Y, Krimmer A, Litnovsky A, Marchuk O, Neubauer O, Offermanns G, Panin A, Pokol G, Schrader M, Samm U: Status of the R&D activities to the design of an ITER core CXRS diagnostic system. Proceedings of the 28th Symposium On Fusion Technology (SOFT-28). ***FUSION ENG DES*** 96-97: pp. 129-135. (2015)

See also: R-Q.1, R-R.2

R-P. Laser plasma

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

Plasma mirrors for KrF lasers with high efficiency. — Perhaps the ultimate method to remove prepulses of ultrashort laser pulses is based on the self-induced plasma shuttering or plasma mirror technique. If the intensity of the laser pulse falling onto a transparent solid material is chosen so that only the leading edge of the main ultrashort pulse is above the threshold for plasma production, prepulses or the pedestal of lower intensity will be transmitted. Only the main pulse will be reflected from the steep density gradient. Whereas plasma mirrors have been successfully applied in experiments with infrared lasers, they have not been used in visible and UV systems due to the larger penetration depth and the lower reflectivity. We demonstrated an efficiently reflecting plasma mirror arrangement reaching nearly 70% reflectivity for a KrF system. This opens the possibility for its integration to our present laser system.

Characterization of gas clusters for high-harmonic generation. — Recently we found evidence for a red shift of high harmonics due to the nanoplasmas of the clusters which could be used even for determining the typical size and density of clusters. In order to gain full insight into the processes Rayleigh-scattering was used to determine the features and sizes of the clusters. Different nozzles for used for these experiments. Besides our previously used nozzles Laval-nozzles were used as well which was characterized by other groups. Fig. 1 illustrates both the experimental arrangement and the observed image by a CCD detector. Note that for a high spatial resolution a CCD detector, whereas for a more sensitive measurement a photomultiplier (PMT) was used. The temporal and spatial evolution of clusters has mapped and is being compared with the results of high-harmonic spectra.

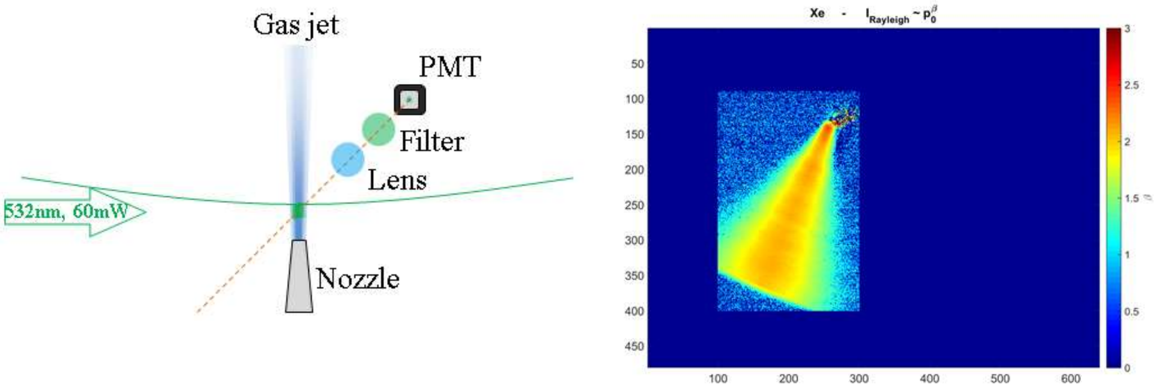

Figure 1. Arrangement for Rayleigh scattering and scattered light on the CCD detector.

Relativistic harmonics from a 2-cycle laser. — The collaboration with the Max-Planck-Institut für Quantenoptik has been continued on the field of high harmonics and isolated attosecond

[#] Ph.D. student

generation from plasmas generated on the surfaces of solids. The ~5fs pulses of the LWS20 laser system of the MPQ is used for these purposes. First the contrast of the pulse had to be improved which was carried out by the MPQ team using XPW+plasma mirror. We had to apply tight focusing of the laser beam by short focal length off-axis parabola, and thus we could achieve 10^{20} W/cm^2 focused intensity. We could obtain high harmonics up to the 60th order, which was limited by the spectrometer. It means that the harmonics were generated by the relativistic oscillating mirror (ROM) mechanism, which will probably enable us to progress toward the generation of isolated harmonics. The figure below is illustrated the harmonic spectra generated by the 5fs laser pulse. The right hand side of the spectrum corresponds to the highest, 60th order. For these 2-cycle laser pulses the carrier-envelope phase may change in each shot, therefore it was monitored throughout the experiments. Conversion measurement and data acquisition is in progress.

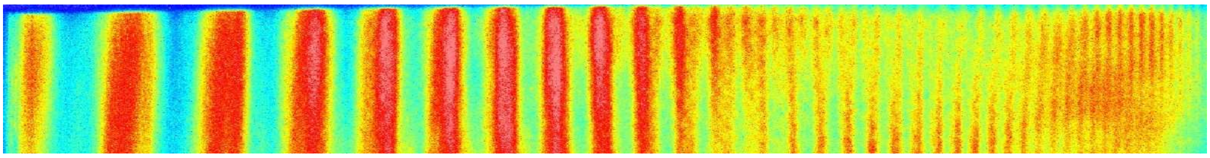

Figure 2. *High harmonics spectrum with a 5 fs laser, $I \approx 10^{20}$ W/cm^2.*

Electron acceleration in underdense plasmas described with a classical effective theory. — An effective theory of laser–plasma-based particle acceleration is presented. The plasma treated as a continuous medium with an index of refraction n_m in which a single electron propagates. Because of the simplicity of this model, we did not perform particle-in-cell (PIC) simulations in order to study the properties of the electron acceleration. We studied the properties of the electron motion due to the Lorentz force and the relativistic equations of motion were numerically solved and analyzed. The results were compared to PIC simulations and experimental data. In spite of the simplicity of our model our results agree with experimental data within a factor of two both for the accelerating gradient and for the maximal energy gain.

Grant

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

International cooperation

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

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6. Pocsai MA, Varró S, Barna IF: Electron acceleration in underdense plasmas described with a classical effective theory. ***LASER PART BEAMS*** 33: pp. 307-313. (2015)

Book chapter

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8. Földes IB, Varju K: Electron Trajectories in High Harmonic Generation. In: *Short Wavelength Laboratory Sources: Principles and Practices.* Eds.: Bleiner D, Costello J, Dortan F, O'Sullivan G, Pina L, Michette A, London: The Royal Society of Chemistry, 2015 pp. 150-162. (ISBN:978-1-84973-456-1)

See also: R-D.5

R-Q. Beam emission spectroscopy

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

Fusion energy could provide long term safe energy source for the humankind without any byproduct of greenhouse gases or long term radioactive nuclear waste. The fundamental physics of fusion plasmas is studied in recent fusion devices and solutions for various technical challenges are developed. For the better understanding of the underlying physics high spatial and temporal resolution measurements of multiple plasma parameters is crucial, which is the subject of the group's activity A significant part of the beam emission spectroscopy (BES) research group resources were focused on the fast evolving fusion research programs in China and in South Korea. The Chinese BES experiment was installed and started in 2014; the first scientific results were achieved in 2015. The main object of the diagnostic is to provide high frequency edge plasma profiles, but edge turbulence and fast transient phenomena could also be studied. We participated the entire measurement campaign of the Korean KSTAR tokamak in 2015. Our responsibility was the operation of the diagnostics which were built and installed by the Hungarian BES team. These systems provide valuable results for various studies and teams, beside our own research programs. An additional Far East research collaboration could start as a new tokamak (JT-60SA) is being built in Japan with significant EU participation. In 2015 a feasibility study and partly conceptual designs were prepared for BES diagnostics on JT-60SA. This could be the first milestone of long term collaborations. As in previous years we also took part in the European fusion research program. Scrape off layer plasma studies were carried out at the JET tokamak in UK and at ASDEX Upgrade tokamak in Germany. Also the BES system observation system has been refurbished at Compass tokamak in Czech Republic resulting higher quality measurements. (Fig. 1).

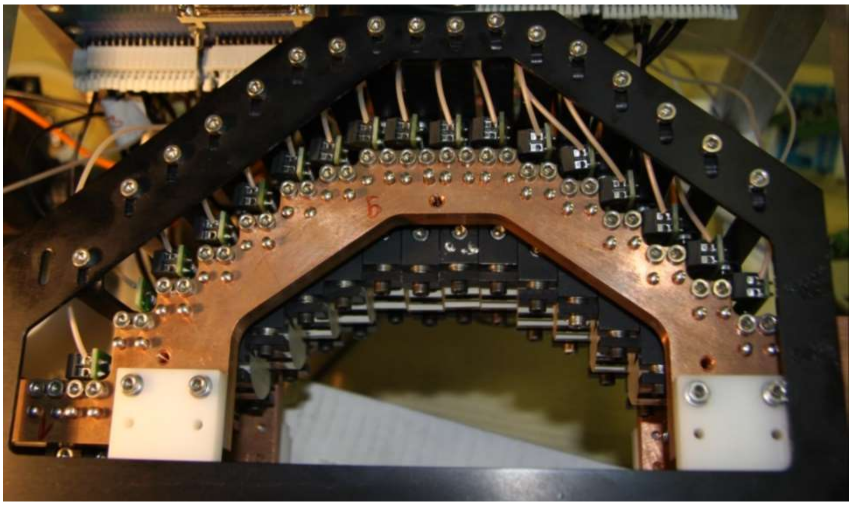

Figure 1. *The Compass BES refurbished detector system. The detector consists of 18 large surface individual avalalanche photodiodes.*

[#] Ph.D. student

[A] Associate fellow

International cooperation

Eurofusion Consortium

Publications

Articles

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See also: R-R.2, R-R.3

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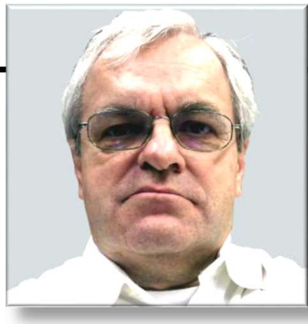
See also: R-R: ASDEX Upgrade Team, Wendelstein 7-X

R-T. Space Technology



János Zoltán Nagy[#], András Balázs, Attila Baksa, László Hevesi, István Horváth, Zoltán Pálos, Bálint Sódor, Sándor Szabó, Lajos Szalai, Sándor Szalai[E], Gábor Tróznai, Pál Gábor Vizi[#]

Our team takes part in several programs which are already in the implementation phase that is operating in space: these are the Rosetta and Obstanovka programs. We also participate in projects which are in preparation and development phase and will get in operational phase in the future.

In general the realization of space research missions usually require several years or even decades. The development of the Rosetta project started in 1993. This project took more than twenty years for design and manufacturing, and then finally ten years to travel through space and nearly two years for operation near the comet to acquire scientific data around the nucleus and on the surface. The spacecraft Rosetta was launched from Kourou on 2nd March 2004. On 12th November 2014, the lander module performed the first successful landing on a comet, on 67P/Churyumov–Gerasimenko (Figure 1). It was the first time in the history of space research that a space probe landed on a comet. The fault tolerant Command and Data Management Subsystem and its software (CDMS hardware and software of Philae lander) were developed by our team together with the Hungarian SME SGF Ltd. After separation from the Orbiter the CDMS controlled all the lander module functions, operation of the scientific instruments, radio connection with the orbiter unit and the.on-board computer which was developed by us. It autonomously controlled the operation of the Philae probe after separation.

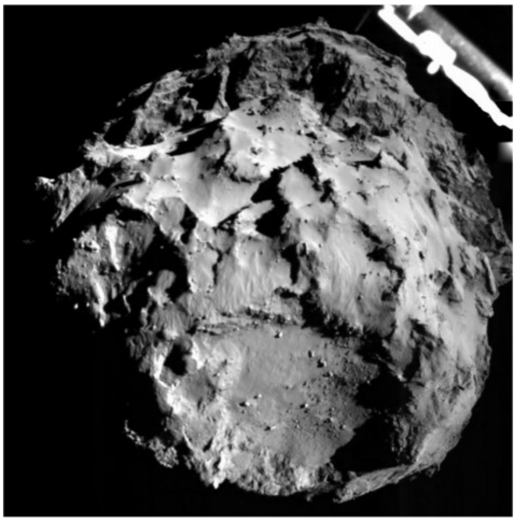


Figure 1. *Picture of the comet landing zone taken by the onboard camera of Philae.*

In 2015 the operation and functioning and data transmission of the lander unit on the comet surface operated intermittently as planned. Scientific data processing and evaluation are to be performed by our physicist colleagues (Figure 2). We participated in the activity of Philae

[#] Ph.D. student

[E] Professor Emeritus

Steering Committee which controlled and organized the long term science operation of the mission.

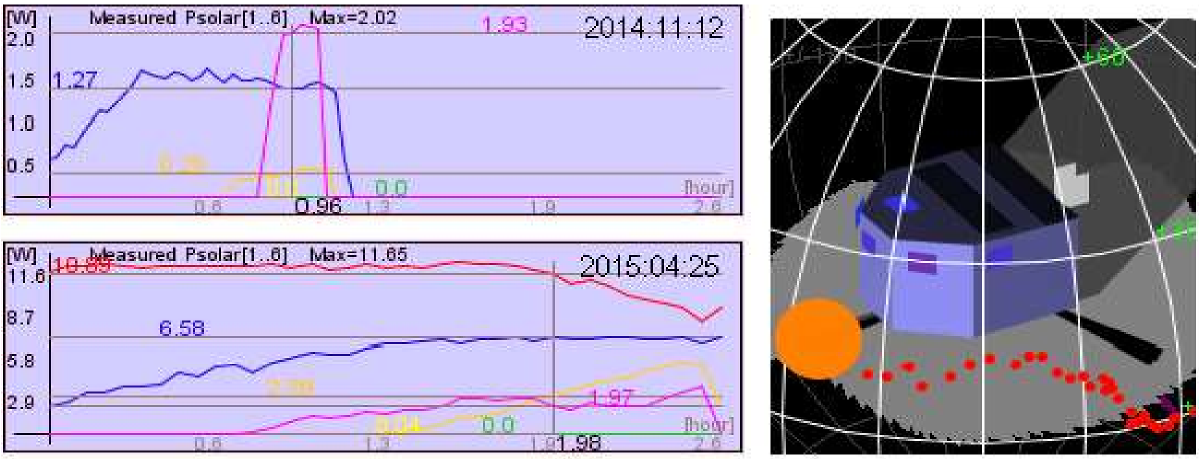


__Figure 2.__ In-situ measured power profiles of solar panels/generators, and reconstructed Sun trajectories after Philae woke up at the end of April 2015

For the Obstanovka experiment, that operates on the Russian part of the International Space Station we developed and manufactured onboard data acquisition and control system containing three processors with distributed intelligence, which worked for more than two years in space until the end of February 2015 when a Solar flare probably caused failure in the power supply system (Figure 3).

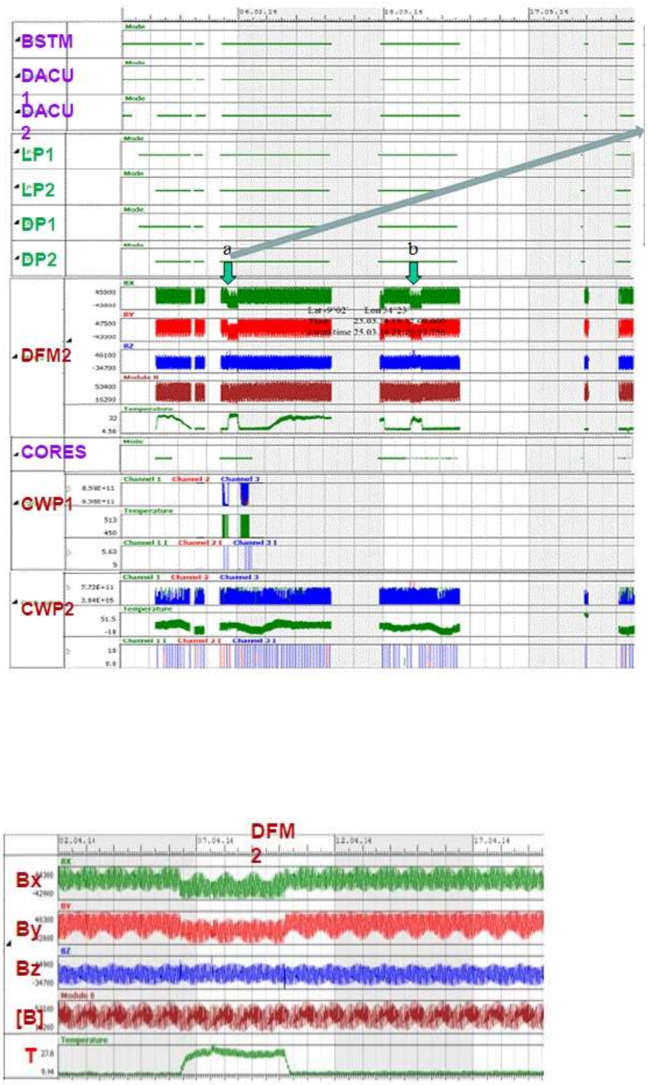


Figure 3. *Telemetry data of Obstanovka, and enlarged magnetic data.*

Currently we are developing and manufacturing DC/DC power supply units for different space experiments e.g. for the PEP instrument on the Juice mission and for the Plasma Ion Camera on BepiColombo mission. In 2015 the Juice mission was reconfigured in order, to minimize weight and power, which meant that we had to redesign our block schemes too (Figure 4). The mission faces in extreme conditions and the requirements to be fulfilled are detailed on hundreds of pages. Realization of hardware started at the end of 2015.

Flight unit and spare flight unit of the DC/DC power supply unit for Plasma Ion Camera of BepiColombo was delivered. In 2015 the technological model of DC/DC unit was modified following changes of flight model (Figure 5).

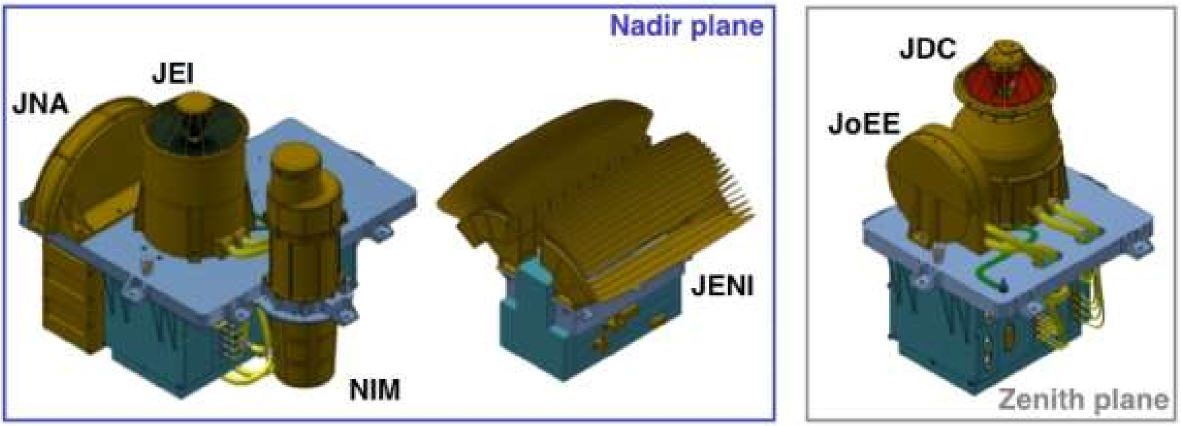


Figure 4. *The arrangement of the 6 Juice sensors of PEP for which we develop power supply units, three cards in Nadir plane equipment. The planned launch is 2022, after 7.5 years cruise to Jupiter the 3.5 years long data acquisition phase starts in the Jovian system.*

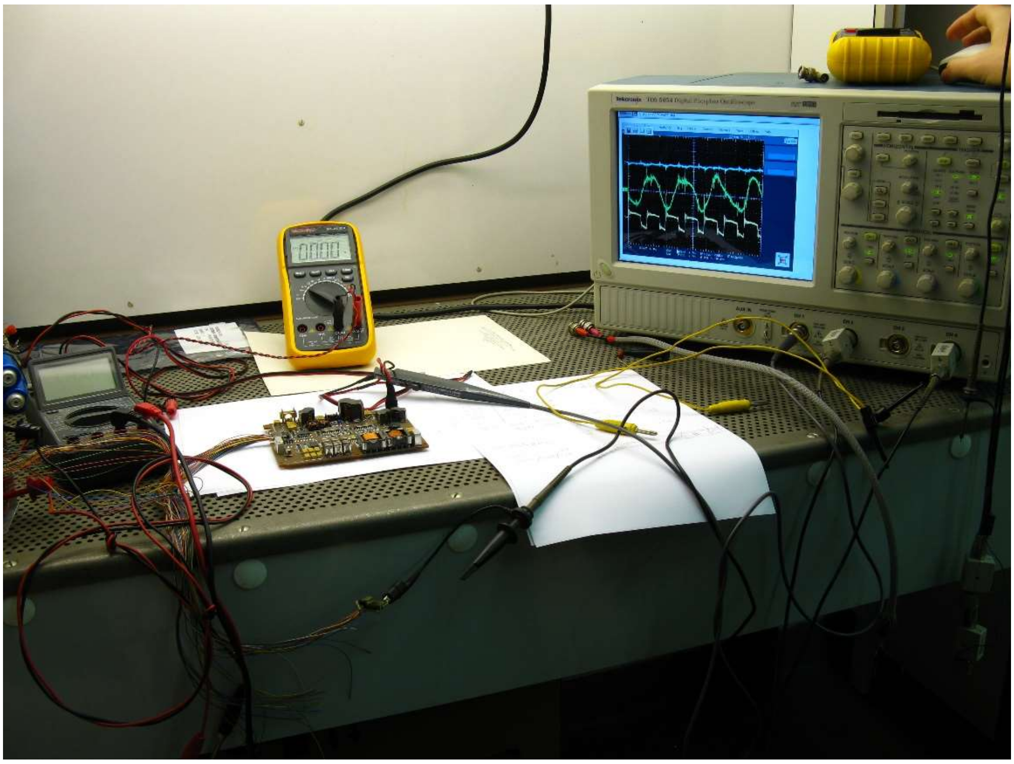


Figure 5. *Test of DC/DC power supply unit for Plasma Ion Camera of Bepi/Colombo.*

Grants

PECS-4200098078 Participation in the development of the CDMS for the Rosetta Lander (S. Szalai, 2011-2015)

PECS-4200098080 Participation in the development of the RPC experiment on board for Roseta Orbiter (S. Szalai, 2013-2015)

PECS-4200098091 Participation in the SERENA/PICAM instrument on MPO of the BepiColombo mission (S. Szalai, 2013-2015)

PECS- 4000109793 Participation in the JUICE mission (as subcontractor to the SGF Ltd.) (S. Szalai, 2013-2017)

International cooperation

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

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Computational Sciences Research Group

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

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

In January 2014 the group won its first EU FP7 ICT project within the Future Internet PPP. The XIFI project will establish federated infrastructure components, with functional components that satisfy the interoperability requirements for the European Future Internet core platform. Though computer networks are manmade, Internet does not have a blueprint, so in some sense it is very much similar to complex dynamical systems in physics and similar methodology is required to analyze and understand them. The XIFI open federation will leverage existing public investments in advanced infrastructures and support advanced large-scale deployment of FI-PPP early trials across a multiplicity of heterogeneous environments and sector use cases that should be sustained beyond the FI-PPP programme. With the project partners we have integrated the Wigner cloud node, installed and tested the virtualization framework and the flexibly configurable modules. In 2015, our group – as the only one from the previous round - has won further support for the continuation and extension of the project in the FI-Core framework.

In December 2014 already in the new framework programme H2020 the group has won a new project in which bioinformatics tools will be used for outbreak detection. The health of humans and animals around the world is increasingly under threat due to new and recurring epidemics and foodborne disease outbreaks, which place pressure on health services and the production of livestock. These epidemics also reduce consumer confidence in food and negatively impact trade and food security. The longer it takes from the start of an outbreak of for example Ebola, influenza or salmonella until it is detected and stopped, the greater the consequences. The most important factor in being able to limit the consequences and costs of such outbreaks is the ability to quickly identify the disease-causing microorganisms that are causing the disease. Also there is the need for knowledge about the mechanisms that cause the disease, and how the bacteria are transmitted to and between humans. The goal of the COMPARE project is a better surveillance system for infectious diseases, to speed up the detection of and response to disease outbreaks among humans and animals worldwide through the use of new genome technology. Our group is mainly responsible for the advanced database system which will store and share the genomic data collected by researchers all over the world. We develop a "virtual research environment", where interested partners can log in, and use the already installed tools, software and data together with their own to do research. The front-end is the "Jupyter Hub" which handles the login, then makes possible to upload/download smaller files, write documents (in "markup" language, which then shows as a webpage). Most importantly it is possible to write scripts (unix, R, Python ...) and run them on the cloud machine, analyze results, generate tables and figures. The whole pipeline with the results can be then shared as webpages. Our hope is that this can accelerate collaboration and workflow development, and also allows to do really transparent shareable science.

