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# **Wigner RCP 2013**

**Annual Report**

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Wigner Research Centre for Physics  
Hungarian Academy of Sciences  
Budapest, Hungary  
2013

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Wigner RCP 2013 – Annual Report

Edited by V. Blázsik-Kozma, G. Konczos, G. Kriza, B. Selmeçi, E. Szilágyi, and P. Ván

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***Dear Reader,***

Budapest, 31 March 2014

***Lévai Péter József***  
Director General

## **Awards and prizes**

### **Awards of the State of Hungary and Government of Hungary**

- F. Mezei, G. Oszlányi, A. Sütő, Széchenyi Award
- Z. Szőkefalvi-Nagy Officer's cross of the Order of Merit of Hungary (civil division), 2013
- A. Czitrovsky, Officer's cross of the Order of Merit of Hungary (civil division), 2013

### **Awards of the Hungarian Academy of Sciences**

- Z. Kurucz, Award for Young Scientists of the MTA 2013
- P. Schlosser, Mention of Secretary General of MTA, 2013
- O. Kálmán, Mention of Secretary General of MTA, 2013

### **International awards**

- Gy. Pergerné-Klupp, Newton International Fellowship

### **Professional awards**

- P. Dombi: Pál Selényi Award of the Hungarian Physical Society
- P. Király: Albert Fonó medal of the Hungarian Astronautical Society
- I. Korolov, Annual Applied Research Prize of the Wigner RCP SZFI
- M. Pápai, Vértes Attila Award for Young Scientists
- G. Pető, László Kalmár Award of the Loránd Eötvös University
- Gy. Tóth, Annual Publication Prize of the Wigner RCP SZFI
- B. Újfalussy: Pál Gombás Award of the Loránd Eötvös Physical Society

### **Awards of foundations and associations**

- O. Kálmán, Junior Prima Prize 2013, Prima Primiissima Foundation

### **"Momentum" Program of the H.A.S., 2013**

- Gy. Vankó
- D. Varga

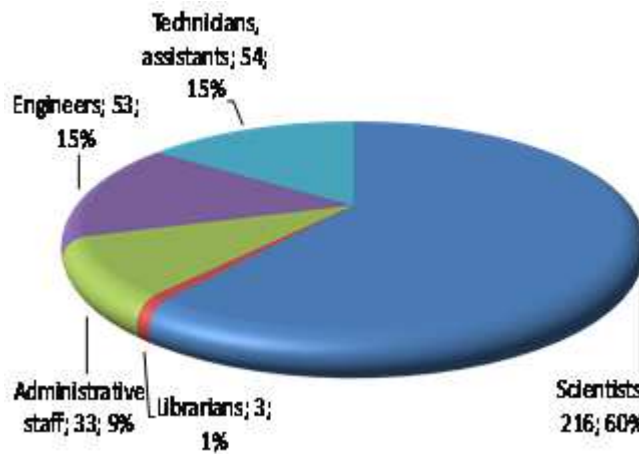
### **Bolyai János Scholarship of MTA**

- G.G. Barnaföldi 2013-2015
- G. Bortel, 2011-2014
- P. Dombi, 2011-2014
- Á. Hegedűs, 2012-2015
- É. Kováts, 2012-2014
- E.A. Somfai 2013-2015
- Gy. Tegze 2013-2015
- G. Vankó, 2012-2014
- M. Vasúth 2013-2015
- A. Vukics, 2012-2014