Grants

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

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

Laboratory of Rehabilitation-Technology

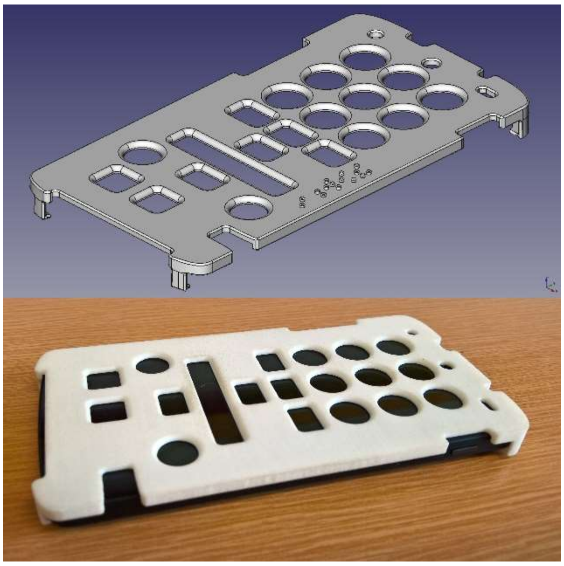
József Laczkó, András Arató, Norbert Márkus, Szabolcs Malik, Mariann Mravcsik[#]

Mobile communication devices for blind, deaf-blind and autistic people. — Augmentative and Alternative Communication (AAC) is a way of communication which aids people who are unable to communicate by speech or cannot use common communication tools (e.g. phones) due to lack of adequate abilities. Special tools and equipments are developed for this reason. We installed fifteen "MOST" (Mobile SlateTalker) devices on Nexus5 smartphones running on the Android 4.4 operating system for blind people. With a special vibrating version, this can be used by deafblind users as well. We developed a self-teaching world-new method for deaf-blind people to use the morse-braille vibrating program. We also designed and created braille masks for Nexus 5 with the use of 3D printing for blind users.We have developed a „speech prosthesis" as a mobile app for Android tablet computers. It has been installed for about 70 users. We also developed TalkNote. This is a new kind of AAC app for Android devices aimed at non-verbal autistic users.

Artificial control of human movements, Human – Machine interfaces. — In the field of human motor control and medical rehabilitation we cooperated with the National Institute for Medical Rehabilitation in Budapest. We provided functional electrical stimulation (FES) driven rehabilitation protocols for people with paralyzed limbs. Using FES technology, people whose limbs are paralyzed may be able to produce active muscle forces and perform certain limb movements, as their muscles are stimulated electrically and their limb movements are controlled artificially by given stimulation patterns. In 2015, six new, spinal cord inured individual participated in this program (after the previously trained 20 participants) and performed active lower limb movements bicycling on a stationary bike. Beside improving rehabilition protocols for the lower limbs, we extended our research on upper limb movements. We measured, analyzed and modeled kinematic and myoelectric characteristics of upper limb movements of able-bodied people. We recorded and analyzed arm-cycling movements (performed on an ergometer) of 24 young, able-bodied people and investigated the variances of these movements. The data, collected in these measurements gave an input to statistical analysis of kinematic and electromyographic properties of cyclic limb movements. This helps us to reveal motor control principles. The external, physical environment influences limb movement patterns and motor performance. Particularly, the effect of external forces (crank resistance) on the variances of angular joint rotations and on muscle activity patterns were studied. The effect was significant on muscle activity patterns but not on kinematic properties of the studied motor tasks. These results help to enhance rehabilitation protocols for people who lost their motor functions due to neural based movement disorders. Measured muscle activity patterns are averaged across healthy subjects and the averaged patterns can be used to define stimulation patterns for FES assisited arm-cycling movements. The use of FES technologies may improve cardiovascular and respiratory

[#] Ph.D. student

functions of people with motor disabilities and the psychological effect is invaluable since they know they genrate active forces with their own muscles, what they would not be able to do without these technologies.



We have upgraded the design of our Braille mask for MObile SlateTalker using 3D printing technology. This mask is easy to remove facilitating the use of screen readers and protects the phone. The unique 3D design allows adding tactile Braille name tags for blind users.

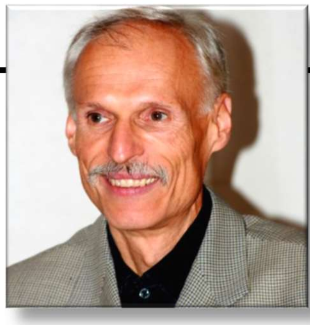
Measurement of arm muscle actvities with surface electrodes palced on the skin above the muscles and measurement os joint positions with ultrasound sensitive markers placed on anatomical landmarks on the arm of an arm-cycling person. Relation of joint rotations and muscle actvities are computed from mesaured data.

International cooperation

Northwestern University, Chicago IL, USA, Human-Machine interface

INSTITUTE FOR
SOLID STATE PHYSICS AND OPTICS

S-B. Complex Systems



Ferenc Iglói, Róbert Juhász, István Kovács, Gergely Roósz, Attila Virosztek, András Sütő[E]

The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Critical behavior of disordered systems. — Modeling long-range epidemic spreading in a random environment, we consider a quenched, disordered, d-dimensional contact process with infection rates decaying with distance as $1/r^{d+\sigma}$. We study the dynamical behavior of the model at and below the epidemic threshold by a variant of the strong-disorder renormalization group method and by Monte Carlo simulations in one and two spatial dimensions. Starting from a single infected site, the average survival probability is found to decay as $P(t) \sim t^{-d/z}$ up to multiplicative logarithmic corrections. Below the epidemic threshold, a Griffiths phase emerges, where the dynamical exponent z varies continuously with the control parameter and tends to $z_c = d + \sigma$ as the threshold is approached. At the threshold, the spatial extension of the infected cluster (in surviving trials) is found to grow as $R(t) \sim t^{1/z_c}$ with a multiplicative logarithmic correction and the average number of infected sites in surviving trials is found to increase as $N_s(t) \sim (\ln t)^\chi$ with $\chi = 2$ in one dimension.

Non-equilibrium dynamics of quantum systems. — We study nonequilibrium dynamics of the quantum Ising chain at zero temperature when the transverse field is varied stochastically. In the equivalent fermion representation, the equation of motion of Majorana operators is derived in the form of a one-dimensional, continuous-time quantum random walk with stochastic, time-dependent transition amplitudes. This type of external noise gives rise to decoherence in the associated quantum walk and the semiclassical wave-packet generally has a diffusive behavior. As a consequence, in the quantum Ising chain, the average entanglement entropy grows in time as $t^{1/2}$ and the logarithmic average magnetization decays in the same form. In the case of a dichotomous noise, when the transverse-field is changed in discrete time-steps, τ, there can be excitation modes, for which coherence is maintained, provided their energy satisfies $\varepsilon_k\tau \approx n\,\pi$ with a positive integer n. If the dispersion of ε_k is quadratic, the long-time behavior of the entanglement entropy and the logarithmic magnetization is dominated by these ballistically traveling coherent modes and both will have a $t^{3/4}$ time-dependence.

The total momentum of quantum fluids. — The probability distribution of the total momentum P is studied in N-particle interacting homogeneous quantum systems at positive temperatures. Using Galilean invariance, we prove that in one dimension the asymptotic distribution of $P/N^{1/2}$ is normal at all temperatures and densities, and in two dimensions the tail distribution of $P/N^{1/2}$ is normal. We introduce the notion of the density matrix reduced to the center of mass, and show that its eigenvalues are N times the probabilities of the different eigenvalues of P. A series of results is presented for the limit of sequences of positive definite

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[E] Professor Emeritus

atomic probability measures, relevant for the probability distribution of both the single-particle and the total momentum.

Unified data representation theory. — Representation of large data sets became a key question of many scientific disciplines in the last decade; however, there was no underlying theoretical framework linking these problems. Here, we show an elegant, information theoretic data representation approach as a unified solution of network visualization, data ordering and coarse-graining. The representation of network nodes as probability distributions provides an efficient visualization method and, in one dimension, an ordering of network nodes and edges. Coarse-grained representations of the input network enable both efficient data compression and hierarchical visualization to achieve high quality representations of larger data sets. Our unified data representation theory will help the analysis of extensive data sets, by revealing the large-scale structure of complex networks in a comprehensible form.

Grant

OTKA K109577: Ordering and dynamics in many body systems (F. Iglói, 2013-2017)

Publications

Articles

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2. Kovács IA, Mizsei R, Csermely P: A unified data representation theory for network visualization, ordering and coarse-graining. ***SCIENTIFIC REPORTS*** 5: Paper 13786. 10 p. (2015)

3. Sütő A: The total momentum of quantum fluids. ***J MAT PHYS*** 56:(8) Paper 81901. (2015)

S-C. Long range order in condensed systems

Balázs Újfalussy, Péter Balla[#], Gábor Csire[#], Krisztina Kádas, Annamária Kiss, Zsolt Maksa, Dávid Molnár, Karlo Penc, Levente Rózsa, István Tüttő[A], Lajos Károly Varga, Ádám Vida, Levente Vitos

Superconductivity in layered heterostructures. — The theory of Bardeen, Cooper, and Schrieffer (BCS) successfully describes the universal properties of conventional (s-wave) superconductors, but it can not be applied easily to inhomogeneous systems where the wave number is not a good quantum number. The generalization of the well-known Hartee-Fock method with the introduction of the concept of mixed particle-hole excited states yields the Bogoliubov-de Gennes (BdG) equations. In this description, the standard momentum operators are replaced by field operators, which have the advantage that they are able to describe inhomogeneous systems. However, this is only a mean-field theory and can not be considered as a predictive approach to allow the computation of material-specific properties. For that purpose, a density functional theory (DFT) was constructed by Oliveira, Gross and Kohn. In this theory, the ground state energy is proved to be a unique functional of the charge density and the so-called anomalous density. Based on the first-principles BdG equations, 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. For the first time, we have extended the screened Korringa-Kohn-Rostocker (SKKR) method for the solution of the Kohn-Sham-Bogoliubov-de Gennes (KSBdG) equation which allowed us to investigate the quasiparticle spectrum of superconducting heterostructures. In order to compare our results with normal state-electronic structure calculations, a scalar-relativistic generalization of the BdG equations within Multiple Scattering Theory was also derived. To illustrate the power of the new method, it was applied to Nb/Au heterostructures. First, for simplicity, Au overlayers of BCC(100) lattice structure on a Nb BCC(100) host have been investigated. While such a material is unlikely to exist for greater Au thicknesses, by assuming layer by layer growth, it resulted in an easily understood system of quantum well states. The effect of the superconducting host on the quasiparticle

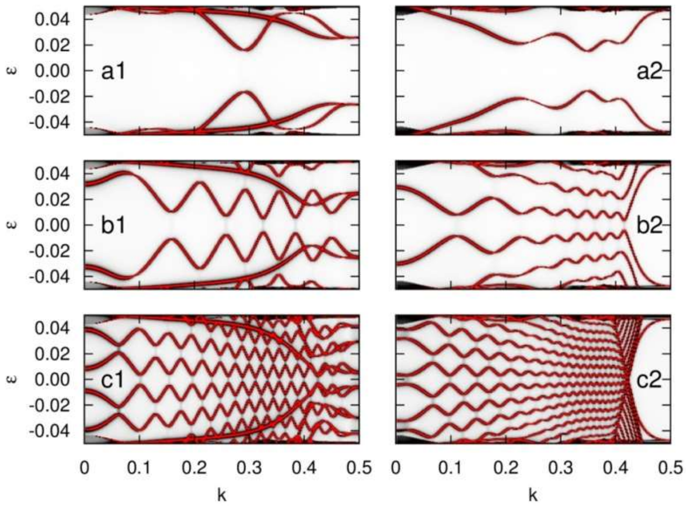

***Figure 1**. The Andreev band structure of bcc (1) and fcc (2) Au on Nb(001). The layer-resolved band structure is summed for all Au layers and is shown for various layer thicknesses (a:3, b:6, c:24 atomic layers)*

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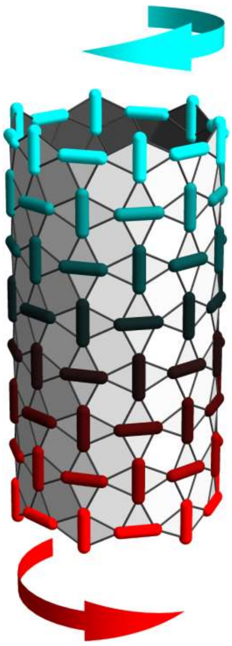
spectrum of Au overlayers can be more easily identified by these states than on a more complex band structure of a real material. Calculations for a more realistic geometry are in progress. We showed that the Quantum Well states which we found to exist in the normal state band structure calculations become bound Andreev states (ABS) due to Andreev scattering. The major result of our investigations is that the ABS have dispersion, which can be obtained only by the BdG-SKKR method. We also found that the proximity of a superconductor in the studied heterostructures induces the mirroring of the electronic bands, and opens up a gap at each band crossing, and the gaps are strongly k-dependent in the two-dimensional Brillouin zone (Figure 1). We have seen that this induced gap remains constant for each layer for a given Au thickness; however, the size of the gap decays as function of the Au thickness. We also investigated the properties of the surface state at the Au surface and found that the gap does not appear in the energy spectrum of these states, probably because they are localized to the surface and consequently do not take part in the Andreev scattering process.

High-Entropy Alloys. — The $Al_xMoNbTiV$ (x = 0–1.5) high-entropy alloys (HEAs) adopt a single solid-solution phase having the body-centered cubic (bcc) crystal structure. We employed the ab initio exact muffin-tin orbitals method in combination with the coherent potential approximation to investigate the equilibrium volume, elastic constants, and polycrystalline elastic moduli of $Al_xMoNbTiV$ HEAs. A comparison between the ab initio and experimental equilibrium volumes demonstrates the validity and accuracy of the present approach. Our results indicate that Al addition decreases the thermodynamic stability of the bcc structure with respect to face-centered cubic (fcc) and hexagonal close-packed lattices. For the elastically isotropic $Al_{0.4}MoNbTiV$ HEAs, the valence electron concentration (VEC) is about 4.82, which is slightly different from VEC$\sim$ 4.72 obtained for the isotropic Gum metals and refractory high-entropy alloys (HEAs).

We collected the available basic properties of nearly 100 HEAs with a single fcc or bcc phase. HEAs crystallizing in the fcc structure are mainly composed of the late 3d elements (LTM-HEAs), whereas HEAs consisting of the early (refractory) transition elements and the LTM-HEAs containing an increased level of bcc stabilizer form the bcc structure. Guided by the solid solution theory, we investigate the structure and hardness of HEAs as a function of the VEC and the atomic size difference (d). The fcc structure is found for VEC between 7.80 and 9.50, whereas the structure is bcc for VEC between 4.33 and 7.55. High strength is obtained for an average valence electron number VEC ~ 6.80 and for an average atomic size difference d~6%. Based on these empirical correlations, one can design the high-entropy alloys with desired hardness.

Hall effect in a quantum magnet. — We studied the effect of topology in the $Sr_2Cu(BO_3)_2$ quantum magnet. This is an insulator in which the constituent spins are pairwise entangled, i.e., pairs of electrons interact in such a way that their spins cancel each other. An excitation of this system corresponds to breaking a pair which turned out to be topological in nature. At low temperatures, we found that the excitations show features very similar to electrons in the quantum Hall effect. The bulk remains insulating, while the edges carry Hall currents. As these excitations carry no electrical charge, there is no Hall voltage. However, as they still carry energy, the Hall current will transport heat from one edge of the sample to the other. The topological nature of the excitations can be tuned with a small applied magnetic field. At



a critical value of the field, the excitations form a new kind of 'Dirac cone', forming a magnetic analogue of graphene.

Figure 2. *Topologically protected edge-states (blue and red) at the edges of an imaginary $Sr_2Cu(BO_3)_2$ layer wrapped as a cylinder. The excitation on the upper and lower edge move in opposite directions.*

Grants and international cooperation

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

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

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

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

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

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

Oak Ridge National Laboratory, Magnetic interactions in distorted systems, (B. Újfalussy, 2014-2015)

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S-E. Non-equilibrium alloys

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

Magnetocaloric effect. — In order to extend the upper range of the operational region of the magnetic cooling, it would be desirable to prepare FeZrB(Cu) amorphous alloys having relatively high Curie point and high magnetic entropy change at the same time.

Magnetic properties and magnetocaloric effect were studied in the $Fe_{92-x}Zr_7B_xCu_1$ amorphous alloy series (x = 0–23 at.%). Enhancement of the magnetocaloric effect was observed in the B-rich side (x > 15 at.%) which correlates well with the anomalous increase of the saturation magnetic moment per Fe atom in this concentration range. Research into $Fe_2(B_{1-y}ETM_y)$ amorphous alloys (ETM = Zr, Nb, Ti and V; y = 0–0.55 atomic fraction for Zr and to 0.25 atomic fraction for the rest) reveals an unexpected increase of the iron magnetic moment when early transition metals are substituted for B up to y = 0.1–0.25 atomic fraction. This behavior is attributed to the highly attractive B–ETM interaction. Similar mechanism is thought to explain the anomalous increase of the iron magnetic moment and hence the magnetocaloric effect in the boron-rich $Fe_{92-x}Zr_7B_xCu_1$ amorphous alloys. Universal scaling of the magnetic entropy change curves is also used to detect differences between $Fe_{92-x}Zr_7B_xCu_1$ alloys.

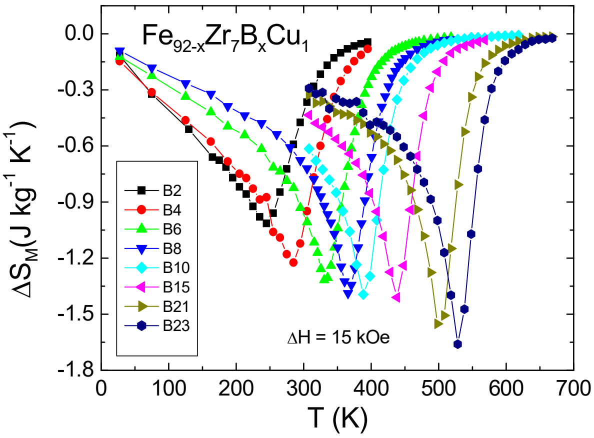

Figure 1. Magnetic entropy change as a function of temperature for $Fe_{92-x}Zr_7B_xCu_1$ amorphous alloys for a magnetic field change of 1.5 T. The boron contents are shown by labels. The lines are guide to the eye.

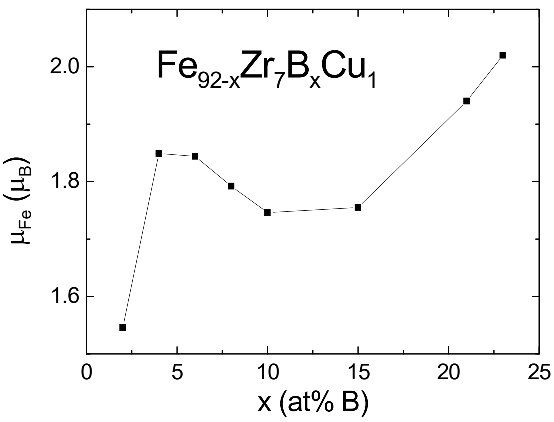

***Figure 2.** Saturation magnetic moment per Fe atom at 5 K as a function of boron content for $Fe_{92-x}Zr_7B_xCu_1$ amorphous alloys. The line is guide to the eye.*

Multilayer interfaces. — Interfaces play a decisive role in all the physical properties of nanometer scale layer structures. Mössbauer spectroscopy being sensitive to the atomic scale

[A] Associate fellow
[E] Professor Emeritus

neighborhood of the ^{57}Fe atoms can give unique information on the extent of the chemical mixing at the interface without being significantly disturbed by topological features of the layers.

The chemical mixing at the "Al on Fe" and "Fe on Al" interfaces was studied by molecular dynamics simulations of the layer growth and by ^{57}Fe Mössbauer spectroscopy. The concentration distribution along the layer growth direction was calculated for different crystallographic orientations, and atomically sharp "Al on Fe" interfaces were found when Al grows over (001) and (110) oriented Fe layers. The Al/Fe(111) interface is also narrow as compared to the intermixing found at the "Fe on Al" interfaces for any orientation. Conversion electron Mössbauer measurements of the trilayers Al/^{57}Fe/Al and Al/^{57}Fe/Ag grown simultaneously over Si(111) substrate by vacuum evaporation support the results of the molecular dynamics calculations.

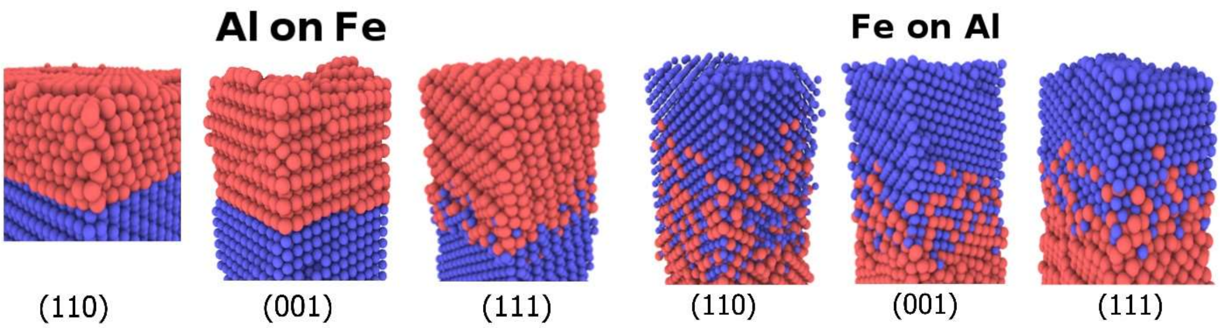

Figure 3. *Structures from molecular dynamics simulations of layer growth for different substrate orientations. Blue and red spheres are the Fe and Al atoms, respectively.*

Grants

OTKA K101456 Mössbauer and Magnetic Study of Intermetallic Compounds (I. Vincze, 2012-2016)

OTKA K112811 Magnetic Multilayers Modified by Amorphous Alloys (J. Balogh, 2015-2018)

International cooperation

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

National Center for Scientific Research "Demokritos" (Athens, Greece) (J. Balogh)

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Articles

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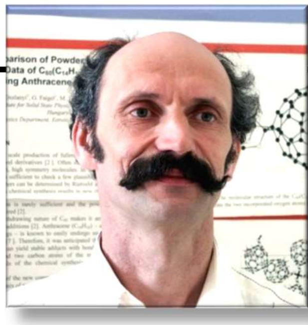
S-F. Laboratory for advanced structural studies



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

The Laboratory for Advanced Structural Studies (LASS) carries out research in three areas: carbon based materials, the theory of phase transformations and x-ray related methods. In the last year, we have reached significant results in the first two 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 highly porous crystalline solids. In the previous period, we started to develop a new family of MOFs with Zn-based secondary building units (SBUs) and 1,4-cubanedicarboxylate linkers. We synthetized four new frameworks of different compositions, and determined their structures by single-crystal x-ray diffraction. We prepared diverse structures: polymer sheets and 3D frameworks with high surface area, as well as neutral and ionic macromolecules and interpenetrated networks. This year, we continued the structural studies of these materials and extended the family with two new members. In collaboration with the thermoanalytical group of the Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, we carried out thermogravimetry-mass spectrometry measurements on the first four crystals. We could determine the chemical compositions and the thermal stabilities of these materials. These studies give the background for the future activation and supramolecular modifications of the MOF structures. The two new materials are: i): two interpenetrated networks of monoclinic structure with 6-connected, tetranuclear SBUs, the simplified chemical formula is $Zn_4O(C_8H_6(COO)_2)_3(DMF)$; ii): a more complex network with 8(10)-connected, hexanuclear SBUs, the simplified chemical formula is $Zn_6(OH)_2(C_8H_6(COO)_2)_5(DEF)_2$. Here DMF is dimethylformamide and DEF is diethylformamide.

Infrared spectroscopy on carbon based systems. — Our research included various topics on fullerenes, carbon nanotubes and solar cell materials. Our most important results concerned the investigation of the phase diagram of expanded superconducting fulleride salts of the composition $Cs_xRb_{3-x}C_{60}$. We studied a series of isostructural materials with varying composition, resulting in different chemical pressure in the crystal. Thus a pressure-temperature space was constructed and various physical properties studied in wide international collaboration. Our own results obtained by temperature-dependent infrared spectroscopy underlined the metal-insulator transition through the coupling of electrons and molecular vibrations. We identified a new phase between the metallic and insulating structure, which we termed "Jahn-Teller metal". Starting from this phase and lowering the temperature, a special non-BCS superconducting state is obtained. We published these

Ph.D student

results in Science Advances and the paper also gained substantial publicity in the popular science press. We also studied the reactivity of carbon nanotubes in sidewall-functionalization reactions and proved that the effect of bundling strongly influences the selectivity of reactions involving charge transfer as a first step.

Theory of phase transformations. – We have investigated various aspects of crystalline freezing within atomistic and coarse-grained continuum models:

(1) Polycrystalline materials play an important role in our everyday life. They consist of a large number of crystalline grains, which form by the interplay of crystal nucleation and growth. The properties of these materials are determined by the size, shape and composition distributions of these grains, i.e., the microstructure. After identifying a set of conditions the models need to obey, we have developed an improved, physically consistent multi-phase-field model, which predicted a limiting grain size distribution that is closer to the experiments than the predictions from previous works (Figure 1). A similar approach was adopted in developing a hydrodynamics-coupled multi-component Cahn-Hilliard model, which is employed to model phase separation in multi-component liquids (Figure 2).

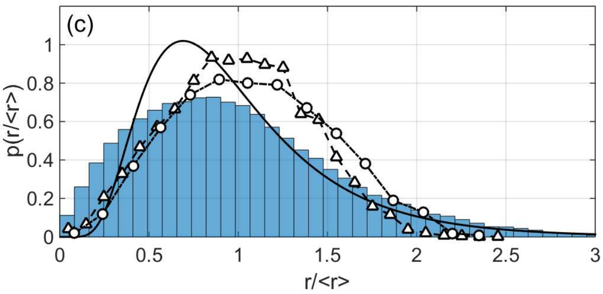


Figure 1. *Limiting grain size distribution predicted by our physically consistent multi-phase-field theory (histogram) compared to experiments (continuous line) and earlier models (triangles and circles).*

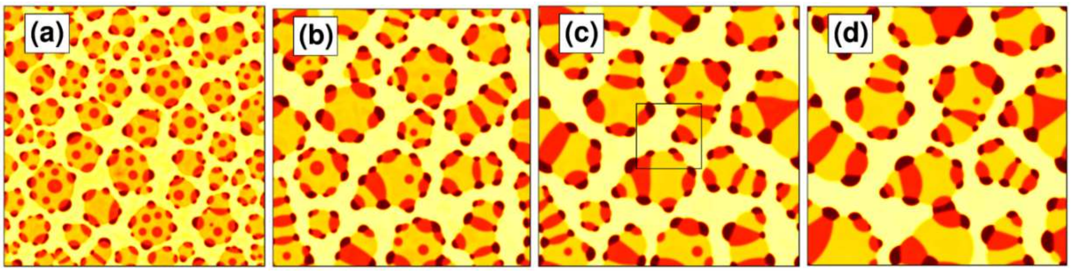


Figure 2. *Time development of a four-component liquid-emulsion system starting from a homogeneous state in our multi-component Cahn-Hilliard model which is coupled to hydrodynamics. Time increases from left to right.*

(2) Some of our technical alloys are formed by simultaneous solidification of two or more solid phases, a mechanism called eutectic solidification. A remarkable discovery made in this field recently is that under appropriate conditions, eutectic dendrites form, which show a spiraling surface pattern during growth. We have carried out systematic phase-field studies of the phenomenon, and determined the scaling properties of the dendrite tip radius and the eutectic wavelength, and observed a random selection from the possible surface patterns (i.e., target pattern, single to five-armed spirals, Figure 3) driven by the fluctuations.

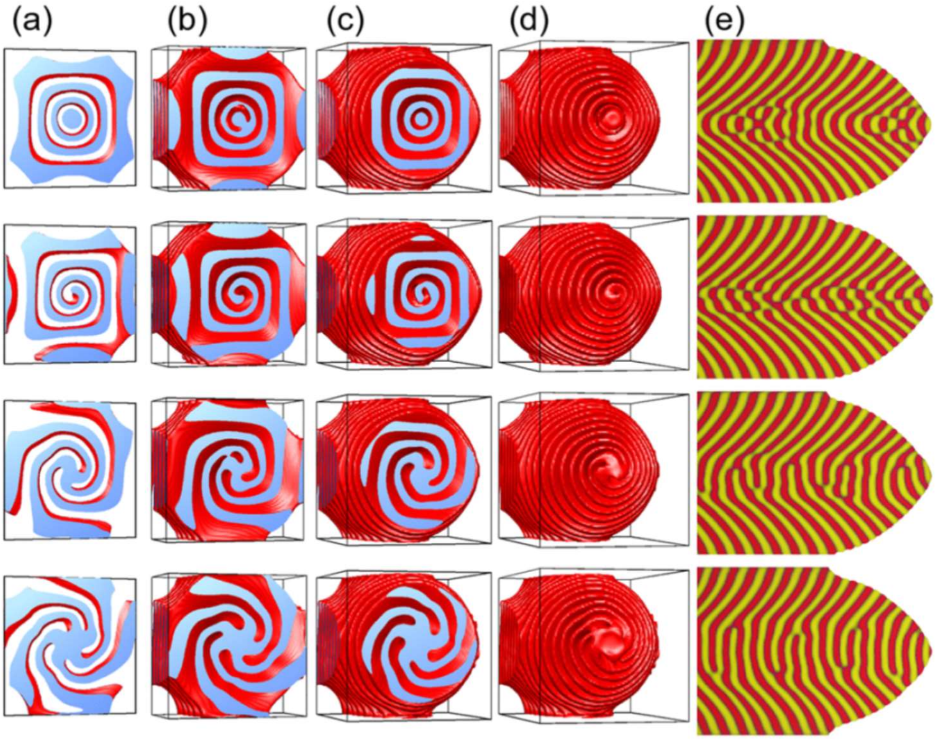


Figure 3. *(a) – (c): Cross sections of eutectic dendrites at different depths from the peak in case of target pattern, 1, 3 and 5-armed spirals. (d) Inner structure of the dendrite when one solid phase is made transparent. (e) Longitudinal cross sections.*

(3) Protein nanotubes are promising candidates to form nano-networks and for sensor applications.

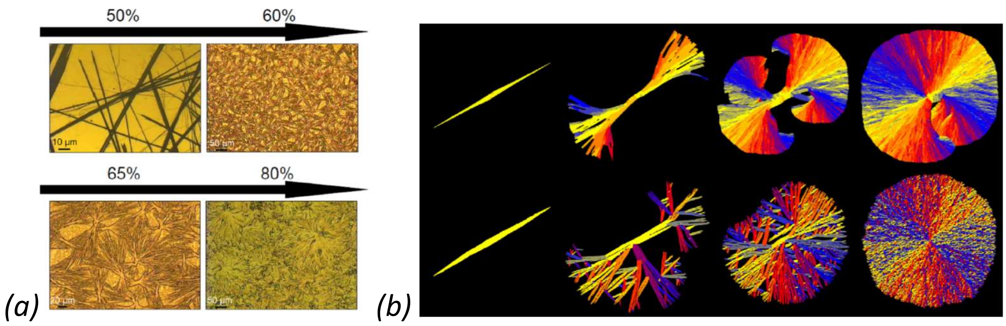


Figure 4. *Change of growth morphology as driving force increases (a) in protein nanotube experiments and in (b) phase-field simulations (different colors mean different crystalline orientations). Driving force increases from left to right. On panel (a) the air humidity is also depicted.*

In collaboration with colleagues in the University of Tel Aviv, we have studied the formation of these materials. A comparison of our simulations to the experiments of our collaborators (Figure 4) indicates that the morphology of protein spherulites can be controlled via changing the humidity, which in turn influences the driving force for solidification.

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ESA PECS Contract No. 40000110759/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2015–2016).

ESA PECS Contract No. 40000110756/11/NL/KML: MAGNEPHAS III – Modelling of growth and transformation kinetics (L. Gránásy, 2015–2016).

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

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

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

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

International cooperation

CNR-IMEM Institute, Parma, Prof. Cesare Frigeri

Faculty of Physics, University of Vienna, Prof. Jannik C. Meyer

Department of Chemistry, Durham University, Prof. Kosmas Prassides

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

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

S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Dávid Iván[#], Kálmán Tompa[E], Tamás Verebélyi[#], Francis I.B. Williams[A]

Water rotation barriers on protein molecular surfaces. — The primary aim of our studies of aqueous protein solutions is the characterization of their dynamic interaction with solvents by the analysis of wide-line solid-state ^{1}H NMR spectra. The experimental characterization of hindered-rotation barriers for the hydration water molecules and the mapping of their energetic heterogeneity are critical for understanding the functional interactions of proteins with their environment.

Molecular motion in the interfacial "ice" starts at temperatures significantly lower than in bulk ice (0 °C). When the temperature of a frozen protein solution increases, water molecules in the hydrate layer of the protein start to move in the range of 180-250 K. We studied the melting for several proteins in seeking a comprehensive interpretation of the entire process.

The melting diagram (Figure 1) of a frozen protein solution can be related to a solvent-driven dynamic transition of the protein. The number of the mobile water molecules in the protein-water interfacial region can be determined by analyzing the ^{1}H NMR signals. Information can be gained about the homogeneous and heterogeneous local hyperfine-field contributions and of rotational and translational diffusion of water molecules.

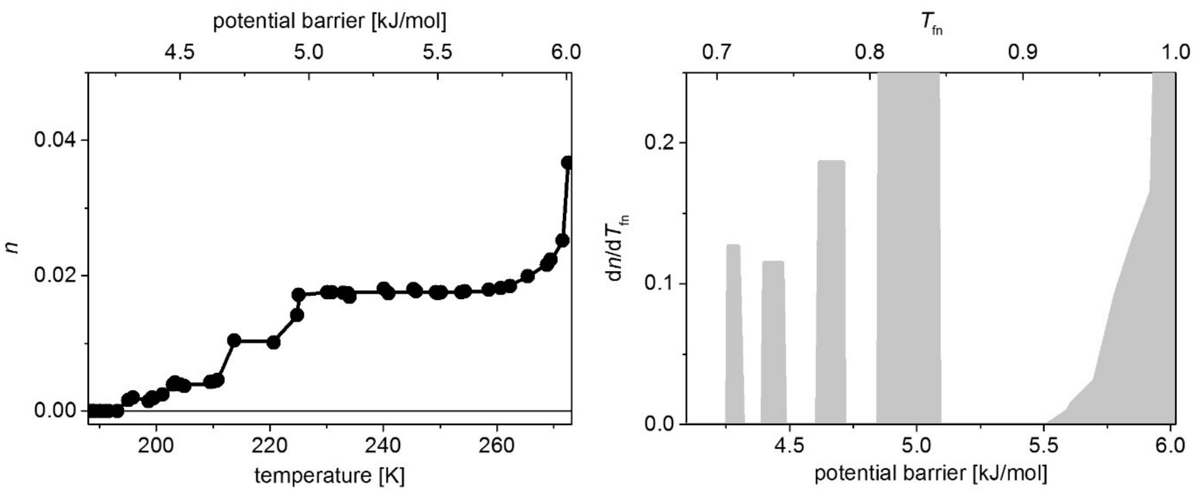

Figure 1. *Hydration properties and water rotation barriers at the molecular surface of the globular protein hen egg white lysozyme dissolved in water. Mobile water fraction (n) as a function of temperature and the corresponding potential barriers (left panel) determined by wide-line NMR and its differential quotient (right panel) as a function of potential barriers and normalized temperature (T_{fn} = T/273 K).*

[#] Ph.D student

[E] Professor Emeritus

[A] Associate fellow

The melting diagrams show the fraction of water molecules which already move, on the NMR time scale, at a given temperature. Since the rotational energy barrier of a particular type of molecular motion in the interface is proportional to $k_B T$, the temperature derivative of the melting curve provides information about the distribution of energy barriers. This, in turn, characterizes the protein-solvent interaction over the interfacial region. The barrier distribution gives insight into the structure of the protein itself. In the case of the globular protein lysozyme, we find gaps in the energy barrier distribution (right hand panel of Figure 1), whereas in disordered proteins (e.g. ERD10) the distribution is continuous.

Organic-inorganic solar cell materials. — One of the most promising new directions in solar cell research is the use of organic-inorganic perovskite compounds which show remarkable photovoltaic power efficiencies in excess to 20%. The most studied member of this family is methylammonium lead iodide ($CH_3NH_3PbI_3$). Despite extensive research in the past years, the electronic properties of this material, in particular the long electron-hole diffusion length, are poorly understood. It is expected that the reorientations of the methylammonium molecule of finite electric dipole moment influence the electronic properties. To gain insight into this molecular motion, we performed ^{207}Pb NMR measurements over a broad temperature range. We find that the spin-lattice relaxation rate which is most sensitive to molecular motion exhibits a strong increase when the temperature of a structural phase transition at 165 K is approached from above, and exhibits an almost 2 orders of magnitude drop below.

International cooperation

Joint Project supported by the Korean Research Council of Fundamental Science & Technology (KRFC) and Hungarian Academy of Sciences (Hungarian project leader: P. Tompa, Institute of Enzymology, Research Centre for Natural Sciences; participating scientists of Wigner RCP: K. Tompa, M. Bokor, 2014-2016)

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See also: S-F.5.

S-J. Gas Discharge Physics

Kinga Kutasi, Aranka Derzsi, Zoltán Donkó, Péter Hartmann, Ihor Korolov, Anikó Zsuzsa Kovács[#], Péter Magyar[#], Pál Mezei, Károly Rózsa[A]

Our research activities are related to the different physical and chemical aspects of low temperature – non-equilibrium – plasmas at low (10-1000 Pa) and atmospheric pressures, and to their possible use for future emerging technologies. Furthermore, we also make use of the plasma environment of the low-pressure gas discharges to study atomic processes, as well as the collective phenomena occurring in many-particle systems using the dusty (strongly-coupled) plasma as model system. In the following, we briefly introduce some of our recent achievements grouped around our four main research directions.

Gas discharge physics. — Most of our research has concentrated on the behavior of charged particles in low-ionization-degree plasmas excited by radio-frequency waveforms. We have experimentally investigated the breakdown of hydrogen and deuterium gases and carried out numerical simulations to gain detailed insight into the build-up of electrical current conduction across the gas. Numerical, particle-based simulations have been developed to understand the plasma-chemical processes taking place in reactive oxygen plasmas. Studying the effects of "tailoring" the driving voltage waveform (by applying multiple consecutive harmonics of a base harmonic radio-frequency signal), we followed the changes in the dynamics of the electrons and ions in the plasmas and demonstrated the possibility of controlling the ion energy distribution functions, which are of great importance in surface processing plasma applications. The interaction between the plasma and the surrounding surfaces was also investigated via including surface processes (electron reflection and secondary electron emission from surfaces) in the discharge models. Simulations as well as experiments have been conducted with different gases to uncover the effects of negative ions, and more generally, effects of ion dynamics on the properties of capacitively coupled plasmas driven by customized voltage waveforms. Nonlinear and resonance effects occurring in these plasmas have also been addressed by computational simulations.

Strongly coupled plasmas. — Heat conduction in strongly magnetized, highly correlated plasmas has been investigated via molecular dynamics simulations. In a classical ideal plasma, a magnetic field is known to reduce the heat conductivity perpendicular to the field, whereas it does not alter the one along the field. We have shown that in strongly correlated plasmas, which occur at high pressure and/or low temperature, a magnetic field reduces the perpendicular heat transport much less and even enhances the parallel transport. These observations have been explained by the competition of kinetic, potential, and collisional contributions to the heat conductivity. Molecular-dynamics (MD) simulations of a strongly coupled binary ionic mixture have revealed the appearance of sharp minima in the species-resolved dynamical density fluctuation spectra. This phenomenon was found to be

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

reminiscent of the well-known Fano anti-resonance, occurring in various physical processes. We gave a theoretical analysis using the quasi-localized charge approximation, and demonstrated that the observed phenomenon in the equilibrium spectrum is a novel manifestation of the Fano mechanism.

Dusty plasmas. — Experiments and particle-based kinetic simulations were performed to obtain the equilibrium levitation height of dust particles in plane-parallel electrode discharges in low-pressure argon gas, established by combined RF and DC excitation. Non-equilibrium molecular dynamics simulation studies were performed on the dynamic (complex) shear viscosity of a 2D Yukawa system. Results include the identification of a non-monotonic frequency dependence of the viscosity at high frequencies and shear rates, of an energy absorption maximum (local resonance) at the Einstein frequency of the system at medium shear rates, of an enhanced collective wave activity, when the excitation is near the plateau frequency of the longitudinal wave dispersion, and the emergence of significant configurational anisotropy at small frequencies and high shear rates.

Discharge plasmas for surface treatment. — Oxygen content and UV radiating active plasmas, as well as afterglows have great potentials for modification of surfaces. For biomedical applications, the modification of polymer surfaces are required for further grafting. We have developed an afterglow system, based on a flowing surface-wave microwave discharge, which makes possible the treatment of the in- and outside walls of small-diameter heat-sensitive polymer tubes. We have determined the operating conditions and the afterglow characteristics in order to optimize the application (Figure 1).

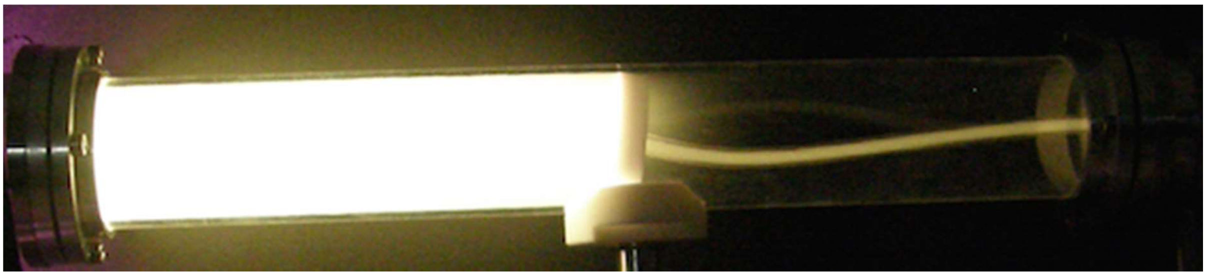

Figure 1. *Afterglow reactor set-up for treatment of heat sensitive tubes.*

Grants

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

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

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

NKFIH K-115805: Complex plasmas in action (P. Hartmann, 2015-2019)

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

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

International cooperation

Boston College

Ruhr Universität Bochum

Baylor University Texas

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

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

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

West Virginia University (Julian Schulze)

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See also: S-Q.2

S-K. Liquid Structure

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

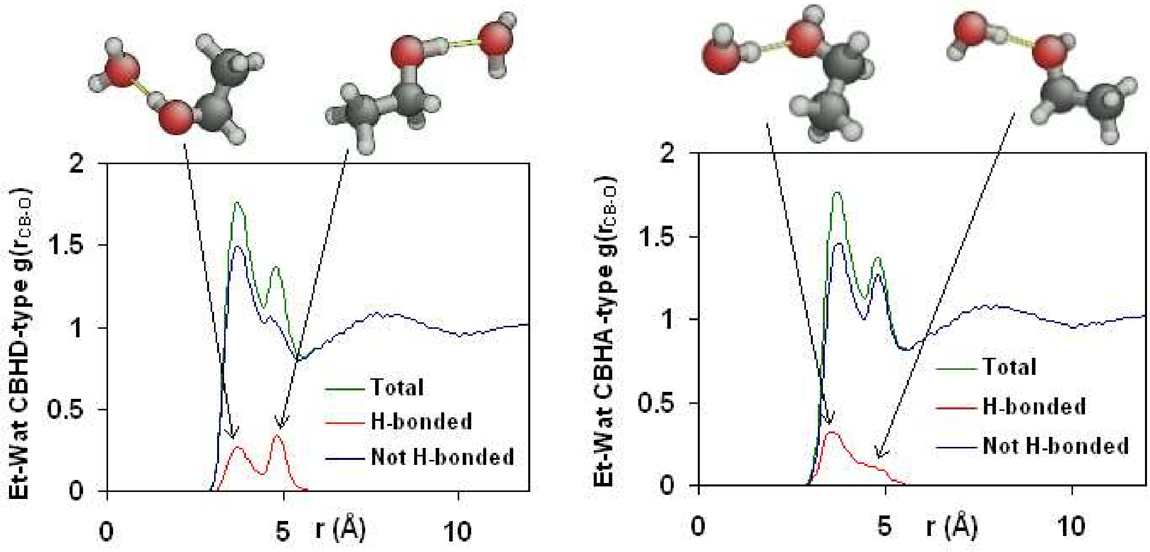
Understanding disordered structures. — The main activity of our research group is the investigation of the microscopic structure of liquids, amorphous materials and disordered crystals. We combine experimental data, such as total scattering structure factors (TSSF) from X-ray and neutron diffraction (XRD and ND, respectively) and extended X-ray absorption fine structure (EXAFS) spectra, with computer modeling tools, such as Reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations. As a result of such an approach, large sets (containing tens of thousands) of atomic coordinates ('particle configurations') in simulation boxes are provided that are consistent (within errors) with experimental data. These configurations are then subjected to various geometrical analyses, so that specific questions concerning the structure of a material may be answered. Below, we provide some selected results from the year of 2015.

Molecular liquids. — The structure of *liquid water* has been revisited using isotopic substitution neutron diffraction. The application of polarized neutron beams allowed us to separate the coherent and incoherent contributions to the total scattering; this way, reliable coherent structure factors could be obtained (for the first time) for H_2O/D_2O mixtures with very high (up to 100 %) H-content. At the same time, the huge incoherent inelastic background could be determined over a very wide scattering vector range, thus providing experimental data for functions that have been searched for decades.

Series of MD simulations for *ethanol-water mixtures* with 20 to 80 molar % ethanol content, as well as for pure ethanol and water were performed. XRD experimental data have been approximated nearly quantitatively, providing a good basis for revealing details of the atomic structure. Coordination numbers and hydrogen bonds/molecule values were calculated, revealing that the oxygen-oxygen first coordination numbers overestimate the average number of hydrogen bonds/molecule. The center of molecule distributions indicate that the ethanol-ethanol first coordination sphere expands with increasing water concentration while the size of the first water-water coordination sphere does not change. The distribution of the distance between the methyl carbon atom and the O-atom of its hydrogen-bonded pair differs for the following two cases: (1) the methyl carbon atom belongs to the hydrogen donor (CBHD), and (b) the methyl carbon atom belongs to the hydrogen acceptor ethanol molecule (CBHA) (see Figure 1).

Covalent glasses. — Short range order of *glassy* $Ge_{20}Ga_{10}Se_{70}$ *and* $Ge_{20}Ga_{5}Se_{75}$ was investigated by ND and EXAFS at the Ge, Ga and Se K-edges. Large scale structural models were obtained by RMC fitting simultaneously four experimental datasets. It was found that both Ge and Ga are predominantly fourfold coordinated. Models giving the best agreement

[A] Associate fellow



a) b)

Figure 1. *Distributions of the distances between the methyl C-atom (C_B) of an ethanol molecule and the O-atom of a water molecule, g(r_{CB-O}), for the MD simulation with 80 molar % ethanol. C_B belongs (a) to an H-donor ethanol (CBHD) and (b), to an H-acceptor ethanol molecule (CBHA).*

with experimental data show that Ga has a complex effect on the Ge-Se host matrix: i) it enters the covalent network by forming Ga-Ge bonds; ii) by decreasing the number of Se atoms around Ge, it contributes to the formation of Se-Se bonds, which may explain the higher solubility of lanthanide ions; iii) the average coordination number of Se increases due to the Ga-Se 'extra' bonds. The higher average coordination of the network may be responsible for the increase of T_g upon adding Ga to Ge-Se glasses.