## Key figures and organizational chart

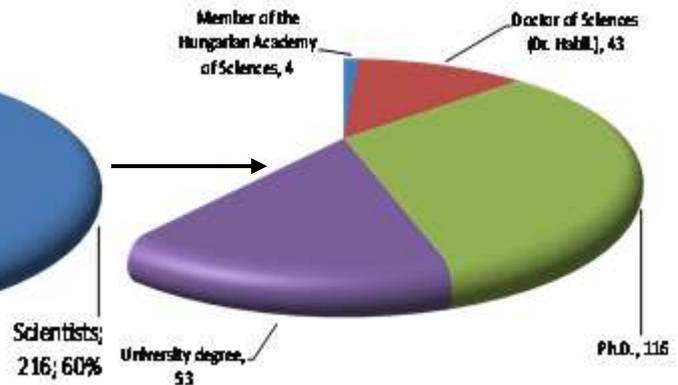
### Permanent staff by profession

Total: 359



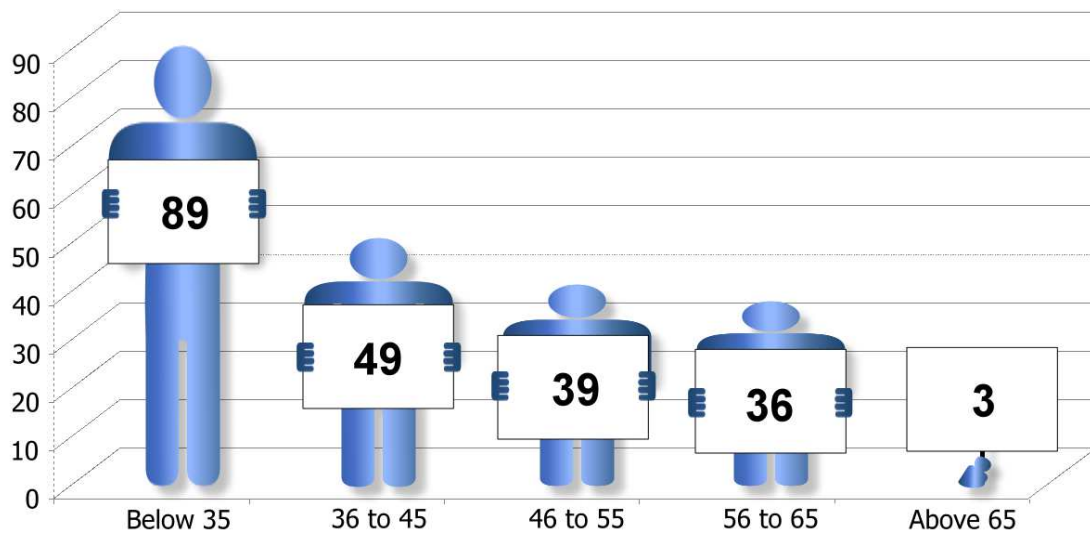
### Scientists by degree/title

Total: 216

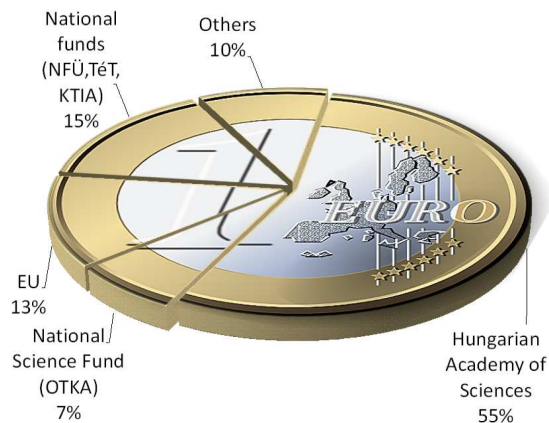