Metallic glasses. — *$Cu_{47.5}Zr_{47.5}Al_5$ metallic glass* was studied by high-energy XRD, ND with isotopic substitution, electron diffraction and EXAFS. The atomic structure of the glass was modeled by RMC and MD simulations. RMC modeling of seven experimental datasets enabled reliable separation of all 6 partial radial distribution functions. A peculiar structural feature of this ternary alloy is the formation of the strong Al–Zr bonding, which is supposed to determine its high viscosity and enhanced bulk glass formation. Comparison of Cu-Cu, Cu-Zr and Zr-Zr correlations in $Cu_{47.5}Zr_{47.5}Al_5$ glass and $Cu_{10}Zr_7$, CuZr B2 and $CuZr_2$ crystalline structures elucidates their similarities and differences and explains why $Cu_{10}Zr_7$ appears first upon devitrification of the glass (see Figure 2).

Grants

OTKA K083529: Investigations concerning the structure of complex liquids (L. Pusztai, 2011-2015)

EU-FP7-NMI3-II, No. 283883 Neutron Scattering and Muon Spectroscopy Integrated Initiative: Neutron diffraction (L. Temleitner, 2012-2015)

SNK-63/2013 (MTA-BAS Hungarian-Bulgarian bilateral) Investigation of the short- and long range order in multifunctional materials (E. Sváb, 2013-2015)

TET_12_MX-1-2013-0003 Hungarian-Mexican bilateral (L. Pusztai, 2015-2016)

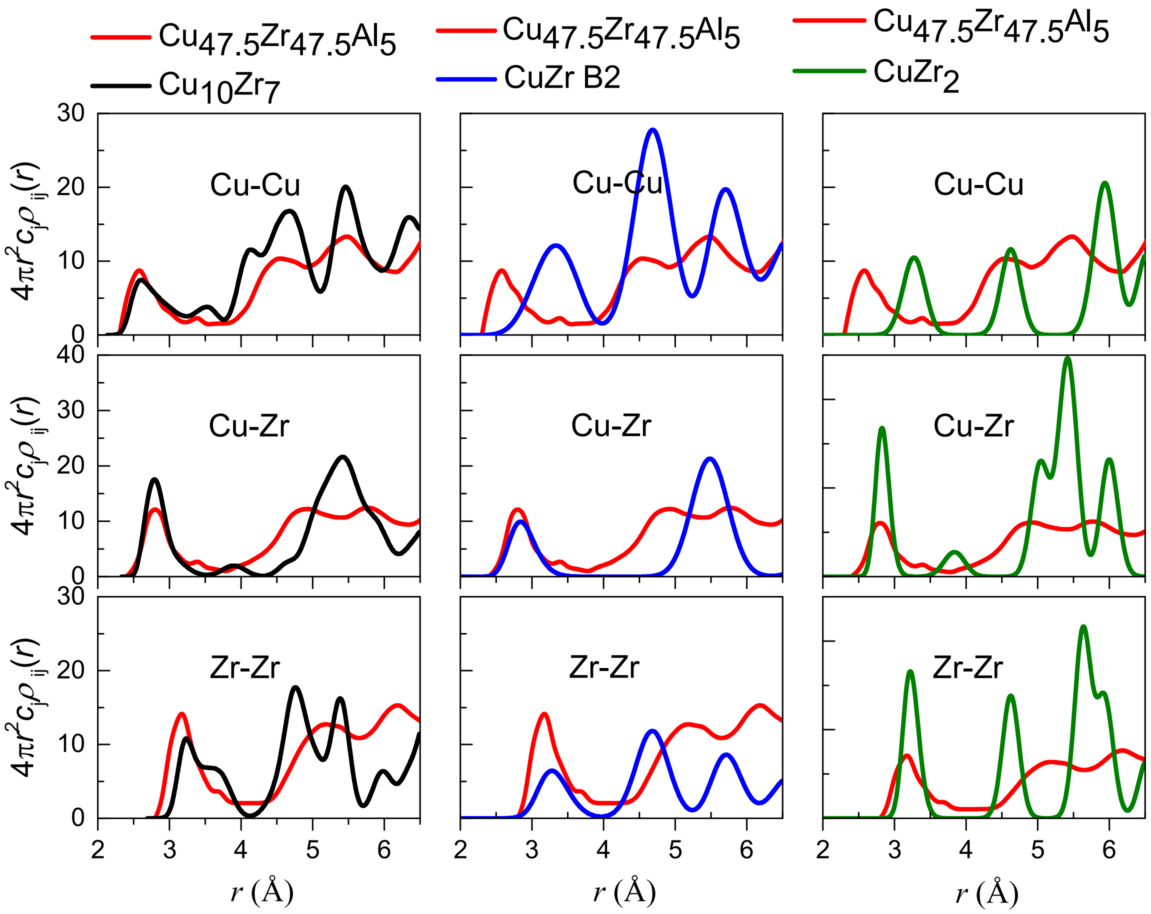


Figure 2. *Partial radial distribution functions of $Cu_{47.5}Zr_{47.5}Al_5$ metallic glass and $Cu_{10}Zr_7$, CuZr B2 and $CuZr_2$ crystal structures*

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14. Pethes I, Kaban I, Wang R-P, Luther-Davies B, Jóvári P: Short range order in Ge–As–Se glasses. ***J ALLOY COMPD*** 623: pp. 454-459. (2015)
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S-L. Nanostructure research by neutron scattering

Adél Len, László Almásy, Katalin Bajnok, Gergely Eszenyi, Margit Fábián, György Káli, Gergely Nagy, László Rosta[A], Noémi Kinga Székely, Gyula Török[A], Renáta Ünnep[#], Tamás Veres

Our group operates four large-scale instruments at the Budapest Research Reactor, used by the national and international research community: “Yellow Submarine” Small Angle Neutron Scattering (SANS) spectrometer, “Athos” cold triple-axis spectrometer, “PSD” thermal neutron diffractometer with a position-sensitive detector and the “TOF” time-of-flight instrument. They are used for the study and analysis of structure and properties of condensed matter.

Steels. — Rolling with shear (RS) is a novel method of continuous severe plastic deformation applied for improvement of the mechanical properties of steel. The technology ensures high plasticity of the material without decreasing the strength. This allows cold drawing of wires without intermediate softening annealing. Samples processed with standard (ST) technology and with RS technology were measured at the Yellow Submarine spectrometer (Figure 1c). SANS results (Figure 1a) explained the density and conductivity behaviour of ST and RS processed wires. The average size of the cracks and nanopores (Figure 1b) was smaller and less anisotropic for the RS than for the ST wires, confirming the dynamic healing of the nanosized defects during the cold drawing of the wires.

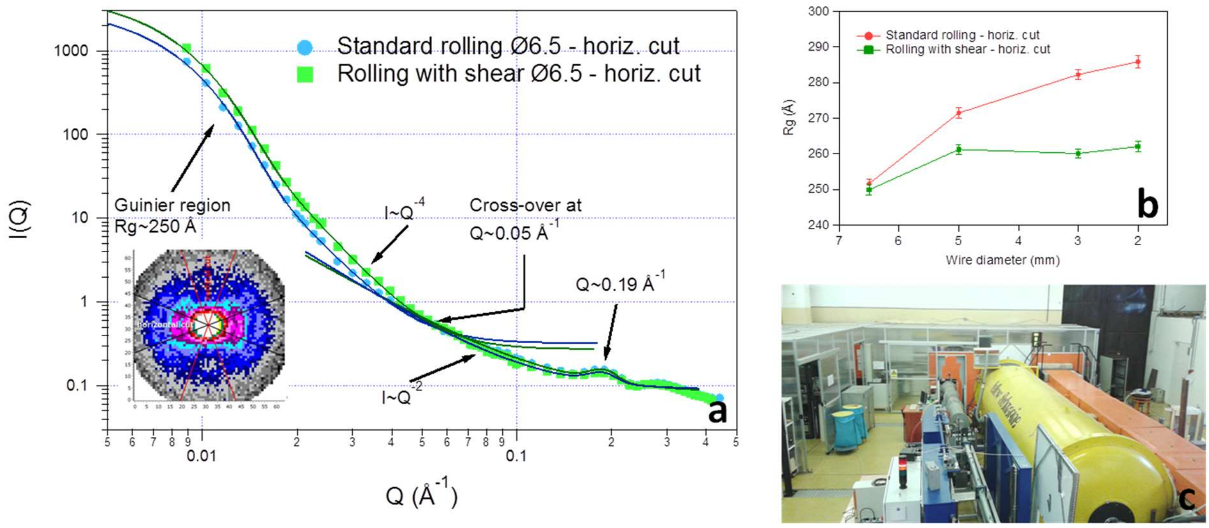

Figure 1. *SANS 2D maps and radial averaged curves for ST and RS steels (a); comparison of radii of gyration for ST and RS steels (b); Yellow Submarine SANS instrument (c).*

Polymers. — We studied ageing behaviour of thermoplastic polyurethanes, of various hard-segment / soft segment ratios. They have been treated by gamma irradiation and aged at elevated temperatures and humidity. Besides the standard physico-chemical techniques, the

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[#] Ph.D student

microstructure changes have been followed by neutron and X-ray scattering. It was found that hydrolysis and chain scission were the prevalent reactions during humid aging, and the high energy impact of the gamma radiation induced the formation of new bonds between adjacent chains, therefore producing a large interconnected network at the highest radiation doses studied. During the prolonged storage at high humidity, the shortening of the polyurethane chains promoted crystallization, as revealed by small-angle scattering.

Nanostructure of archaeological objects. — Several types of archaeological objects, such as high tin-contained nomadic bronze mirrors (University of Leipzig), weapons from the Copper and Bronze Age (Archaeological Institute of the HAS), three tin-lead busts of the 18th century Messerschmidt Collection (Museum of Fine Arts, Budapest), a terracotta relief commemorating the Plague Epidemic in Vienna in 1679 by Fischer von Erlach (Museum of Fine Arts, Budapest) and medieval eastern steel weapons from the Wallace Collection (London) were studied by various metallurgical, neutron and X-ray techniques. Eleven bronze nomadic Carpathian mirrors from the 4-5th century were measured at the TOF and the PGAA (Prompt Gamma Activation Analysis) instruments. Besides the elemental analysis made on PGAA, the TOF measurements revealed that the delta-bronze phase was the most characteristic nanocomponent of the mirrors. This phase is rigid, and easily polishable, a feature that serves the original function of the object. These measurements demonstrated the high-level knowledge of the masters that made possible the production of the best quality mirrors of this age.

Borosilicate glasses. — In the past year, 26 different borosilicate glass types, suitable for the storage of high-activity radioactive waste were produced, characterized and optimized. The samples were manufactured in a high-temperature furnace, followed by fast cooling. The matrix/waste ratio was optimized by the addition of actinides and lanthanides in various concentrations. The samples were then characterized by neutron diffraction and modelled using the reverse Monte Carlo simulation method.

Grants

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

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

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

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

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

International cooperation

Paul Scherrer Institute, Switzerland (Renáta Ünnep) - Aveiro Institute of Materials, Portugal (László Almásy) - Joint Institute for Nuclear Research, Russian Federation (László Almásy) - Petersburg Nuclear Physics Institute, Russia (Gyula Török) - Institute Laue Langevin, France (László Rosta) - Institute of Macromolecular Chemistry, Czech Republic (László Almásy) -

Institute of Chemistry, Poland (László Almásy) - Laboratoire Léon Brillouin CEA-CNRS, France (László Rosta) - Institute of Chemistry Timisoara of Romanian Academy, Romania (László Almásy, Adél Len) - Institute of Chemical Technology, Prague (Adél Len) - Key Laboratory of Neutron Physics and Institute of Nuclear Physics and Chemistry, China (László Almásy) - Donetsk Institute for Physics and Engineering named after A. A. Galkin, Ukraine (Adél Len) - Université Cadi Ayyad, Marrakech, Morocco (Adél Len) - Institute of Occupational Medicine and Environmental Health, Poland (László Almásy) - Institute of Theoretical and Applied Mechanics, Czech Republic (Adél Len)

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"Enhancing the Characterization, Preservation and Protection of Cultural Heritage Artefacts" (2014-2015).

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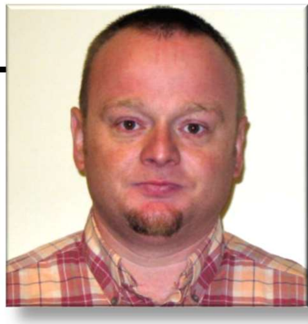
See also: R-M.2, R-M.4

S-M. Neutron optics



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

Neutron instrumentation development. — The focusing small-angle neutron scattering spectrometer (FSANS) developed and installed at the Budapest Neutron Centre has reached the commissioning stage. The instrument has a two-fold mission: 1) extends the accessible scattering vector range of the highly demanded BNC YS SANS towards smaller q values; 2) provides a versatile test bench for future development of neutron optical devices. It is able to accommodate a larger variety of collimation optics: classical pinhole collimation, multibeam converging collimation, magnetic focusing and reflective focusing by means of elliptical mirrors. The sample and detector positions can be adjusted to allow variation of incoming beam position and direction. A 4-chopper flight time definition system is used for energy determination required by scattering vector computation. It also allows accurate and extensive mapping of the wavelength-dependent transfer functions of the tested optical devices.

The development and construction of a prototype of the position-sensitive neutron detector based on thin solid boron converter layers was achieved. Neutron-sensitive layers were produced by sputtering technique. The layers were characterized in terms of thickness uniformity and absolute thickness by transmission measurements. These parameters are essential for the detection efficiency and homogeneity. Optimal layer thickness has been determined by numerical simulation. The prototype of the detector has been characterized by homogeneity, position resolution and efficiency measurements.

Researchers of the group actively contributed to the detector development and moderator investigation workpackages of the ESS Brightness project and provided scientific input to the Hungarian in-kind contribution to the construction of the European Spallation Source: optimization of the secondary instrument of MIRACLES (Multiple Resolution Analyser Crystal for Life and Energy Science); development of a new time-focusing concept for time-of-flight quasi-backscattering (scattering angle is of a few degrees smaller than 180 degrees) analyzer for the same instrument; neutron guide system optimization for the NMX (neutron macromolecular diffractometer) instrument.

Neutron holography. — Measurement and evaluation of the hologram of a Cd-contaminated Sn single-crystal allowed for the first time the determination of three-dimensional displacement vectors of host atoms around impurity atoms using atomic resolution neutron holography. The addition of Cd impurities slows down the β→α phase transition of Sn but the microscopic reason was not known. The experiment showed a contraction of the lattice

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[A] Associate fellow

[#] Ph.D student

[E] Professor Emeritus

around the impurity, similar to the effects of external pressure. The 3D displacement showed that the BCT lattice of β-Sn is distorted towards the diamond structure of α-Sn.

Structural investigation of hybrid silica gels. — Methyl, vinyl, phenyl, isobutyl substituted silica gels have been synthetized by sol-gel process. In order to find the optimal conditions for the *in situ* immobilization of the Cellulase from *Trichoderma sp.,* complementary physicochemical characterization methods have been employed. The obtained biocomposites activity has been assayed by the enzymatic bioconversion of cellulose to monomeric sugars, with significant commercial interest.

Grants and international cooperation

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

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

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

Chinese Academy of Sciences - Institute of High Energy Physics – China Spallation Neutron Source: Neutron scattering instrumentation development for the China Spallation Neutron Source built in Dongguan.

Publications

Articles

1. Orbán J: Serial delay-line readout for position sensitive neutron beam monitor. ***POLLACK PERIODICA*** 10:(1) pp. 53-60. (2015)

2. Putz A-M, Cecilia S, Ianăşi C, Dudás Z, Székely KN, Plocek J, Sfârloagă P, Săcărescu L, Almásy L: Pore ordering in mesoporous matrices induced by different directing agents. ***J POROUS MAT*** 22: pp. 321-331. (2015)

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S-N. Laser applications and optical measurement techniques

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

Aerosol drug delivery/deposition in human lungs. — A novel Raman spectroscopic method has been developed that can be used to study the deposition of aerosol drugs and other airborne substances in realistic human airway replicas. In this procedure, silicon substrates were attached to the internal surface of 3D printed hollow airway walls in order to collect the deposited drug. Their surface was analysed by mapping Raman spectroscopy. Intensity maps of characteristic Raman peak of the medication were found to be in good agreement with optical microscopic images of the scanned areas.

A computational fluid dynamics (CFD) model developed for the determination of flow characteristics and estimation of particle deposition in airways was validated by experimental measurements of velocity profiles with laser Doppler anemometry in an idealized airway model. A good correlation was found between the velocity profiles and velocities obtained by numerical modelling and the experimental measurements performed with similar conditions and input parameters. The CFD model predicted the flow to be laminar in the trachea region of the airway model, with a remarkable role of the airway geometry in the flow characteristics at subsequent generations. This behaviour was supported by the experimental data as well. According to our results, the CFD model is able to determine the flow characteristics at least to the 3rd generation of the airway model.

Study of optical properties of aerosols. — Measurements of ambient urban aerosols were conducted by simultaneously using optical particle spectrometry based on elastic scattering and photo-acoustic spectrometry and filter deposition technique. Of all methods used in this study, only the Dual-Wavelength Optical Particle Spectrometer (DWOPS) technique allows the direct assessment of the complex refractive index as well as the corresponding particle size. The imaginary part of the refractive index reflects the absorbing properties of particles in question. The fact that DWOPS determines the size and the complex refractive index of each detected particle allows inferring the number concentrations of absorbing ambient aerosols as a function of their absorptivity.

EXMET – Interferometric measurement methods. — In cooperation with the University of Miskolc, we have developed a Michelson-type interferometer, using a frequency stabilized laser and high-quality optical elements for the investigation of vibrations. The instrument was installed into a rigid box on the top of an optical bench. A new LabView software was also developed to control the measurements and evaluate the acquired data.

Optical thin-film structures consisting of nanoscale laminated layers. – We have continued our research towards the development of optical thin-film structures containing

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

nanooptically thin layers for advanced applications in laser physics and information technology.

Service laboratory for optical measurements. — We have continued the utilization of our surface profiler based on white-light interferometry. We have developed a new method which combines surface diagnostics with aerosol science: aerosol drug samples on impactor plates are investigated by the interferometric surface profiler to determine the exact volume of deposited species. We have performed aerosol measurements by optical and spectroscopic methods in the frame of academic cooperation and industrial contracts (HOYA Co., H-ION Ltd.).

Participation in TAMOP Educational Program for ELI. – In the frame of this project, we have prepared several lectures for Msc and PhD students and organized a workshop, where several lectures were presented in the "Fundamentals of optics in the scope of ELI-ALPS" topic. Laboratory practices were also organized for students and masters.

Grants

KTIA_AIK_12-1-2012-0019: "Theoretical and experimental investigation of aerosol deposition in human airways in case of frequent lung diseases (asthma, COPD)" (A. Nagy, 2013-2015)

TeT_10-1-2011-0725 Austro-Hungarian Bilateral Co-operation, Study of optical properties of aerosols and their climate relevance with dual wavelength optical particle spectrometer (A. Nagy, 2013-2015)

EAC 2011, 82013-00 European Aerosol Conference (A. Czitrovszky, 2011-2015)

TAMOP-4.1.1.C-12/1/KONV-2012-0005: Preparation for educational and R&D activities related to the Hungarian ELI project in the concerned sectors (Project leader: M. Veres, 2014-2015; participating scientist: A. Czitrovszky)

OPTILAB – WIGNER RCP No. WG-76/2014 (Karpat Ferencz, 2015)

EXMET 93010-14: Development of interferometric measurement methods (A. Czitrovszky, 2014- 2015)

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

HAS – Wigner RCP 81033-15: Deposition of aerosols (supplement) (A. Nagy, 2015)

HION - Wigner RCP: Investigation of sampled industrial aerosols by Raman spectroscopy, optical and electron microscopy (A. Czitrovszky 2015-2016)

HOYA - Wigner RCP: Measurements of industrial indoor aerosol pollution (A. Czitrovszky, 2014-2015)

International cooperation

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

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

Publications

Articles

1. Fekeshgazi IV, Sidenko TS, Czitrovszky A, Veresh M, Trukhan VM, Shoukavaya TV: Raman Spectra of Gyrotropic Cadmium Diphosphide Crystals. ***J APPL SPECTROSC*** 82:(3) pp. 367-373. (2015)

Conference proceedings

2. Fried M, Major C, Juhász G, Petrik P, Horváth Z: Expanded beam speetro-ellipsometry for big area on-line monitoring. Conference on Optical Measurement Systems for Industrial Inspection IX. Munich, Germany: 22.06.2015 – 25.06.2015, ***PROC SPIE*** 9525: Paper 95251S. 12 p. (2015)

3. Kerekes A, Veres M, Himics L, Tóth S, Czitrovszky A, Nagy A, Oszetzky D, Kugler S, Koós M: Determination of the distribution of inhaled drugs in human airways by Raman spectroscopy. ***NATO SCIE PEACE SECU,*** 39: pp. 437-442. (2015)

Patents

4. Horváth ZGy, Juhász G, Fried M, Major C, Petrik P: Imaging optical device with a pinhole camera. Japanese Patent JP2010528281

5. Veres M, Nagy A, Czitrovszky A, Oszetzky D, Rigó I, Kerekes A, Himics L, Borossáné Tóth S: Determination of size distribution and mass of deposited aerosol particles by white light interferometry, submitted to the Committee of Intellectual Properties of Wigner RCP

See also: S-P.5, S-P.21, S-R.3

S-O. Femtosecond lasers for nonlinear microscopy

Róbert Szipőcs, Dóra Haluszka[#], Ádám Krolopp, Lajos Vass

Femtosecond fiber lasers for nonlinear microscopy. — In 2014, we developed a pulsed Yb-fiber oscillator and amplifier system with a variable repetition rate in the 1 to 36 MHz range in collaboration with our industrial partner, R&D Ultrafast Laser Ltd. The laser is used for our hand-hold 3D nonlinear microscope system (*FiberScope*), and allows *in vivo* imaging of murine skin at an average power level as low as 5 mW at a 200 kHz sampling rate. The system has the main advantages of the lower price of the fs laser applied, fiber optics flexibility, a relatively small, light-weight scanning and detection head, and no risk of thermal or photochemical damage of the skin. This year, we have tested the *FiberScope* system for different *in vivo* murine skin samples. Among others, using SHG imaging of the collagen, we could investigate and follow the effects of obesity on dermal collagen alterations. For demonstration purposes in cosmetology and nanomedicine, we also used our 2PEF/SHG imaging system for *in vivo* visualization and monitoring the uptake of Alexa Fluor 546 labelled nanomedicine by Langerhans cells for 24 hours. The SHG image of the collagen (shown in Figure 1, left) was recorded at ~5 mW average power. The pixel dwell time was set to 5 µs, which corresponds to our 200 kHz sampling rate. On the right side of Figure 1, we show the result of an *in vivo* penetration measurement of Alexa-546 labelled nanoparticles (AF546-DV) in murine skin, using the same device optimized for combined 2PEF/SHG measurements.

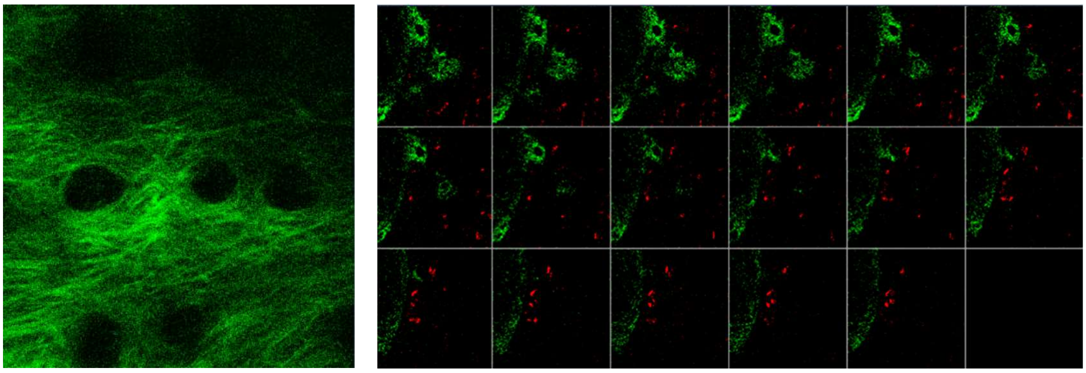


Figure 1. *Left: SHG image of collagen recorded at 5 mW average power (measured directly above the skin) from an Yb-fiber laser operating at a 1.89 MHz repetition rate. Right: in vivo penetration measurement of Alexa-546 labelled nanoparticles (AF546-DV) in murine skin. Excitation wavelength: ~1030 nm, z-stack image (128x128 pixels/frame). Green: SHG signal of collagen. Red: fluorescence signal of AF546-labelled nanoparticles 1 hour after of the topical treatment by nanomedicine of the skin. One can observe that the Langerhans cells, which are a part of the immune system, accumulate the AF546-labelled nanoparticles.*

[#] Ph.D student

The variable repetition-rate, sub-picosecond pulsed Yb-fiber oscillator and amplifier system itself has the drawback of a limited tuneability in the 1020-1060 nm spectral range. By this year, we have developed a highly efficient wavelength conversion method, which is based purely on optical fibre technology. This fact is demonstrated in Figure 2 (left), where a colour photo image of the wavelength converted Yb-fiber laser output reaching a white screen is shown. As one can observe, the fiber laser has a visible, red output due to the fact that most of the optical power is concentrated at around 700 nm. On the right side of Figure 2, the same picture is shown as taken by a IR viewer: here, one can observe the hexagonal symmetry of the photonic crystal fiber (PCF) used for frequency conversion in this experiment.

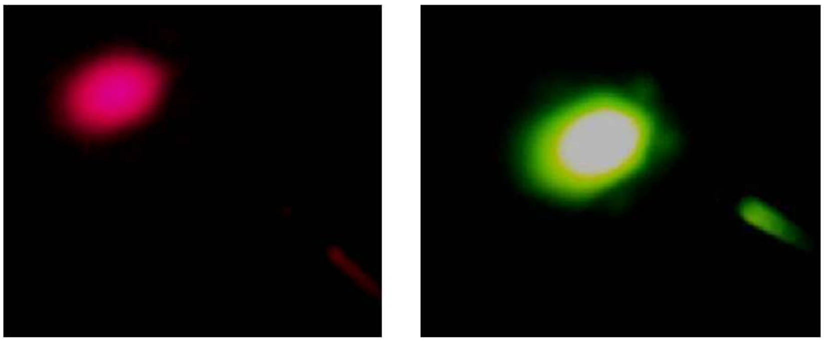


Figure 2. *Left: Colour photo image of the fiber laser output after frequency conversion in a PCF. Right: the same picture taken by the use of an IR viewer.*

CARS microscopy. — In parallel with our cutting-edge non-linear microscope developments (such as the *FiberScope* system mentioned above or our combined CARS / Stimulated Raman Scattering (SRS) data acquisition system developed and tested for lipid, protein and NO detection), we performed a high number of experiments using our anti-Stokes Raman scattering (CARS) imaging system. The measurements were related to *in vivo* optical disease diagnosis in dermatology (such as characterization of obesity, see our related paper in Microscopy Research and Techniques), or in neurology (such as characterization of animal models developed for studying sclerosis multiplex (SM)), in collaboration with our scientific partners: Semmelweis University, Department of Dermatology and University of Szeged, Department of Neurology, respectively. In neurology, we performed a quantitative analysis of the myelin loss in a cuprizone model of SM depending on the drug treatment. Using the CARS imaging system we installed at Szeged University in the summer of 2014, we could record the CARS images shown in Figure 3.

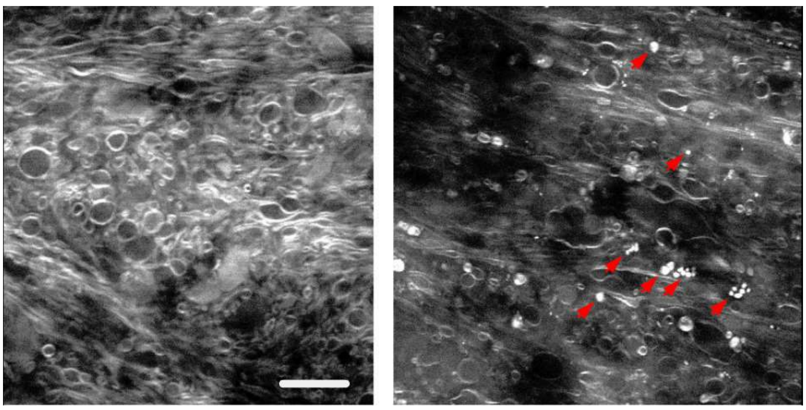


Figure 3 CARS image of normal myelin fibers (control) in the white matter of a mouse brain slice (left), and after cuprizone treatment resulting in myelin loss and lipid droplets indicated by red arrows (right).

Grants

TECH-09-A2-2009-0134 National Technology Program, – Development of fiber integrated nonlinear microendoscope for pharmacological and diagnostic examinations based on novel fiber laser technology (R. Szipőcs, 2009-2015)

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

Publications

Articles

1. Haluszka D, Lőrincz K, Molnár G, Tamás G, Kolonics A, Szipőcs R, Sarolta Kárpáti, Norbert M Wikonkál: In vivo second-harmonic generation and ex vivo coherent anti-Stokes Raman scattering microscopy to study the effect of obesity to fibroblast cell function using an Yb-fiber laser based CARS extension unit. ***MICROSC RES TECHNIQ*** 78:(9) pp. 823-830. (2015)

2. Grósz T, Kovács AP, Mecseki K, Gulyás L, Szipőcs R: Monitoring the dominance of higher-order chromatic dispersion with spectral interferometry using the stationary phase point method. ***OPT COMMUN*** 338: pp. 292-299. (2015)

3. Haluszka D, Lőrincz K, Csákányi A, Vass L, Krolopp Á, Kolonics A, Szipőcs R, Kárpáti S, Wikonkál N: Nemlineáris mikroszkópia alapjai és alkalmazási lehetôségei a dermatológiában (Principles of non-linear microscopy and application possibilities in dermatology). ***BŐRGYÓGYÁSZATI ÉS VENEROLÓGIAI SZEMLE*** 91:(1) pp. 34-39. (2015)

4. Lőrincz K, Bánvölgyi A, Haluszka D, Keszeg A, Márton D, Kuroli E, Szipőcs R, K Scharfetter-Kochanek, M Wlaschek, Kárpáti S, Wikonkál N: Hosszú távú PUVA kezelés bőröregítő hatásának vizsgálata egereken (Analysis of skin aging during long term PUVA treatment on mice, in Hungarian). ***BŐRGYÓGYÁSZATI ÉS VENEROLÓGIAI SZEMLE*** 91:(1) pp. 18-22. (2015)

S-Q. Crystal physics

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

Crystal growth of sLN and KLN. — Computer-controlled pulling and rotation systems were set up for 4 crystal growth apparatuses providing gradually variable rotation and pulling rate during the growth process. Based on Raman spectroscopy, a Mg concentration mapping of lithium niobate ($LiNbO_3$, LN) crystals was developed ensuring the growth of high quality stoichiometric sLN:Mg just above the threshold concentration; this required also the extension of the high-temperature top-seeded solution growth technique by semi-continuous feeding during growth. The impact of Ti^{4+} and Ta^{5+} dopants on the crystallization of potassium lithium niobate ($K_3Li_2Nb_5O_{15}$, KLN) and its phase transition was explored based on UV absorption and temperature dependent dielectric measurements.

Spectroscopy of $LiNbO_3$ and lithium yttrium orthoborate ($Li_6Y(BO_3)_3$, LYB) single crystals. – An incorporation model based on optical absorption spectroscopic results was successfully developed for optical damage resistant (Mg, Zn, In, Sc, Hf, Zr, Sn, etc.) and rare-earth dopants in $LiNbO_3$ crystals. It was shown by SIESTA quantum-chemical calculations that the ODR ions preferably incorporate at neighboring lattice sites, creating small defect structures.

The population relaxation kinetics of the $^4I_{11/2}$ – $^4I_{13/2}$ – $^4I_{15/2}$ transitions of Er^{3+} ions was determined by a saturation spectroscopic method both for congruent and stoichiometric $LiNbO_3$, and the splitting of the spectral holes due to magnetic field was measured in $LiNbO_3$:Er, $LiNbO_3$:Yb, and $Li_6Y(BO_3)_3$:Yb crystals (Figure 1). The sensitivity of the spectral holes to magnetic field is much higher than that of a typical Zeeman-splitting process. Spin-Hamiltonian tensor-parameters of the Er^{3+} dopant in LYB were evaluated from angular dependent EPR spectra with the magnetic field rotated in 4 different crystallographic planes, required for an unambiguous characterization of the dopant's low-symmetry incorporation site and electronic structure (Figure 2).

$Li_2B_4O_7$-based dosimeters and detectors. – Thermostimulated and various X-ray, cathodo- and photoluminescence spectra of the tissue-equivalent dosimetry material LTB activated by Ag and/or Cu doping were used to describe the recombination processes on the atomic level. This can be used for an optimization of dosimetric and neutron detector applications in medicine and industry.

Analytical methods for advanced materials and environmental control. – Solid (powder) sampling high-resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS-GFAAS) methods were elaborated and used for the determination of the Li and Na (flux) additives in yttrium orthosilicate polycrystalline scintillator materials. The methods were validated with the application of internationally certified reference materials.

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

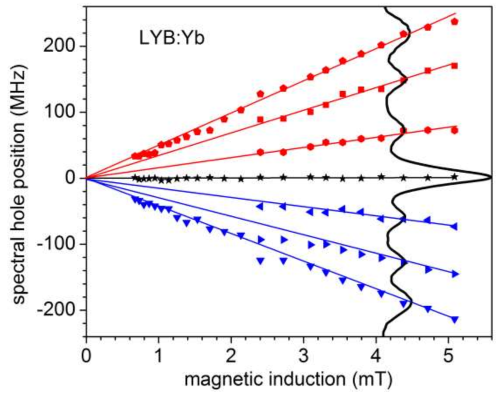


Figure 1*. Splitting of the spectral hole due to the presence of magnetic field in ytterbium-doped LYB single crystals*

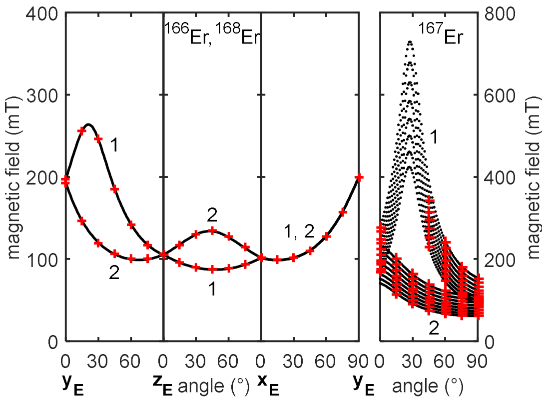


Figure 2*. Angular dependence of the EPR lines in a LYB:Er^{3+} single crystal due to both non-magnetic Er isotopes and the magnetic ^{167}Er isotope resulting in hyperfine splitting.*

The quenching mechanism between SiC nanocrystal – one of the most hopeful nanomaterials for *in vivo* applications in human medicine – and Bovine Serum Albumin (BSA) was found to be mainly static with a weak dynamic component. Thermodynamic calculations showed that both hydrogen and hydrophobic interactions are present in the SiC-BSA binding.

A combination of convective-diffusive vapor-transport models was described to extend the calculation scheme for sensitivity (in terms of the characteristic mass, m_0) in graphite furnace atomic absorption spectrometry. The new model was tested for 18 elements. The calculated m_0 data gave a fairly good agreement with the corresponding experimental m_0 values.

The deposition of atmospheric aerosols causing soiling/blackening was determined in four Belgian cultural heritage buildings, installed with different heating/ventilation systems. The studies demonstrated clearly reduced levels of deposited water-soluble aerosols compared to uncontrolled indoor environments.

Grants

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

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

International cooperation

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

Osnabrück University (Germany), Small polarons in luminescent $LiNbO_3$: From bulk to nanocrystals (Zs. Kis, participants: G. Corradi, I. Hajdara, L. Kovács, K. Lengyel, G. Mandula, Zs. Szaller)

Paderborn University (Germany), Paramagnetic resonance spectroscopy of rare earth doped oxide crystals (G. Corradi)

Publications

Articles

1. Anaf W, Bencs L, Van Grieken R, Janssens K, De Wael K: Indoor particulate matter in four Belgian heritage sites: Case studies on the deposition of dark-colored and hygroscopic particles. ***SCI TOTAL ENVIRON*** 506–507: pp. 361-368. (2015)

2. Bencs L, Laczai N, Mezei P, Cserfalvi T: Detection of some industrially relevant elements in water by electrolyte cathode atmospheric glow discharge optical emission spectrometry.
SPECTROCHIMICA ACTA PART B-ATOMIC SPECTROSCOPY 107: pp. 139-145. (2015)

3. Bencs L, Laczai N, Ajtony Z
Model calculation of the characteristic mass for convective and diffusive vapor transport in graphite furnace atomic absorption spectrometry. ***SPECTROCHIM ACTA B*** 109: pp. 52-59. (2015)

4. Laczai N, Péter Á, Kovács L, Bencs L, Lorincz E: Synthesis and characterization of $Y_2(SiO_4)O$:Ce with LiF and NaF additives. ***SOLID STATE SCI*** 45: pp. 23-29. (2015)

5. Lengyel K, Péter Á, Kovács L, Corradi G, Pálfalvi L, Hebling J, Unferdorben M, Dravecz G, Hajdara I, Szaller Z, Polgár K: Growth, defect structure, and THz application of stoichiometric lithium niobate. ***APPL PHYS REV*** 2:(4) Paper 040601. (2015)

6. Mandula G, Kis Zs, Lengyel K: Real-time dynamic calibration of a tunable frequency laser source using a Fabry-Pérot interferometer. ***REV SCI INSTRUM*** 86:(12) Paper 123104. 5 p. (2015)

7. Ryba-Romanowski W, Lisiecki R, Beregi E, Martín IR: Spontaneous and stimulated emission in Sm^{3+}-doped YAl_3 $(BO_3)_4$ single crystal. ***J LUMIN*** 167: pp. 163-166. (2015)

8. Unferdorben M, Szaller Z, Hajdara I, Hebling J, Pálfalvi L: Measurement of Refractive Index and Absorption Coefficient of Congruent and Stoichiometric Lithium Niobate in the Terahertz Range. ***J INFRARED MILLIM TE*** 36:(12) pp. 1203-1209. (2015)

Article in Hungarian

9. Szaller Zs, Tichy-Rács É: Ultraibolya tartományban működő nemlineáris optikai egykristályok. ***TERMÉSZET VILÁGA*** 146:(3) pp. 121-124. (2015)

Conference proceeding

9. Laczai N, Bencs L, Péter Á, Kovács L: Polikristályos ittrium-oxi-ortoszilikát előállítása és elemanalitikai vizsgálata (Preparation and analytical study of polycrystalline yttrium-oxi-orthosilicate, in Hungarian). In: Magyar Kémikusok Egyesülete 2. Nemzeti Konferencia, Hajdúszoboszló, Hungary, 31.08.2015. – 02.09.2015. Budapest: MKE, p. n.a..

WIGNER DATACENTER

Gábor Pető, Kármen Almási, Balázs Bagó, Péter Bányai, Ferenc Cseh, László Erdélyi, Szabolcs Hernáth, Ildikó Kovács, Miklós Madurovicz, Viktória Mészáros, Dezső Mihalovics, Imre Molnár, Zoltán Nagy, János Sajben, Domokos Szabó, Péter Szabó, Balázs Szentiványi, Gábor Szentiványi, Ferenc Török, Endre Tóth, Ágnes Vona

Operation. — When the construction of the Wigner Datacenter was completed in 2013 it became necessary to conclude operational support contracts because of the expiry of the comprehensive warranty. The new contracts resulted in the involvement of three new partner companies.

Outstanding results. — The operation of the IT capacity, which has been continuously increasing since January 2013, as well as the efficiency of the staff play important roles in ensuring partners' satisfaction: **the confirmed availability** of the Datacenter infrastructure for 2015 was **99.998%**, more than the 99,990% undertaken in the contracts. The successful work of the Datacenter is confirmed by the fact that the hosting contract, which was to be in force till the end of 2015, was extended by CERN, the biggest user of the Datacenter for another year as early as May instead of the due date in October.

It is the mission of the Datacenter to launch further high value-added services. In the first half of 2015 the IT devices ensuring the capacity of the **Wigner Cloud were installed** (close to 1000 processor cores and 1 PB of raw storage capacity), later, in the second half of the year the construction of **OpenStack-based cloud was started**, followed by the operational tests and trial operation, so that by the end of the year it got to the phase of "real-life-like" testing. At the same time the acquisition of a flexibly scalable tape storage unit was concluded, which will be available for the research projects in the first phase with 1.5 PB capacity and direct expandability to 6 PB.

In May 2015 we managed to win the support of the Academy for the realization of the **MTA Cloud**. The project aims to set up an OpenStack-based cloud federation with the participation of MTA SZTAKI (Institute for Computer Science and Control), under the leadership of the MTA Wigner RCP Datacenter.

The role of CLOUD in research support. — Nowadays it has become a necessity to use cloud configurations for storing large amounts of data generated during research, or for performing complex, memory-hungry compute-intensive tasks. Their role is crucial for scientists so they could devote all their attention to their research projects exclusively; they do not have to care about time-consuming tasks like purchasing equipment that becomes obsolete over the time. Clouds can be used in a leasing agreement as needed for running research calculations, or for storing big data. There is no need to pay for even one extra minute when using the service, so the costs can be planned and calculated accurately. Its usage is not restricted to any fixed location, so it may become essential in large-scale domestic and international consortium-type collaborative research projects (eg. Horizon 2020).

Important events. — After serious preparatory work the **MTA Cloud** was finally presented on May 11, 2015 to the more than 250 participants in the Ceremonial Hall of the Hungarian Academy of Sciences Headquarters. The participants received users instructions illustrated with practical examples. After the presentations researchers and IT professionals had the opportunity to ask their questions and formulate suggestions concerning the design and the usage of the cloud service. The outstanding level of participation is partly due to the wide-range needs assessment. Sent out questionnaires were filled out by more than 260 researchers, helping the long-term work of the project team with their constructive proposals. This fact also proved the high level of interest.

On April 21, 2015 at the Budapest University of Technology and Economics Gábor Pető, head of the Datacenter and Szabolcs Hernáth, manager responsible for the IT services gave presentations to participants of the XII. Simonyi Conference. Gábor Pető spoke about the **infrastructure and operation of the TIER-0 Datacenter,** which started its operation two years ago with the highest cutting-edge technology of its class, while Szabolcs Hernáth presented the cloud concept - its scope of usage and its benefits – and about the Wigner Cloud under construction at that time.

On October 15, 2015, also within the framework of Simonyi's Day Gábor Pető presented the Wigner Cloud to the Wigner RCP staff. During the course of this interactive demonstration Mr Peto answered the questions of the interested audience, going into a few practical details.

On October 13, 2015 Szabolcs Hernáth also held a presentation concerning the 3-year experience of operation of the Wigner Datacenter at the Brookhaven National Laboratory in Upton (New York) at the HePIX (High Energy Physics Information eXchange) workshop.

Consequential impacts. — During the past year a large number of high-level domestic and foreign delegations and senior officials visited the Wigner Datacenter. In addition to the visit of Csaba Kőrösi, leader of the Environmental Sustainability Directorate of the President's Office, we should also mention the visit of Mr. Xiao QIAN, Chinese Ambassador, Mr. Mahmoud Vaezi Joze, Iranian Minister of Infocommunication, and Mr. Ahmed Berbar, Algerian Deputy Minister of Information. The outgoing Director General of CERN, Prof. Rolf-Dieter Heuer and Mr. Wayne Salter, leader of the CERN IT computing facilities group also visited the Datacenter. The Datacenter accommodated for the 2015 autumn meeting of the EIROforum workteam, organized by Mr. Frederic Hemmer, the Head of CERN's IT Department. In addition to all the above, in 2015 the Wigner Datacenter hosted Polish, Vietnamese, Bulgarian and Romanian delegations, representatives of multinational corporations and international bodies as well. The Datacenter took an important role in conducting of several events, such as the CERN-Wigner Open Days, GPU Days, Girls' Day opening ceremony, events of the IT, Telecommunications and Electronics Enterprises Association (IVSZ. In the autumn, a group of students from Lausanne also had a chance to gain an insight to the operation of the Datacenter.

THE RESEARCH LIBRARY

Anikó Kutnyánszky, Andrea Harsányi, Emese Szabó, Ilona Verle, Szabolcs Bálint

The library's main task is to provide information resources and materials for 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 RCP.

On 31 December 2015, the stock of the library consisted of 66720 print monographs and conference proceedings, 65 electronic books with remote access, 41099 periodical/journal issues and 40 893 research reports. In 2015 we had a subscription for 76 periodical titles (49 print and 27 online) and there were 69 monographs (print books) and 1 e-book added to the collection. From the newly acquired materials 29 were purchased, and 41 items were donated.

During the year a total of 117 books were sorted out from the collection, out of which 6 copies were donated to other libraries. The duplicate copies of periodicals were also offered to partner libraries, and 3 volumes were donated.

Within inter-library loan services 123 library items were provided to our library users and we fulfilled 51 document requests from other libraries and external partners. In 2015 we had a network of 21 partner institutes in Hungary and abroad.

The library has its own website, which is accessible to the general public, except for the subscription-based contents that are only available for the academic staff.

In 2012 we started a revision process of the library stock to take inventory. In the first phase the items on loan were checked, which was finished by the end of 2013. Unfortunately, the work had to be suspended due to changes in the number of the library staff. From November 2015 the process was continued with the revision of non-circulating items and reference materials. A total of 3208 items were checked and this part of the work was closed by the end of the year. We will go on with revising the circulating books, the biggest part of the stock, which is scheduled to be started in January 2016.

We also continued to build the online catalogue like the previous years. 100% of the reference materials in the reading-room were processed in the first half of 2015, and additional 834 records were added to the catalogue within retrospective conversion during the year.

In the fall of 2015 Wigner Cloud storage service was launched, which makes it easier for us to share and manage our files, registers and records, thus contributing to a more efficient library service.

Like in 2014, a training session was held again in September 2015 for 8 participants. Our aim is to familiarize new researchers and scholars of the institutes with the library and its services, emphasizing the use of online search tools and academic databases.

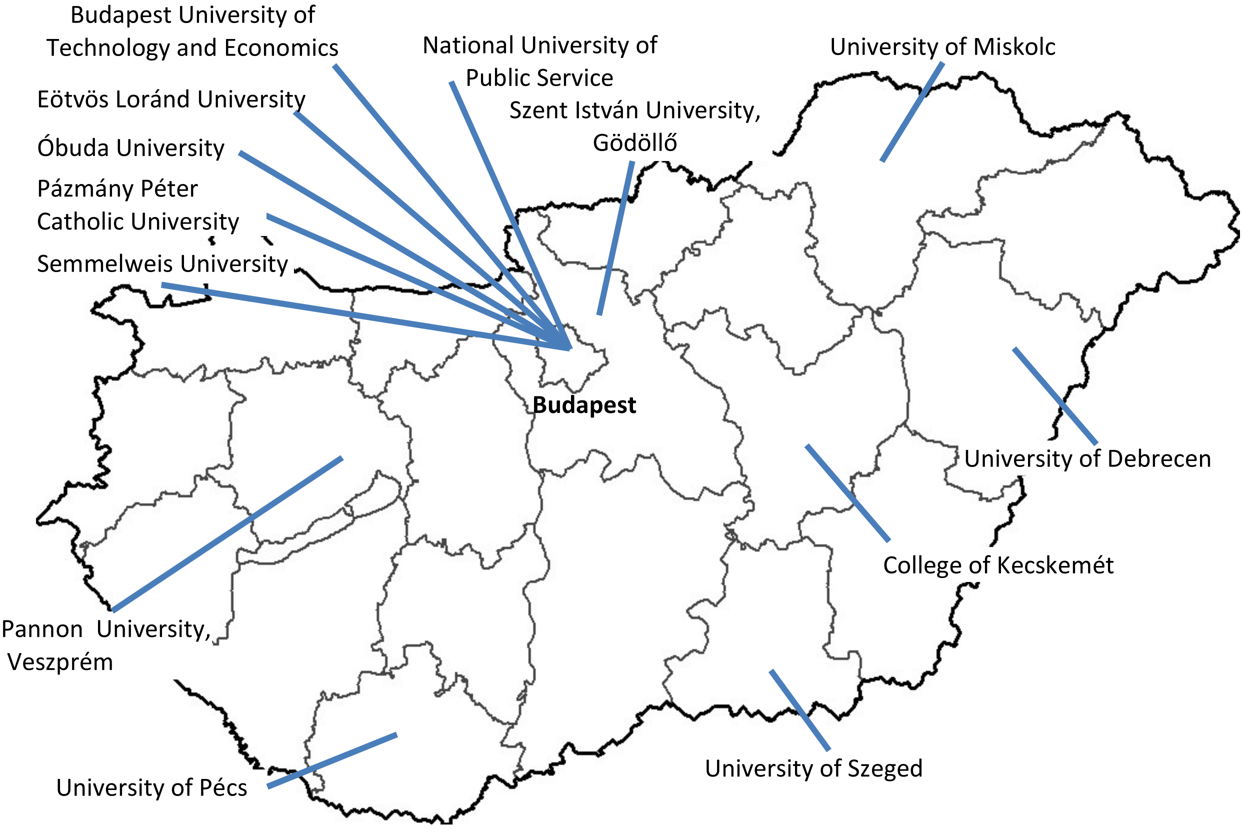
2 new librarians joined our team in May and October, so we are currently a staff of 5, like in the good old days. Two of our colleagues have successfully completed a web-editing training and a course on "Bibliometric methods – how to measure science", respectively.

Members of the library team participated in 13 professional events and conferences. The 10th IGeLU (International Group of Ex-Libris Users) conference was held in Budapest on 2-5 September 2015. As we use the Aleph Library Management System in our library, we were interested and involved in this event, and one of our colleagues volunteered in the conference organizing team.

It was our pleasure to invite some colleagues from the Library of the Alfréd Rényi Institute of Mathematics, HAS, to visit us at the end of the year. Besides sharing our experiences and best practices in the form of a colloquial meeting, the guests were shown around the whole campus and visited the nuclear research reactor at the Centre for Energy Research and the laser laboratory at the Institute for Solid State Physics and Optics.

SUPPLEMENTARY DATA

Education



Graduate and post-graduate courses

Eötvös Loránd University, Budapest

- Algebraic Bethe Ansatz and its applications (F. Woynarovich)
- Algebraic quantum field theory (P. Vecsernyés)
- Applications of synchrotron and neutron radiation for structural studies (G. Vankó)
- Cognitive neuroscience, (L. Négyessy)
- Computational neuroscience (Z. Somogyvári)
- Electrodeposition of metals (L. Péter)
- Electrons in solids (I. Tüttő)
- Integrable quantum field theories (Z. Bajnok)
- Introduction to general relativity (M. Vasúth)
- Introduction to gravitation and high energy physics (M. Vasúth)
- Introduction to gravitational theory and high-energy physics (G.G. Barnaföldi, M. Vasúth, BSc/MSc)
- Investigation of the inner structure of compact stars (G.G. Barnaföldi)
- Low temperature plasma physics (Z. Donkó)
- Macromolecules (S. Pekker)
- Many-body problems I-II. (G. Szirmai)
- Modeling the neural system (G. Orbán)
- Modern solid state physics (I. Tüttő)
- Nanomagnetism (J. Balogh)
- Nanophase metals (I. Bakonyi)

- Neutron physics (M. Márton)
- Neutron techniques - part of the material science course (L. Rosta)
- Nuclear solid-state physics I-II (D.L. Nagy)
- Optics and relativity theory (Gy. Dávid and J. Cserti, D. Varga)
- Physics of jets (P. Lévai)
- Pattern formation in complex systems (Á. Buka and T. Börzsönyi)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Quantum electrodynamics in resonators (J. Asbóth)
- Selected topics in experimental high-energy physics (F. Siklér, A.J. Zsigmond, D. Varga, G. Hamar, A. László)
- Solid state physics (J. Sólyom)
- Statistical learning in the neural system (G. Orbán, M. Bányai, D. Nagy, M. Gaspar)
- Superconductivity (I. Tüttő)
- The phase-structure of the strongly interacting matter (P. Lévai)
- Theory of open quantum systems (L. Diósi)
- Topological insulators (J. Asbóth)

Budapest University of Technology and Economics

- Astrophysics 1 (K. Szegő)
- Coherent control of quantum systems (Z. Kis)
- Group theory in solid state physics (Gy. Kriza)
- Infrared and Raman spectroscopy (K. Kamarás)
- Introduction to fusion plasma physics (S. Zoletnik)
- Introduction to superconductivity (Gy. Kriza)
- Introduction to theoretical plasma physics (A. Bencze)
- Lectures on category theory (G. Böhm)
- Low temperature plasma physics (Z. Donkó)
- Magnetohydrodynamics in low dimensional systems (A. Bencze)
- Modern solid state physics (A. Virosztek)
- Neutron physics (M. Márton)
- Physics of the heliosphere (G. Erdős)
- Spectroscopy and the structure of matter (K. Kamarás)
- Theoretical solid state physics (A. Virosztek)
- Theory of magnetism II. (A. Virosztek)
- Trends in material science (Á. Gali)
- Variational methods in the basics laws of physics (T.S. Biró, MSc BME)

Óbuda University, Budapest

- Chemistry and physics of polymers (S. Pekker)

Semmelweis University, Budapest

- Complexity of the brain (P. Érdi)
- Neocortex: from structure to function, (L. Négyessy)
- Neuroelectricity (Z. Somogyvári)

Szent István University Gödöllő

- Biophyics (Z. Szőkefalvi-Nagy, both in Hungarian and in English, two courses)

University of Debrecen

- Experimental particle physics (D. Horváth)

University of Pécs

- Biorobotics, (J. Laczko)
- Control systems (J. Füzi)
- Digital control (J. Füzi)
- Electronics (J. Füzi)
- Introduction to quantum optics (T. Kiss)
- Linear algebra (I. Márton)
- Mathematics I., (J. Laczko)
- Mathematics II, (J. Laczko)
- Neuroinformatics (J. Laczkó)
- Numerical methods (P. Ádám)
- Open quantum systems (P. Ádám)
- Probability theory (B. Nagy)
- Probability theory (P. Ádám)
- Resonant light-matter interaction (P. Ádám)
- Statistical physics (K. Szlachányi)
- Stochastic processes in the economy (P. Sinkovicz)
- Theoretical mMechanics (K. Szlachányi)
- Theoretical physics III. (P. Ádám)
- Theory of control and regulation, (J. Laczko)

University of Szeged

- Applications of statistical physics (F. Iglói)
- Calculus for informatics students (G. Pusztai)
- Calculus I for physics students (G. Pusztai)
- Calculus II for physics students (G. Pusztai)
- Disordered systems (F. Iglói)
- Introduction to the physics of laser plasmas (I.B. Földes)
- Introduction to statistical physics (F. Iglói)
- Linear algebra for physicists (L. Fehér)
- Linear spaces and operators (G. Pusztai)
- Quantum field theory (L. Fehér)
- Symmetries in physics (L. Fehér)
- Statistical physics (F. Iglói)

University of Physical Education

- Special biomechanics (B. Újfalussy, TE)

Others

- Artificial intelligence, Milestone Institute (Orbán G.)
- Life science journal club and seminar, MTA Wigner RCP, Budapest (M. Bányai, M. Gáspár, D. Nagy, G. Orbán)
- Neural computation, BSCS (M. Bányai)
- PATTERN study group, MTA KOKI, Budapest (G. Orbán)
- Statsitics and the brain, BSCS, Budapest (G. Orbán)

Laboratory practices and seminars

Eötvös Loránd University, Budapest

- Differential equations (T. Gombor)
- Graphical processors for scientific applications (D. Berényi and M.F. Nagy-Egri)
- Experiments on liquid crystals (Á. Buka, N. Éber, P. Salamon)
- Laboratory course in general chemistry (G. Bazsó)
- Laboratory course in inorganic chemistry (G. Bazsó)
- Laboratory practice in solid state physics and materials science (M. Bokor)
- NMR and Cherenkov photometry, nuclear analitics laboratory (P. Pósfay)
- Nuclear techniques & X-ray spectroscopy (Z. Németh)
- Particle and nuclear physics detectors laboratory (G. Hamar, D. Varga, coordinated by M. Csanád)
- Raman spectroscopy, part of the biophysics laboratory practice (M. Veres)
- The theory of C++ programming (Sz.M. Harangozó)

Budapest University of Technology and Economics

- Biomedical computing practices (B. Sódor)
- Chemical and biomedical measurement technology (B. Sódor)
- Engineering thermodynamics 2 (R. Kovács)
- Infrared and Raman spectroscopy (K. Kamarás)
- Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (K. Lengyel)
- Introductory physics (D. Szemes)
- Introductory physics (A. Csóré)
- Laboratory practice (M.A. Kedves, B. Raczkevi)
- Laboratory practice in chemistry (Gy. Károlyházy)
- Laboratory practice in physics (G. Thiering, B. Somogyi)
- Physics 2i (D. Szemes)
- Physics II. practice (G. Thiering)
- Raman spectroscopy, part of the course experimental methods in materials science (M. Veres)
- Small-angle neutron scattering - part of the neutron methods laboratory practice (A. Len, L. Almásy)
- Thermal physics, mechatronics (P. Ván)
- Thermodynamics and heat transfer (R. Kovács)

College of Kecskemét

- Quantum mechanics (V. Ivády)

University of Pécs

- Linear algebra (J. Laczko)
- Mathematical methods in physics IV. (P. Ádám)
- Mathematics I., (J. Laczko)
- Mathematics II. (J. Laczko)
- Neuroinformatics (J. Laczko)
- Statistical physics (K. Szlachányi)
- Theoretical mechanics (K. Szlachányi)

University of Szeged

- BSc laboratory project practice (I.B. Földes)
- Calculus for informatics students(G. Pusztai)
- Calculus I for physics students (G. Pusztai)
- Calculus II for physics students(G. Pusztai)
- Linear spaces and operators (G. Pusztai)
- Summer practice, KrF laser-plasma interactions (I.B. Földes)

IPP Prague

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

Mirrotron Ltd

- Backgrouds of neutron science (M. Markó)
- Optimization of the neutron guide (M. Markó)
- Polarization systems for neutron instruments (J. Füzi)

Diploma works

Eötvös Loránd University, Budapest

- G. Balassa, Multiple Scattering in High-Energy Heavy Ion Collisions (Supervisor Gy. Wolf)
- K. Boros: Electrodeposition of nickel-cadmium alloys (Supervisors: L. Péter and K. Neuróhr)
- G. Bíró: Application of New-generation High-energy Detector Simulators for the Investigations of Identified Hadron Spectra (G.G. Barnaföldi)
- D. Englert, Study of particle correlations in high-energy p-Pb collisions with the CERN-CMS experiment (Supervisors: F. Siklér and G.I. Veres, MSc)
- V. Fisch, Testing of a front-end electronics for the CMS Phase 1 Pixel detector (Supervisor V. Veszprémi, MSc)
- A. Fülöp: Network models of cerebral cortex interactions (Supervisor: L Négyessy, Msc)
- G. Galgóczi (Supervisor: G. Hamar, D. Varga, BSc)

- D. Herrmann: Interpretation of temperature at different atmospheric heights (Supervisor: A. Opitz)
- R. Haminda, Thymosin-β4 and stabilin: hydration and molecular interaction in aqueous solution. (Supervisors M. Bokor and A. Perczel, BSc)
- B. Kacskovics, Spin dependence of gravitational waveforms from pulsar OJ287 (Supervisor: M. Vasúth, BsC)
- K. Kapás (Supervisor: G. Hamar, D. Varga, BSc)
- Sz. Karsai, Investigation of Compact Star Interior (G.G. Barnaföldi)
- G. Kasza: Investigation of the direct photon spectra of high-energy heavy ion collisions (BSc, Supervisor: T. Csörgő)
- A. Kherlenzaya: Preparation and properties of magnetic nanoswires (Supervisor: I. Bakonyi)
- E.B. Kiss (Supervisor: G. Orbán)
- Z. Laczkó, The complete solution of the boundary Lee-Yang model, (supervisor: Z. Bajnok)
- J.E. Maróti, Forecasting gravitational waves (Supervisor: M. Vasúth, BsC)
- D. Molnár Investigation of the properties of high entropy alloys by ab initio calculations (Supervisor: L.K. Varga)
- B. Nagy: Analysis of the data from the Rosetta space mission (Supervisor: K. Szegő)
- G. Németh: Investigation of nanostructures by near-field infrared spectroscopy
- L. Oláh: Synthesis and characterization of self-assembly supramolecular gold(I) complexes, Diploma work 2015 (Supervisor: A. Deák)
- K. Szabó: Planetary space weather at Mars (Supervisor: A. Opitz)
- L. Vanó, Edge plasma turbulence studies utilizing beam emission spectroscopy on MAST, (Supervisor: D. Dunai)
- J. Város, The Δ-decay in Effective Field Theories (Supervisor P. Kovács)
- Á. Vida, Preparation and investigation of high entropy alloys (Supervisor: L.K. Varga)

Budapest University of Technology and Economics

- D. Iván, Measurement of diffusion in aqueous solutions of proteins. (Supervisors M. Bokor and F. Simon, MSc)
- R. Kovács, The Thermodynamical Assumption of Wave-transport, -dispersion, and -absorption (P. Ván)
- Á. D. Major, Determination of pKa values for silicon carbide nanoclusters (Supervisor: Á. Gali, BSc)
- D. Nagy, Numerical modelling of red blood cells (Supervisor E. Somfai, BSc)
- G. Nyitrai: High-resolution quality control system for particle detectors. (Supervisor: D. Varga, Bsc)
- Zs. Szendi, Classical Electrodynamics and Hydrodynamics (Supervisors T.S. Biró and G. Takács)
- M. Timár, Investigation of low energy optical properties of a π-conjugated polymer, (Supervisor: Ö. Legeza, G. Barcza)
- L. Zsuga, Study of ELM related MHD activities (Supervisor: S. Zoletnik)

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 (Supervisor: R. Szipőcs)

University of Pécs

- O. Csetényi, Electronic supplement for the Chapter "Energy" of the OFI physics textbook for 9th graders (Supervisor P. Ádám)
- I. Horváth, Electronic supplement for the Chapter "Motion" of the OFI physics textbook for 9th graders (Supervisor P. Ádám)
- A. Szám, Periodic single-photon sources (Supervisor P. Ádám)
- M. I. Janecska, Traveling-wave realization of the non-classical states of light (Supervisor P. Ádám)
- K. Varga-Umbrich: Study of coherent excitation and ionization of alkali atoms by strong laser pulses. (Supervisor M.A. Kedves)

University of Szeged

- Á. Bálind, Tensor calculus with mechanical applications (Supervisor: G. Pusztai)
- Zs. Kovács, Investigation of plasma mirror arrangements (Supervisor: I.B. Földes)

Széchenyi István University of Győr

- Sz.J. Balogh: Preparation of external networks of muon tomographs for monitoring volcanic activity. (Supervisor: G. Hamar, MSc)

Ph.D students

Eötvös Loránd University, Budapest

- K. Bajnok, 5-7th century pottery production in transdanubia (Supervisors: L. Rosta, T. Vida and Gy. Szakmány)
- D. Barta, Dispersion of gravitational waves in interstellar media (Supervisor: M. Vasúth)
- G. Bazsó, Structural investigation of biomolecules by matrix isolation and laser techniques experiment (Supervisor: Gy. Tarczay)
- G. Bíró, Investigation of particle production in high-energy heavy ion collisions (Supervisors: G.G. Barnaföldi and G. Papp)
- G. Csire, Quasiparticle spectrum of superconductor-normal metal heterostructures (Supervisor: B. Újfaussy)
- K.Z. Csukás, Initial value formulation of general relativity (Supervisors: I. Rácz)
- Z. Darázs, Quantum control with measurements (Supervisor: T. Kiss and A. Csordás)
- M. Dolgos, Diffusion study in metastable phases (Supervisor: L. Bottyán)
- A. Dombi, Quantum dynamics of atomic motion in multimode optical resonator fields (Supervisor: P. Domokos)
- T. Gombor: Holography and the gauge gravity duality (Supervisor: Z. Bajnok)
- Sz.M. Harangozó, High-momentum nuclear effects in heavy ion collisions at CERN LHC (Supervisors: G.G. Barnaföldi and G. Papp)

- L. Holló, The AdS/CFT correspondence (Supervisor: Z. Bajnok)
- G. Homa: Quantum information and irreversibility (Supervisor: L. Diósi)
- M. Horváth, Generalized Boltzmann equation (Supervisors: A. Jakovác and T.S. Biró)
- Sz. Karsai, Investigation of the strongly-interacting matter in compact stars (Supervisors: G.G. Barnaföldi and E. Forgács-Dajka)
- G. Kiss, Microstructure gaseous particle detectors (Supervisor: D. Varga)
- J. Konczer: Integrable methods in the AdS/CFT correspondence (Supervisors: Z. Bajnok, Á. Hegedűs)
- G. Kónya, Many-body physics in cavity QED (Supervisor: P. Domokos)
- B. Korbuly: Phase-field modeling of complex polycrystalline patterns (Supervisor: L. Gránásy)
- N. Laczai: Preparation and study of polycrystalline scintillator materials (Supervisor: L. Bencs)
- P. Magyar, Response functions and collective excitations of strongly coupled plasmas (Supervisor: Z. Donkó)
- K. Márton, Ultrarelativistic hadron-nucleus collisions at the CERN SPS (Supervisors: A. László and D. Varga)
- D. Molnár, Investigation of high entropy alloys (Supervisor: L. Varga)
- D. Nagy: Normative model of episodical memory (Supervisor: G. Orbán)
- M.F. Nagy-Egri, Numerical solutions of Einstein equations (Supervisor: I. Rácz)
- F.J. Nemes Elastic scattering of protons at the TOTEM experiment at the LHC (Supervisors: T. Csörgő and M. Csanád)
- K. Németh, Chemical modification and optical spectroscopy of single-walled carbon nanotubes (Supervisor K. Kamarás)
- É. Oláh, Particle physics teaching in secondary school (within the Teacher's PhD program of ELTE, Supervisors: D. Horváth and D. Varga)
- É.M. Oláh: Teaching particle physics in high school (Supervisor: D. Horváth)
- L. Oláh, Identified particles by ALICE HMPID (Supervisors: G. G. Barnaföldi, D. Varga)
- L. Oláh, Research and development of particle detectors for muon tomography and the ALICE experiment (Supervisors: G.G. Barnaföldi and D. Varga)
- P. Pósfay, Functional renormalization group method for the description of compact stars (Supervisors: G.G. Barnaföldi and A. Jakovác)
- L. Rátkai: Dynamics of crystalline self-organization within continuum theory (Supervisor: T. Pusztai)
- D. Réfy, H-mode pedestal studies with beam emission spectroscopy diagnostics (Supervisor: S. Zoletnik)
- B. Szabó, Shear zones in dry granular materials (Supervisor: T. Börzsönyi)
- B. Török: Learning of temporal processes (Supervisor: D. Németh, G. Orbán)
- É. Tichy-Rács: Synthesis, crystallization and spectroscopic investigation of rare-earth alkali borate scintillator materials (Supervisor: K. Lengyel)
- M. Timár: Investigation of strongly correlated systems by renormalization methods and approximation of high-dimension fields by tensor factorization (Supervisors: Ö. Legeza, G. Barcza)
- R. Ünnep, The ultrastructure and flexibility of thylakoid membranes in different photosynthetic organisms as revealed by small angle neutron scattering (Supervisors: L. Rosta and Gy. Garab)

- T. Verebélyi, NMR and DSC study of protein solutions (Supervisor: K. Tompa)
- M. Verebélyiné Dósa: Space weather at the inner planets (Supervisor: G. Erdős)
- Á. Vida, Preparation, investigation and application of high entropy alloys (Supervisor: L. Varga)
- A.J. Zsigmond, Measurement of Z boson production in heavy ion collisions with the CMS detector at the LHC (Supervisors: F. Siklér and G.I. Veres)
- S. Zsurzsa, Doctoral school of physics (Supervisor: I. Bakonyi)

Budapest University of Technology and Economics

- P. Balla, Optical properties of magnetic materials (Supervisor: K. Penc)
- D. Beke, Synthesis and analysis of silicon carbide based nanoclusters (Supervisor: Á. Gali)
- B. Botka, Optical and Raman spectroscopy of carbon nanotube based hybrid materials (Co-supervisor: K. Kamarás)
- D.R. Cserpán: Estimation of input signals based on multielectrode array measurements, Doctoral School of Informatics (Supervisor: Z. Somogyvári)
- A. Gilyén, Dynamics and control of quantum networks (Supervisor: T. Kiss)
- D. Iván, Magnetic field types, pulse combinations, and their solid-state NMR-spectrometric applications in living material science. (Supervisors: M. Bokor and F. Simon)
- Gy. Károlyházy, Controlled generation of point defects in silicon carbide (Supervisor: Á. Gali)
- M. Lampert, Turbulent and zonal flow studies in fusion plasmas (Supervisor: S. Zoletnik)
- F. Podmaniczky: Dynamics of solidification, pattern and defect formation in phase-field crystal theories (Supervisor: L. Gránásy)
- L. Rózsa, Exotic magnetism in thin films (Supervisor: B. Újfalussy)
- B. Somogyi, Semiconductor biomarkers for biological imaging: A first principles study (Supervisor: Á. Gali)
- A. Szakál, Investigation of application possibilities of atomic resolution neutron holography (Supervisor: L. Cser)
- T. Szarvas, Wave propagation and modelling of quantum optical processes in structured dielectric media (Supervisor: Z. Kis)
- D. Szemes: Dynamics of light-activated functional molecules studied with ultrafast spectroscopy (Supervisor: Gy. Vankó)
- 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 (Supervisor: L. Cser)

Linköping University, Sweden

- V. Ivády, Investigation of point defects for quantum bit applications (Supervisor: Á. Gali)

National University of Public Service

- P.G. Vizi, Micro- and nano-robots of war, aerospace and security technology

Óbuda University, Budapest

- J. Nagy, Development of small satellites in the Earth's environment carrying onboard scientific measurements and data acquisition system (Supervisor: A. Molnár)

Paderborn University, Germany

- S. Arceiz Casas: EPR characterization of crystal defects for quantum optical applications (Co-supervisor: G. Corradi)

Pázmány Péter Catholic University, Budapest

- B. Jákli: Control of biomechtronic robotic arm (Supervisor: L. Négyessy)
- A. Valy: Neuromorph control of limb movements (Supervisor: J. Laczko)

Semmelweis University, Budapest

- M. Ashaber: First steps of tactile cortical processing in primates (Supervisor: L. Négyessy)
- Zs. Benkő: Exploring causality for understanding dynamical behaviour of cortical areas based on multichannel electrode system measurements (Supervisor: Z. Somogyvári)
- P. Katona (Supervisor: J. Laczko)
- E. Pálfi: The role of somatosensorycortical inhibition in tactile functions of primates (Supervisor: L. Négyessy)

Szent István University Gödöllő

- T. Baross, The application of the hot isostatic pressing (HIP) welding for fusion reactor conditions (Supervisor: G. Veres)

University of the Basque Country (UPV/EHU)

- G. Vitagliano, Spin squeezing, macrorealism and the Heisenberg uncertainty principle (Supervisor: G. Tóth)

University of Debrecen

- M. Bartók, Search for supersymmetry at the Large Hadron Collider (Supervisor: V. Veszprémi)
- J. Karancsi, Search for new particles beyond the Standard Model (Supervisor: V. Veszprémi)

University of Jyväskylä, Finnland

- M. Vargyas (Supervisors: J. Rak, T. Csörgő)

University of Lund, Sweden

- A. Ster (Supervisors: B.Lörstad, L. Lönnblad and T. Csörgő)

University of Pécs

- M. Aladi, High harmonic generation from atoms and clusters (Supervisor: I.B. Földes)
- R. Bolla, Diagnostics of noble gas clusters (Supervisor: I.B. Földes)
- F. Bódog, Optimalization of periodic single-photon sources (Supervisor: P. Ádám)

- V. Csajbók, Inducing ultrafast currents in dielectrics (Supervisor: P. Dombi)
- A. Kerekes, Development and application of optical measurement methods for the investigation of the deposition of aerosols in the human airways (Supervisor: A. Nagy)
- B. Kollár, Quantum information in quantum-optical networks (Supervisor: T. Kiss)
- I. Márton, Ultrafast photoemission from plasmonics structures (Supervisor: P. Dombi)
- G. Mogyorósi, Traveling-wave realization of non-classical states (Supervisor: P. Ádám)
- E. Molnár, Realization of non-classical quantum states with superposition of coherent states (Supervisor: P. Ádám)
- B. Nagy, Controlling photoelectrons on the nanoscale with plasmonic nanoparticles (Supervisor: P. Dombi)
- M. Posai, (Supervisor: I.F. Barna)
- P. Sinkovicz, Simulation of quantum lattice models with ultracold gases (Superviso:r G. Szirmai)
- Á. Varga, Quantum measurement with maximal information (Supervisor: P. Ádám)

University of Szeged

- T.F. Görbe, Thesis to be defended in 2016 (Supervisor: L. Fehér)
- D. Haluszka: Assessing the application possibilities in dermatologyand potential risks of pulsed lasers used in nonlinear microscopy (Supervisors: N. Wikonkál and R. Szipőcs)
- L. Himics, Nanocrystalline diamonds for advanced applications (Supervisor: M. Koós)
- Zs. Kovács, Laserplasma interactions with KrF lasers (Supervisor: I.B. Földes)
- I. Rigó, Preparation and characterization of plasmonic diamond-gold nanostructures (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

M. Ashaber, A tapintás kérgi feldolgozásának első lépései főemlősökben (First steps of tactile cortical processing in primates), 118p, 2015

É. Bajnóczi, Chemistry of some amphoteric cations (Sn^{2+}, Pb^{2+}, Cr^{3+}) in hyper-alkaline aqueous solutions, 77p, 2015 (DOI: 10.14232/phd.2561)

G. Barcza, Nonlocal density matrix renormalization group applied to strongly correlated systems, 129p, 2015

A. Barna, Ultrarövid, ultraibolya lézerimpulzusok és magas harmonikusok diagnosztikája (Diagnostics of the ultrashort, ultraviolet laser pulses and high harmonics), 96p, 2015.

D. Haluszka: A nemlineáris mikroszkópiában használt impulzusüzemű lézerek diagnosztikai célú felhasználása és potenciális egészségügyi kockázatainak vizsgálata (Assessing the application possibilities in dermatology and potential risks of pulsed lasers used in nonlinear microscopy), 86p, 2015

G. Hamar, Nagy impulzusú részecskék vizsgálata nehézionütközésekben (Investigation of high momentum particles in heavy ion collisions), 120p, 2014

B. Kollár, Disorder and entropy rate in discrete time quantum walks. 154p, 2015, http://fizphd.ttk.pte.hu/vedes/BKdissertation.pdf

A.Zs. Kovács, Erősen csatolt sokrészecskerendszerek kollektív dinamikája (Collective dynamics of strongly coupled many-particle systems), 100p, 2015

E. López-Centella, Quantization of categories: weak bialgebras and weak multiplier bialgebras, 224p, 2015.

F. Nemes, Elastic scattering of protons at the TOTEM experiment at the LHC, 124p, 2015, (http://cds.cern.ch/record/2131667?ln=en)

M. Pápai, Theoretical characterization of electronic states of iron complexes, 152p, 2015 (DOI: 10.15476/ELTE.2014.003)

B. Szabó, Shear zones in dry granular materials, 109p, 2015

K. Szász, Ponthibák azonosítása félvezető szerkezetekben hiperfinom tenzor számításával (Identification of point defects in semiconductors by calculating the hyperfine tensor), 119p, 2015

Zs.Szekrényes, Study of complex nanostructures by infrared spectroscopy, 115p, 2015.

B. Tál: Measurement of transient events in hot magnetized plasmas, 197p, 2015.

Memberships

L. Almási
- Member of the Editorial Board of New Frontiers in Chemistry Journal (Timisoara, Romania)

A. Arató
- National contact of the Association for the Advancement of Assistive Technology in Europe (AAATE)
- Program committee member of the International Conference on Computers Helping People with Special Needs (ICCHP)

P. Ádám
- Member of the Laser Physics Committee of MTA.

K. Bajnok
- Member of the Geochemical, Petrographical and Mineralogical Scientific Board of the Archaeological Comission of the HAS

Z. Bajnok
- Member of the ESF Holograv Steering Committee
- Member of the ESF Holograv Executing Committee
- Member of the Particle Physics Committee of the H.A.S.

I. Bakonyi
- Member of the Solid State Physics Committee of MTA (2011-2014)
- Member of the Editorial Advisory Board (from 2005), Journal of Materials Science and Technology (Bulgaria, Sofia)
- Member of the European Board (from 2006), European Academy of Surface Technology (EAST)
- Member, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
- Member of the Management Committee, COST MP 1407 action

Judit Balogh
- Int. Board on the Application of the Mössbauer Effect (IBAME), 2012-2017

József Balogh
- Member of the Particle Physics Committee of the H.A.S

G.G. Barnaföldi
- Editor of The European Physics Journal A: Hadrons and Nuclei Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
- Member of Physics PhD School at Eötvös Loránd University, Budapest
- Hungarian representative, Board Member of the CERN LHC ALICE Collaboration,
- Group Leader of the Hungarian ALICE Group
- Member of the Eötvös Loránd Physical Society (ELFT)
- Member of the European Physical Society (EPS)
- Hungarian representative, rapporteur, WG2 QCD Topic Leader of the New Compstar COST MP1304 action (2013-2017)
- IAC member of the ISOTDAQ International School on Trigger and Data Acquisition

- LOC member of the ISOTDAQ 2014 International School on Trigger and Data Acquisition 2014
- LOC member of the 7th FIKUT – Workshop of Young Researchers in Astronomy and Astrophysics 2014, Budapest
- LOC member of the CompStar 2015 Meeting, Budapest
- IAC member of the International Conference of the High-pT Physics for the RHIC/LHC Era
- Member of the general assembly of the Hungarian Academy of Sciences
- Wigner Intellectual Property Council member
- IAC member for SQM2015, Dubna, May 15, 2015.

D. Barta

- Member of the Virgo Scientific Collaboration

F. Bazsó

- Programme Committee Member, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne

L. Bencs

- Editorial Board member of ISRN Analytical Chemistry
- Member of the Work Committee for Environmental Chemistry of MTA
- Member of the Hungarian Chemical Society, Spectrochemical Division

T.S. Biró

- Vice director of MTA Wigner FK RMI (Sept.01.2013-)
- Editor-in-Chief (theory) (Oct.01.2013-) of the European Physical Journal A: Hadrons and Nuclei;
- Member of IAC for Sigma Phi 2014 (held in Rhodos, Greece)
- Member of International Advisory Board for Strangeness in Quark Matter (SQM2015 Dubna, Russia);
- Member of the Physics PhD School at TU Budapest (BME)
- Member of the Physics PhD School at Eötvös University (ELTE) Budapest
- External member of the ELTE TTK PhD Council
- Member of the Nuclear Physics Committee at the Hungarian Academy of Science
- Member of the Eötvös Loránd Physical Society (ELFT),
- Chairman of the Zimányi Foundation for Physics,
- Editor of the Wigner Yearbook 2014,
- IAC member of the Sigma Phi 2014, Rhodos
- IAC member of the SQM2015, Dubna
- LOC member of the Zimányi School 2014
- Member of Eötvös Society Council
- Member of the Presidential Publication Committee of the HAS
- Member of the Wigner Scientific Council (WTT)
- Member of the Natural Sciences Committee of the HAS, Chair of the Physics 2 section

L. Bottyán

- Member of MLZ Review Panel Magnetism and Spectroscopy, Elastic Application

G. Böhm

- Member of Expert Panel W&T1: Mathematical Sciences, Fonds Wetenschappelijk Onderzoek – Vlaanderen (Scientific Research Fund – Flanders, 2012 -- 2018)
- Member of the Scientific Committee for: New trends in Hopf algebras and tensor categories (Brussels, Belgium, June 2-5, 2015)

Á. Buka

- Electronic-Liquid Crystal Communications, Editorial Board
- International Liquid Crystal Conference, International Advisory Board
- Solid State Physics Committee of MTA, Member

G. Cseh

- Member of the Hungarian Nuclear Society

L. Csernai

- Member of the Editorial Board, International Journal of Modern Physics E - Nuclear Physics
- Member of Loránd Eötvös Physical Society
- Member of the Academia Europaea
- Member, Academia Europaea, Council
- Member of the Norvegian Scientific Academy
- Member of the Norvegian Academy for Technological Sciences

T. Csörgő

- Academia Europaea (London), elected member (2011-)
- Member, Section Committee, Physics and Engineering Sciences, Academia Europaea (2013-)
- Member, physics PhD School, ELTE, Budapest
- Member, Institutional Board, PHENIX Experiment, BNL
- Member, Executive Council, TOTEM Experiment, CERN LHC
- Member, Editorial Board, TOTEM Experiment, CERN LHC
- Member, CERN LHC Resource Review Board
- Member, International Advisory Committee, WPCF 2013 Conference, Acireale, Italy
- Member, International Advisory Committee, ISMD 2013 Conference, Chicago, USA
- Principal Investigator, PHENIX - Hungary sub-collaboration (2003-2013)
- Principal Investigator, TOTEM - Hungary sub-collaboration
- Member of the Editorial Board, TOTEM experiment at CERN LHC
- Member, Section Committee for Physics and Engineering Sciences, Academia Europaea (London)

A. Czitrovszky

- Member of the ELI_ALPS Scientific Advisory Committee
- Member of the Board of International Aerosol Association
- Member of the Board of European Aerosol Assembly
- Member of the Gesellschaft für Aerosolforschung
- Member of the International Junge Award Committee
- Chairman of the Working Group Instrumentation in EAA
- President of the Hungarian Aerosol Society

- President of the Hungarian Branch of the European Optical Society
- Head of the Optical Chapter of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology (Budapest)
- Member of the Editorial Board of “Fizikai Szemle”
- Chairman of the Optical Chapter of Roland Eötvös Physical Society
- Chairman of the Committee for the Lasers Physics and Spectroscopy in MTA
- Founding member of Ph.D. school at the University of Pécs

G. Debreczeni

- Computing Coordinator of the Virgo Collaboration (Virgo CC)
- Chair of the Virgo Data Analysis Software and Computing Group (VDASC)
- Chair of the Computing Technical Coordination Commitee (CTCC)
- Member and co-chair of the Ligo - Virgo Joint Computing Comitee (Ligo - Virgo JCC)

L. Diósi

- Member of the Management Committee of EU COST Action Fundamental Problems in Quantum Physics
- Member of the Management Committee of EU COST Action Thermodynamics in the Quantum Regime

P.Dombi

- Member of the Commitee of Laser Physics of the Hungarian Acedemy of Sciences
- International Conference on Photonic, Electronic and Atomic Collisions, ICPEAC Program Committee Member
- Conference on Lasers and Electro-optics (CLEO Europe 2015), Program Committee Member
- Journal Editor at Scientific Reports (Nature Publishing)
- Management Committee Member of the COST network “Nanospectroscopy”
- Senior Member of the Optical Society of America

P. Domokos

- Editor of the European Physical Journal D
- Liaison Committee representative of the International Union of Pure and Applied Physics (IUPAP)
- Member of the Laser Physics Committee of MTA

Z. Donkó

- Member of International Scientific Committee, Conference series “Symposium of the Phenomena in Ionized Gases”, from 2006
- Member of International Advisory Board, Conference series “Strongly Coupled Coulomb Systems”, 2007-
- Member of International Scientific Committee, Conference series “Symposium on Application of Plasma Processes,” from 2008
- Member of the Laser Physics Committee of MTA
- Member of OTKA Council on Natural Sciences and Engineering

P. Dombi

- Senior Member of SPIE (Photonics Society), USA

G. Dzsotjan

- Member of the Committee of Laser Physics of the Hungarian Academy of Sciences
- Member of the Doctor of Sciences Committee (Physics) of the Hungarian Academy of Sciences

M.F. Egri-Nagy

- Member of the Virgo Scientific Collaboration

G. Erdős

- National Representative of COSPAR
- Deputy Chairman of the Committee on Astronomy and Space Physics of HAS

N. Éber

- Member of The Open Crystallography Journal, Editorial Board
- Member of the Journal of Research in Physics, Editorial Board
- Member of the Management Committee of the COST Action IC1208

P. Érdi

- Co-Director: Budapest Semester in Cognitive Sciences
- Program co-Chair, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
- Member of the Editorial and Programme Advisory Board of the Springer Complexity publishing program
- Member of the Executive Committee of the European Neural Network Society
- Member of the Editorial Board of the Journal of Applied System Studies
- Member of the Editorial Board of the Cognitive Neurodynamics
- Associate Editor of Neurobiology
- Member of the Editorial Board of the Nonlinear Biomedical Physics Open Access Journal
- Member of the Editorial and Programme Advisory Board of the Springer Complexity Publishing Program, http://www.inns.org/Member of the Board of Governors of the International Neural Network Society
- Editor-in-Chief, Cognitive Systems Research (2015-2018)

G. Faigel

- XFEL In-kind Review Committee member
- XFEL SAC member

K. Fodor-Csorba

- Member of the Hungarian Chemical Society

L. Fehér

- Member of the international editorial board of SIGMA
- Member of the international editorial board of JNMP
- Member of the Particle Physics Committee of the H.A.S.
- Member of International Advisory Committee for: Integrable Systems and Quantum Symmetries (Prague, Czech Republic, June 23 - 27, 2015)

P. Forgács

- Member of the Particle Physics Committee of the H.A.S.
- Member of the Doctoral Council, Physics Section of the H.A.S.
- Member of the Doctoral Council, Doctoral School in Physics, Loránd Eötvös University
- National Scientific Research Fund (OTKA), Physics Panel Member

I. Földes

- Member of the Laser Physics Committee of the HAS
- Member of EPS and ELFT, also of the Laser Physics Committee of the Roland Eötvös Physical Society
- LASERLAB Europe: Users' Representative
- General Assembly member, LASERLAB Europe
- Member of COST Action MP 1208, management committee
- Substitute member of the COST Action MP 1203, management committee
- Member of the Euratom, Inertial Fusion Energy Working Group

T. Fülöp

- Member of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)

J. Füzi

- International Scientific Advisory Council of BNC (Budapest Neutron Centre)
- Editorial Board Member, Pollack Periodica
- Editor, IEEE Transactions on Magnetics, SMM21 Budapest issue
- Member of International DENIM Committee

L. Gránásy

- Member of the ESA Topical Team "Solidification of Containerless Undercooled Melts", SOL – EML
- Member of The Minerals, Metals, and Materials Society, USA
- Solid State Physics Committee of MTA
- Mathematics and Science Committee of AKT
- Elected member of the Academia Europae (London)

P. Hartmann

- Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" Member of International Scientific Committee, 2008-2014

D. Horváth

- Member of the Editorial Board of "Fizika Szemle"
- Member of the CMS Publication Committee
- Member of the IUPAP C11, Commission on Particles and Fields
- Member of the "M-T Szakbizottság"
- "INKP Kuratórium", "MTA Fiz. Osztály", "MTA Részecskefizikai Bizottság"

F. Iglói

- Science Editor – Europhysics News

J. Janszky

- Member of the Laser Physics Committee of HAS

K. Kamarás

- Editorial Board Member, European Physical Journal B

K. Kecskeméty

- Member of the Committee on Astronomy and Space Physics of HAS

Z. Kis

- Member of the Editorial Board of the Physical Review A

T. Kiss

- Member of the Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP)
- Member of the Management Committee of COST Action MP1006
- Member of the Laser Physics Committee of ELFT

G. Kocsis

- Member of the Hungarian Nuclear Society
- Member of the Nukleon Editorial Board
- Member of the EUROfusion JET CDT2 Project Board
- Member of the EUROfusion S1 Project Board
- Member of the Roland Eötvös Physical Society

L. Kovács

- Member of the Hungarian National Committee, International Union of Crystallography
- Member of the International Advisory Committee of EURODIM and ICDIM Conference series
- Member of the Program Committee of the OMEE Conference series
- Member of the Eötvös Loránd Physical Society, Atom, Molecule Physics and Quantum Electronics Division

P. Kovács

- Member of the general assembly of the Hungarian Academy of Sciences

G. Kriza

- Member of the Solid State Physics Committee of MTA (from 2007)
- Member of Ph.D. School of Physics, BME (from 2008)
- Member of Bolyai Fellowship Board, MTA (from 2010)
- Member of MTA Domus Hungarica Scientiarum et Artium Fellowship Board (from 2008)

N. Kroó

- Chair of the Governing Council of the Hungarian Research Infrastructure Program
- Chair of the Rátz High School Prize
- Member of the Hungarian UNESCO Committee
- Chair of the Dennis Gabor International Prize Committee
- Chairman of the Research Infrastructure Expert Group of ERA (EC)
- Member of the High Level Expert Group on Digital Libraries and Scientific Publications (EC)

- Member (former Chair) of the Section of Physical and Engineering Sciences of Academia Europaea
- Member of the Advisory Group on ESOF
- Member of the ELI_ALPS Scientific Advisory Committee
- Editorial Board, Laser Physics Letters

K. Kutasi

- Member of International Scientific Committee, Conference series "International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment," from 2006
- Member of International Scientific Committee, Conference series of "Central European Symposium on Plasma Chemistry" 2013-

J. Laczkó

- Member of the Society for Neuroscience
- Member of the International Society for Motor Control

Ö. Legeza

- Member of the Statistical Physics Scientific Committee, MTA
- Member of the Young Researcher Committee, MTA
- Secretary of the Statistical Physics Section of Roland Eötvös Physical Society (ELFT)
-

P. Lévai

- Member of the Physics PhD. School, ELTE
- Member of the Hungarian CERN Committee
- Member of the CERN Council
- Member of the ESFRI (European Strategy Forum on Research Infrastructure)
- Member of the Committee on Research Infrastructure.
- Member of the Committee on Nuclear Physics.
- Member of the Committee on Particle Physics.
- Member of the IAC of the Quark Matter 2012 Conference (Washington, 2012. 08.13-18)
- Member of the IAC of the 7th International Workshop on High-pT Physics at LHC, (Frankfurt, 2012.03.26-30)
- Member of the IAC of the 8th International Workshop on High-pT Physics at LHC, (Wuhan, 2012.10.21-24)

B. Lukács

- Member of the Astronomical and Space Research Committee of the H.A.S.

F. Mezei

- Chairman of the Physical Society Publication Committe
- American Physical Society
- Academia Europaea, London
- European Neutron Scattering Association (ENSA) Committee
- Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA

— International Council for Scientific and Technical Information, University of California, San Diego, USA

A. Nagy

— Co-chairman of the Working Group Instrumentation in European Aerosol Assembly

D.L. Nagy

— Common Coordination Committee of the Hungarian Academy of Sciences and the Joint Institute for Nuclear Research, Dubna, MTA Representative
— Joint Institute for Nuclear Research, Dubna, Scientific Council, Member
— European XFEL, Council, Member
— FP7 Research Infrastructures Programme Committee, expert
— International Board of the Applications of the Mössbauer Effect, Chair
— European Synchrotron Radiation Facility, Consortium CENTRALSYNC, Steering Committee, Member
— Hyperfine Interactions, Editorial Board, Member
— International Union of Pure and Applied Physics (IUPAP), Commission on Physics for Development (C13), Member
— European Physical Society, Council, Member
— European Strategy Forum on Research Infrastructures, Working Group on Regional Issues, Member
— European Science Foundation, Member Organisation Forum on Research Infrastructures, Member
— Program Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research, Dubna, Member

J.Z. Nagy

— Member of the MANT (Hungarian Astronautical Society)

Z. Németh

— Member of the Materials Sicence Work Committee of the Hungarian Academy of Sciences

K. Penc

— Member of the HAS Solid State Physics Com

L. Péter

— Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
— Representative for Hungary, International Society of Electrochemistry (2011-2016)
— Council Member of Graduate School of Chemistry, ELTE (2009-)
— Editor for Electrochemistry (Open Chemistry; formerly Central European Journal of Chemistry; 2009-)
— Key Reader (Metallurgical and Materials Transactions E, 2014-)
— Member of the Management Committee and training course coordinator, COST MP 1407 action

K. Polgár

— Hungarian Advisor of the International Organization for Crystal Growth

— Member of the International Advisory Committee of the 17th Intern. Conference on Crystal Growth and Epitaxy (ICCGE-17)
— Member of the International Advisory Board of the Fifth European Conference on Crystal Growth (ECCG5)

I. Rácz

— Member of the International Society for General Relativity and Gravitation

L. Rosta

— Member of the European Neutron Scattering Association
— Member of the European Spallation Source, Steering Committee
— Member of the Hungarian ESS Committee

F. Siklér

— Member of the SPS and PS experiments Committee (SPSC)
— Institutional representative at the CMS Collaboration Board
— Member of the CMS Publication Committee, Heavy Ions editorial board
— Member and secretary of the Particle Phyisics Scientific Committee of the HAS; representative at the general assembly of the HAS

E. Somfai

— IOP member
— Member of the American Physics Society

J. Sólyom

— Chairman of the Physics Section of the Hungarian Academy of Sciences

Zs. Sörlei

— Member of the Committee of Laser Physics of the Hungarian Academy of Sciences

L. Szabados

— Scientific advisory panel of the journal Classical and Quantum Gravity
— Member of the Particle Physics Committee of the H.A.S.

T. Szabolics

— Member of the Hungarian Nuclear Society

S. Szalai

— Member of Hungarian Space Research Council
— Member of ARTEMIS-H steering
— Member of Rosetta Lander steering
— Member of the MANT (Hungarian Astronautical Society)

V. Szalay

— CMST COST Action CM1405 Management Committee member

Zs. Szaller

— Member of the Thermoanalitical Committee of HAS

K. Szegő

— Member of Committee on Astronomy and Space Physics of HAS
— Member of IAA
— Member of ERC Starting Grant Evaluation Panel

T. Szepesi

- Member of the Hungarian Nuclear Society

E. Szilágyi

- International Committee of the Conference series of Ion Beam Analysis, member
- Member of the Committee on Solid State Physics

R. Szipőcs

- Member of Optical Society of America

Z. Szőkefalvi-Nagy

- Member of the Editorial Board, International Journal of PIXE
- Member of the International Honorary Committee, PIXE
- Member of the Committee on Atomic and Molecular Physics and Spectroscopy

Gy. Török

- Member of IAEA JRC-1575
- Member of JRC-NET

B. Újfalussy

- Secretary of the Materials Science Group of Loránd Eötvös Physical society
- Secretary general of the Lorand Eotvos Physical Society
- Secretary of the HAS Solid State Physics Committee

R. Ünnep

- Member of the Hungarian Biophysical Society

G. Vankó

- Secretary of the Hungarian Synchrotron Committee, MTA
- Management Committee, EU COST Action MP1203 Advanced X-ray spatial and temporal metrology

L.K. Varga

- Member of the International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM)
- Member of Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)

S.Varró

- Member of the Commitee of Laser Physics of the Hungarian Acedemy of Sciences
- Member of the Committee of the Quantumelectronics Division of the Lóránd Eötvös Physical Society

M. Vasúth

- Member of the Virgo Scientific Collaboration
- MC Member of the NewCompStar EU COST MP1304 action

P. Ván

- Editor of the Continuum Mechanics and Thermodynamics, Springer,
- Secretary of the Society for the Unity of Science and Technology
- Scientific Advisory Board member of JETC'15 (Joint European Thermodynamics Conference,)

- Member of the REPS (Roland Eötvös Physical Society)
- Member of the Physics PhD School at TU Budapest (BME)

P. Vecsernyés

- Member of the Particle Physics Committee of the H.A.S.

G. Veres

- Member of the Hungarian Microscopy Society
- Member of the Hungarian Aerosol Society
- Governing Board Member of the European Joint Undertaking for ITER and the development of Fusion Energy

V.Veszprémi

- Member of the CMS Phase I Upgrade Management Board
- CMS Tracker Institutional Board (ex officio), CMS Tracker Management Board (ex officio)

I. Vincze

- Member of the Council of Doctors at the Hungarian Academy of Sciences

G.Vizi

- board member of the MANT (Hungarian Astronautical Society)

Gy. Wolf

- Hungarian representative of the NuPECC EU FP7 HadronPhysics2, HadronPhysics3, HadronPhysicsHorizon, GSI FAIR, CBM, JRA Thuric, Toric, and Meson-Net projects.
- Leader of the PANS,
- President of the NEFIM
- Member of the NICA
- President of the of the Nuclear Physics Board, Eötvös Loránd Physical Society
- Secretary of the Nulcear Physics Board of the Hungarian Academy of Sciences
- Representative in Physics Department of the Hungarian Academy of Sciences

S. Zoletnik

- European Expert in the EU-Korea fusion collaboration committee;
- International Tokamak Physics Activities (ITPA) "Diagnostics Topical Group" EU representative
- EURATOM Science and Technology Advisory Committee (STAC), deputy chair
- MAST Programme Advisory Committee, Culham, UK
- International Board of Advisors of the Institute of Plasma Physics, Prague
- Governing Board of Fusion for Energy, Barcelona, Spain
- EURATOM Scientific and Technical Committee (STC)
- Editorial Board of Plasma Physics and Controlled Fusion, IOP
- International Tokamak Physics Activities (ITPA) diagnostic topical group vice chair

- Eurofusion General Assembly
- Eurofusion General Assembly Bureau
- International Tokamak Physics Activity Diagnostics Topical Group
- International Board of Advisors of the Institute of Plasma Physics of CAS

Conferences

9th Central European Training School on Neutron Techniques, 4-8 May 2015

The training was organized with the participation of 24 master and PhD students, as well as post-doctoral researchers from 10 Central- and Western-European countries. The scope of the school was to provide insight into neutron scattering techniques and their application for studies on structure and dynamics of condensed matter. Each year it sets up as scope the development of the experimental skills of the participants and the wish to show them the art of the research on large scale facilities, as well as the interpretation of the results obtained in neutron experiments.

11th International Workshop on Electrodeposited Nanostructures (EDNANO-11), 10-12 September 2015

The EDNANO workshops established in our institute are held on an 18-month frequency bases in various European venues. In 2015, it was the third time that Hungary hosted the workshop. Nowadays, this workshop is a unique meeting and offers a forum for specialists of the field, shaping also a research community. 52 registered participants attended the EDNANO-11 workshop from 34 different laboratories in Europe, 3 in Asia and 3 in America. Hotel Margaréta in Balatonfüred provided an excellent a quiet environment for the intense scientific programme that included 34 oral presentations and 20 posters.

42nd Plasma Physics Conference of the European Physical Society, Lisbon Artificial Atoms: from Quantum Physics to Applications", 22-26 June 2015

I.B. Földes was the member of the programme committee

Annual NewCompStar Conference 2015, 15-19 June 2015, 120 participants

This international conference was organized as the annual meeting of the NewCompStar COST action community. The conference took place in Budapest at Hotel Mercure Buda, and was devoted to all aspects of compact stars and related fields.

Balaton Summer School in Physics (T. Vámi, Mafihe Nyári Iskola)

CMS Phase I Pixel Upgrade Workshop, 8-10 June 2015, Visegrád, Hungary (V. Veszpremi)

Conference: "HEPTech Academia Meets Industry on Big Data ICTT 2015" 30-31 March 2015, Budapest, Hungary

Large European Institutes such as CERN, DESY, STFC, FAIR/GSI and ELTE, SZTAKI, WIGNER together with the HEPTech Network organized two Academia-Industry Matching events on Information Technology, focusing on Big Data Applications in Science and Industry. This is the first of these two events, aiming to bring together Academia and Industry to share ideas, potential applications and fostering collaborations in the newly emerging field of Big Data and related topics. It facilitated information exchange among the 87 international participants, address some of the challenges faced by future HEP projects in the controls area and examine new solutions.

Conference on Neural Networks 2015, Killarney, Ireland (co-organizer: P. Érdi)

The motivation for proposing the workshop is to bring together (different- and like-minded) people working on the area of computational modelling and related fields to discuss current state-of-the-art and possible way forward, to initiate new collaborations and research avenues. We also endeavour to include the topic of computational model validation and whether we could take inspiration from established validation techniques in engineering for application in computational neurology and psychiatry.

Computational neurology and psychiatry: do we need it? Workshop at International Joint Conference "Annual NewCompStar Conference 2015", 15-19 June 2015, Budapest, Hungary

The NewCompStar COST Action MP1304 is dedicated to build network and synergy among astrophysics, astronomy, gravitation theory and high-energy nuclear physics fileds. Since Hungary is the full member of the NewCompStar collaboration were could organize the first Annual NewCompStar Conference and Annual Steering Committee Meeting of the COST Action MP1304 in Budapest. We had 83 participants, 20 including 30 invited speakers form US, Turkey, Armenia, Russia, Japan, and certainly, European Union countries. We could also provide support for about 15 young students and postdocs in order to present their results.

Conference "Design and Engineering of Neutron Instruments Meeting (DENIM 2015)", 7-9 September 2015.

The conference was organized as a joint collaboration between the Wigner Research Centre for Physics and The Centre for Energy Research. The event had 139 participants, the meeting featured a large variety of engineering and neutron instrumentation topics. Besides scientists from the organizing institutes, guests arrived from EU, USA, Canada, Australia, Japan and Argentina.

Conference: "Integrating devices and materials: a challenge for new instrumentation, Meeting of the COST Action IC1208 ", 3-4 September 2015

The conference included the meetings of the workgroups WG1-WG4 as well as the 6th management committee meeting of the COST Action IC1208. The conference took place at Hotel Flamenco, Budapest, with the participation of 70 scientists involving most European countries.

Conference "Zimányi School '15: 15th Zimányi Winter School on Heavy Ion Physics", 7-11 December 2015, Budapest, Hungary

This traditional one-week international winter school use 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 15th time, providing an excited platform for discussion between students and world-class experts of the high-energy heavy ion collisions both form theoretical and experimental sides. We had about 20 visitors from the US, Japan, Brazil, and European countries, representing the huge experimental collaborations, such as ALICE, CMS, LHCb from CERN, Switzerland besides STAR and PHENIX from the BNL, USA, and KEK, Japan.

"Data Science @ LHC 2015 Workshop", 9-13 November, 2015, CERN, Geneva

ESS In-kind Delivery Workshop Series

A series of 6 workshops were organized by the Neutron Spectroscopy Department on various themes in order to set-up a collaboration and start a discussion within the ESS and the Hungarian companies interested in the In-kind Delivery for the European Spallation Source, which will be the brightest neutron source of Europe in the near future. The subtitles of the workshops were: Detector Workshop, LINAC Workshop, CAMEA Workshop, NMX diffractometer Workshop, Motion Control & Automation Workshop.

International Conference on Precision Physics and Fundamental Physical Constants (FFK-2015), 12-16 October 2015, Hungarian Academy of Sciences, Budapest, Hungary (D. Horváth)

International Conference on Silicon Carbide and Related Materials 2015

~700 participants; conference on silicon carbide: growth, defect characterization, quantum and traditional applications

"International Workshop on Lithium Niobate", Tianjin, China, 3-5 November 2015.

Co-organized by Y.F. Kong, L. Kovács and J.J. Xu. It was the second meeting of a new series of workshops on the growth, properties and applications of lithium niobate crystals. Beside the 19 invited lecturers from China, Germany, Hungary, Italy, Russia, Ukraine, and USA many Chinese students got acquainted with the recent scientific results on lithium niobate.

LSC-VIRGO Collaborating Meeting, 31 August - 3 September 2015, 220 participants

The international conference was organized as the second annual meeting of the LIGO-Virgo Scientific Collaboration. The conference took place at Kempinski Hotel Corvinus Budapest. Besides scientists from EU, guests arrived from the USA, Japan and India.

PEP19 meeting, 15-17 June 2015

The conference was organized as a joint meeting of PEP team members. The meeting took place in building 3 of our Institute. 22 participants arrived from the USA, Sweden, Finland, Germany, Great Britain, Switzerland and France. The topic of three-day meeting was technical problems of space research instrument of Juice PEP project.

Progress in Motor Control X

The leader of our group was the main organizer and the chair of the international conference of the International society of motor Control. The conference was entitled as "Progress in Motor Control X" and 175 scientists, from 31 countries participated this scientific meeting. The conference took place at the Congress Center of Hotel Novotel Budapest City in July 22-25, 2015. It gave the opportunity to Hungarian attendees to became familiar with the growing scientific field, named "motor control". Beside the scientific value, this research area has an invaluable social significance. For people who lost their motor functions and live with motor impairment, this conference presented the newest available results to rehabilitate and restore lost motor functions.

Rosetta Plasma Consortium Team Meeting, Budapest, 9-11 September 2015

The meeting, organized by our group took place in Budapest and was attended by about 40 scientists from all over the world. The latest results of the plasma observations near Comet Churyumov-Gerasimenko by the Rosetta spacecraft were discussed.

Summer School "Nyáridő a téridőben – Téridő a nyáridőben" Space-time Summer School, 12-18 July 2015, Mindszentpuszta, Hungary

The aim of this summer school was to summarize and extend the knowledge of space-time in many senses, like topology, field theory, gravitational physics. We had about 40 participants including about 25 university students from Hungary. The event was supported by mainly the Heavy ion Wigner Research Group.

Scientific meeting of the Committee on Laser Physics: Light in the science and in the technology, 2015. May 7. Hungarian Academy of Sciences (connected to the International Year of Light)

Summer School on Optics - Symposium on Optical Developments, Siófok, Júni 7-10. 2015.

"The First 27 Years of Reverse Monte Carlo Modelling: RMC-6", 15-19 September 2015

This was the latest event of a triannual conference series focusing on the various aspects of the Reverse Monte Carlo structural modelling technique. Since 2003, the meeting has been organised by our research group, in various locations in Budapest; this time (similarly to the 2012 event) the venue was the Holiday Beach Wellness Hotel (northern Buda). More than 50 scientists from all over the world (geographically, between the USA and Japan) have attended. A special issue, directly linked with the recent conference, of Physica Scripta is under preparation.

Workshop "5th GPU Day, The Future of Many-Core Computing in Science", 20-21 May 2015, Wigner RCP, Budapest, Hungary

The "GPU Day" series has been organized by the Wigner GPU Laboratory for the 5th times in this year. The two-day workshop interconnects scientists, programmers, and parallel-computing experts from all over the world. This year we had 80 participants and visitors from US, Spain, Ukraine, Romania. Several commercial companies visited the event from Hungary and abroad.

Workshop "Entanglement Day 2015", 24-25 Sep 2015

Meeting of researchers working on quantum entanglement, on the national level.

Workshop on the "Integrable Approaches to 3pt functions in AdS5/CFT4, Budapest, 15 - 19 June 2015

The aim of the workshop was to bring together the experts working on different aspects/regimes of the 3pt functions in the AdS5/CFT4 correspondence to share ideas, results and spark new collaborations and activity. The workshop venue was the Physics Building of the Eötvös University and we had around 30 participants from all over the world.

Workshop "Lectures on Modern Scientific Programming", 23-25 November 2015, Wigner FK, Budapest, Hungary

This new international workshop of the Wigner GPU Laboratory is dedicated to widen our knowledge and practice on parallel computing in science. The seminar-series-like event started from the basics of computing and informational technologies, then moved to basic and parallel programming techniques for physicists. We had 60 registered participants mostly from the Hungarian and abroad universities.

Workshop "Zagreb—Budapest Meetup 2015", 28th October 2015, Wigner RCP, Budapest, Hungary

This small workshop is regular meeting between the ALICE groups of the University of Zagreb and the Hungarian ALICE Groups. Our aim is to build a bridge for knowledge-transfer between the two experimental groups, with about 20 participants.

Workshop "Wigner— IOPP CCNU Balaton Workshop 2015", 12th-17th July 2015, Tihany, Hungary

This one-week workshop is dedicated to bring together the high-energy heavy ion community related to the Wigner RCP and the Institute of Particle Physics Central China Normal Univeristy. Our aim was to discuss the recent experimental results and prepare ideas, theories for the later Quark Matter 2015 international conference. This event we had about 40 participants from US, Germany, Cech Republic, and China.

Wigner Colloquia

In the fall of 2014 we have started to organize a series of Wigner Colloquia, inviting international experts to deliver talks on fresh and interesting research topics to the entire community of our research centre. We also have dispatched a modest financial background to support this activity by occasionally reimbursing travel costs to and accomodation costs in Budapest for the invited speakers.

The concept of this series is to offer to our researchers a possibility to meet colleagues from external institutions who work on hot topics and able to present their favorite research to a wide audience of physicists, working both in experiment and theory in fields ranging from high energy particle physics via nuclear and plasma physics to material and life science related problems. We restrict our invitations in number to a few per semiannual blocks.

Wigner Colloquia in 2015

https://indico.kfki.hu/category/42/

06-01-2015	Dr. Máté Lengyel (Computational and Biological Learning Lab, Cambridge University), "Neural network models of hippocampal memory"
10-03-2015	Prof. Joachim Burgdörfer (University of Vienna), "Time-resolved electronic dynamics on the attosecond time scale"
07-04-2015	Dr. Konstantinos Makris (TU Wien), "Parity-time symmetry, singular amplification, and constant intensity waves in non-Hermitian photonics"
12-05-2015	Prof. Ludwig Dmitrievich Faddeev (Steklov Institute of Mathematics, Russian Academy of Science), "Scenario of renormalization for the Yang-Mills theory in 4D"
02-06-2015	Prof. Johann Rafelski (University of Arizona), "Boiling Quarks, Melting Hadrons"
23-06-2015	Prof. Jacob David Bekenstein (The Hebrew University of Jerusalem), "Playing with quantum gravity on the tabletop"
13-10-2015	Prof. Andrei Alekseevich Slavnov (Mathematical Institute, Russian Academy of Science), "60 years of gauge fields"
03-11-2015	Prof. Dezső Horváth (HAS Wigner RCP), "Nobel Prize 2015 in Physics: neutrino oscillations"
17-11-2015	Prof. Kosmas Prassides (Univ Durham, Dept Chem), "Fullerene superconductivity: a personal ongoing voyage into the unexpected"
01-12-2015	Prof. József Fortágh (CQ Center for Quantum Science University of Tübingen), "Interfacing ultra-cold atoms and solids"

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/

Life Sciences Seminars
http://indico.kfki.hu/category/37/

09-01-2015	Gergely Fejos (RIKEN, Japan): Finite temperature chiral symmetry restoration with functional renormalization group methdods (Theoretical physics seminar)
30-01-2015	Leszek Hadasz (Kraków, Poland) : Super Liouville - double Liouville equivalence and its possible extensions (Theoretical physics seminar)
27-02-2015	Noa Mitsui (Visiting Researcher): Thermodynamics of friction (Theoretical physics seminar)
13-03-2015	Miklós Gyulassy (Columbia University): The Strongly Coupled Quark-Gluon-Magnetic Monopole Plasma (Theoretical physics seminar)
03-04-2015	Zoltán Zimborás (University College London): Novel Lie-theoretical theorems and their applications (Theoretical physics seminar)
22-05-2015	Urko Reinosa (Ecole Polytechnique): Perturbative study of the QCD phase diagram for heavy quarks at non-zero chemical potential from a model extension of the Landau-DeWitt gauge (Theoretical physics seminar)
14-09-2015	Alexander Belavin (ITP, Moscow): Frobenius manifolds and Minimal string theory (Theoretical physics seminar)
09-10-2015	Prof. Tamás Sándor Biró (Wigner RCP), "An Introduction to the Non-Extensive Statistical Models of Hadronization" (Theoretical physics seminar)
19-10-2015	Takuya Matsumoto (Nagoya University, Japan): Representations of centrally extended Lie superalgebra psl(2|2) (Theoretical physics seminar)
30-10-2015	Daniel Nogradi (ELTE): Light composite Higgs (Theoretical physics seminar)
03-11-2015	Dr. Balázs Hangya (Research Institute for Experimental Medicine, HAS), "The role of the basal forebrain in learning" (Life Sciences Seminar)
10-11-2015	Dr. József Bíró (BME), "Navigable networks as Nash equilibria of navigation games" (Life Sciences Seminar)
04-12-2015	Dénes Molnár (Purdue University): Elliptic flow from anisotropic escape (Theoretical physics seminar)

Wigner RCP SZFI Seminars

http://www.szfki.hu/seminar

13-01-2015	Kálmán Tompa (Wigner RCP): History and the future at present time (on the border of life sciences and physics)
20-01-2015	Andrea Alberti (Universitat Bonn): Quantum walks with neutral atoms
27-01-2015	Norbert Kroó (Wigner RCP): Strong field plasmonics
03-02-2015	Péter Hartmann (Wigner RCP): Plastic strain and dusty plasmas
10-02-2015	Katalin Gillemot (Wigner RCP): Playing Lego with molecules: the rough path to atomic-sized thermoelectric devices
17-02-2015	Balázs Dóra (Wigner RCP): Loschmidt echo in Luttinger liquids
24-02-2015	Csete Mária (University of Szeged): Plasmonic amplification of light-matter interaction
26-02-2015	Balázs Rózsa (Wigner RCP): Fast three-dimensional laser scanning multiphoton microscopy for medical diagnostics, and brain research
03-03-2015	Ellák Somfai (Wigner RCP): Rheology of soft matter near the jamming transition
10-03-2015	Zoltán Donkó (Wigner RCP): Electron transport in gases as a classical many-body problem
17-03-2015	Judit Sári (PTE, BME-MTA EKF Momentum group): Making visible relativistic covariance in graphene and alpha-(BEDT-TTF)2I3
19-03-2015	Miron Amusia (Racah Institute of Physics, Hebrew University of Jerusalem; A. F. Ioffe Physical-Technical Institute, St. Petersburg, Russia): Atoms and endohedrals as resonators and amplifiers of radiation
19-03-2015	Zoltán Darázs (Wigner RCP): Dynamical properties of quantum systems with few degrees of freedom
23-03-2015	Csaba Tóth (Lawrence Berkeley National Laboratory): BELLA (BErkeley Lab Laser Accelerator), a 1 Hz, 1 PW pulse-peak performance laser system for GeV electron acceleration in plasmas
24-03-2015	Krisztián Szász (Wigner RCP): Identification of point defects in semiconductor structures by hyperfine tensor calculations
26-03-2015	Johannes Richter (Institut für Theoretische Physik, Universitat Magdeburg, Germany): Strongly correlated systems on highly frustrated lattices: The flat-band scenario and beyond
02-04-2015	Jack F. Douglas (National Institute of Standards and Technology, Materials Science and Engineering Division, Gaithersburg): Cooperative Motion and Structural Relaxation in Glass-Forming Materials
07-04-2015	Péter Dusán Ispánovity (ELTE): Deformational avalanches in crystalline materials
09-04-2015	J.D. Whitfield (Vienna Center for Quantum Science and Technology): Theoretical limitations to model chemistry
14-04-2015	Szilvia Pothoczki (Wigner RCP): Structural study of simple molecular liquids
21-04-2015	Zoltán Dudás (Wigner RCP): Sol-gel synthesis and physico-chemical characterization of amorphous silica and crystalline zinc-silicate based materials
22-04-2015	Hajnalka Tóháti (Wigner RCP): Optical spectroscopy of carbon nanotube-based hybrid materials

28-04-2015	Ranjini Bandyopadhyay (Raman Research Institute Bangalore, India): A colloidal clay suspension as a model glass-former: some recent experimental results
30-04-2015	Ihor Korolov (Wigner RCP): Investigation of radio-frequency gas breakdown: simulations and experiments
05-05-2015	István Márton (Wigner RCP): Investigation of electrons created by ultrafast surface plasmons
12-05-2015	Katalin Németh (Wigner RCP): Chemical modification and optical spectroscopic investigation of single-wall carbon nanotubes
19-05-2015	Gabriella Dravecz (Wigner RCP): Al, Si determination by high-resolution graphite-furnace atomic absorption analysis, investigation of the biological applicability of SiC nanocrystals
19-05-2015	Dávid Beke (Wigner RCP): Preparation and characterization of SiC-based nanoclusters
26-05-2015	Katalin Neuróhr (Wigner RCP): Electrochemical deposition and investigation of metallic nanostructures
26-05-2015	László Himics (Wigner RCP): Spectral characterization of the zero-phonon line of Si-vacance centre in nanodiamond thin layers
02-06-2015	Tamás Verebélyi (Wigner RCP): Motion parameters of hydrogen pairs in solid phase of proteins
02-06-2015	Dávid Nagy (Wigner RCP): Non-equilibrium Dicke phase transition by subohmic dissipation
04-06-2015	Nikoletta Laczai (Wigner RCP): Preparation and investigation of polycrystalline yttrium-oxi-ortosilicates
04-06-2015	Edina Szirmai (BME): Spin-FFLO state of high spin fermions in a one-dimensional optical lattice
09-06-2015	Anikó Zsuzsa Kovács (Wigner RCP): Collective dynamics of strongly coupled multiparticle systems
11-06-2015	Dimitrie Culcer (University of New South Wales, Sydney, Australia): Weak antilocalisation of topological insulators with strong spin-orbit scattering
16-06-2015	Gábor Kónya (Wigner RCP): Decay of the soft polariton mode of a Bose-Einstein Condensate in an optical resonator
16-06-2015	Péter Sinkovicz (Wigner RCP): Return time in iterated open quantum systems
16-06-2015	Zoltán Bodrog (Wigner RCP): Modeling single photon sources in SiC and diamond
18-06-2015	Gergely Roósz (Wigner RCP): Dynamics of isolated quantum systems
18-06-2015	Gergely Barcza (Wigner RCP): Phase separation in the system of four-component ultracold atoms
23-06-2015	Hidetsugu Shiozawa (Faculty of Physics, University of Vienna): Magnetic properties of nano metals
25-06-2015	Renáta Ünnep (Wigner RCP): Investigation of the structure of photosynthetic membrane structures by small-angle neutron scattering and electron microscopy
25-06-2015	Viktor Ayadi (Wigner RCP): Theoretical investigation of ultrafast photoemission

30-06-2015	Gábor Csire (Wigner RCP): Quasiparticle spectra of superconducting heterostructures
07-07-2015	Sándor Volkán-Kacsó (California Institute of Technology): Theories of single molecule processes: quantum dot blinking and ATP-ase rotation
14-07-2015	Levente Rózsa (BME): Noncollinear spin configurations in magnetic thin layers
10-08-2015	Márton Vörös (Institute for Molecular Engineering, University of Chicago): Molecular design of nanocrystals for efficient third generation photovoltaics using first principles simulations
11-08-2015	David Statman (Physics Department, and Chemistry Department, Allegheny College, Meadville, USA): Photoinduced reorientation of methyl-red-doped nematics: What we have learned
17-08-2015	Yunzhi Wang (Department of Materials Science and Engineering, The Ohio State University): A Combined Experimental and Simulation Study of Deformation Mechanisms of Order Precipitates in Superalloys
08-09-2015	Jenő Sólyom (Wigner RCP): How to write correctly in Hungarian about physics
15-09-2015	Ken Elder (Oakland University): Honeycomb and Triangular Domain Wall Networks in Heteroepitaxial Systems
22-09-2015	Sándor Bordács (BME): Néel-type Skyrmion Lattice in a Polar Magnetic Semiconductor
29-09-2015	Sándor Ricz (HAS ATOMKI): Investigation of ionization processes by angle- and high-energy-resolution electron spectroscopy methods
06-10-2015	Alexander Blumen (Freiburgi Egyetem, SZFI-s szervező: Kiss Tamás): Dynamics in Complex Systems: From Continuous-Time Quantum Walks to Polymers and Back.
13-10-2015	Salvatore Manmana (Institute for Theoretical Physics, University of Göttingen): Recent developments for finite-temperature dynamics with matrix product state approaches
20-10-2015	Gábor Vattay (ELTE): The effect of critical quantum walk on daisies
27-10-2015	Miklós Erdélyi (University of Szeged): Localization optical microscopy: method, development and application possibilities
03-11-2015	Viktor Chikán (Kansas State University): Building a Better Nanoparticle
04-11-2015	Martin Richardson (University of Central Florida): Development and applications of ultrashort high intensity lasers
10-11-2015	Gábor Halász (Oxford University): Hole dynamics in exactly solvable gapped and gapless spin liquids
17-11-2015	Sándor Varró (Wigner RCP): The 110 Years of the Photon. From Einstein's Light Quanta to Extreme Light
24-11-2015	Gyula Tóth (University of Bergen): Formation of crystal seeds and crystal growth in Molecular Phase Theory
01-12-2015	Xavier Marti (Czech Academy of Sciences): Antiferromagnetic spintronics
08-12-2015	Aranka Derzsi (Wigner RCP): Radiofrequency gas excitations in electronegative gases
10-12-2015	Ralf Stannarius (Dept. of Nonlinear Phenomena, Otto von Guericke Uni Magdeburg): Freely suspended liquid crystal films: liquids in 2D

15-12-2015	Gergely Thiering (Wigner RCP): Investigation of point defects connected to silicon and oxygen in diamond by ab-initio methods
15-12-2015	Gyula Károlyházy (Wigner RCP): Controlled preparation of point defects in silicium carbide