### Scientists by age group

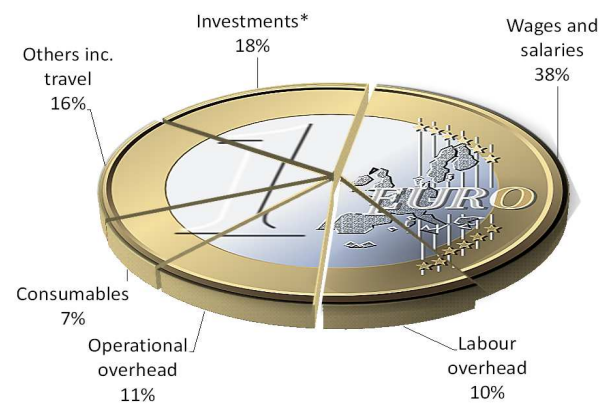
Total: 216



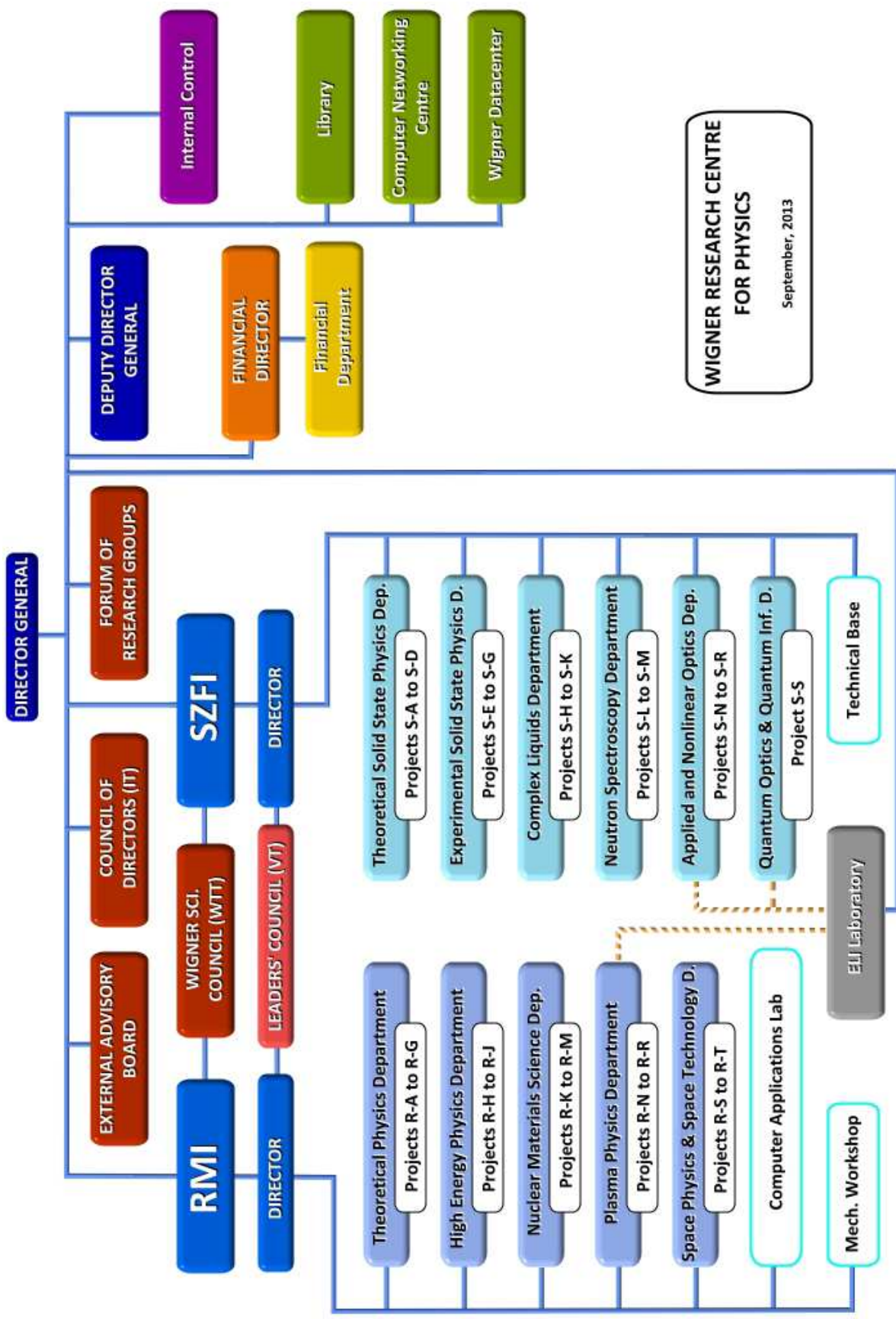
### Income



### Expenditure



\* Investments don't include the costs of Wigner Data Center jointly funded by the Hungarian Government and CERN.



**WIGNER RESEARCH CENTRE  
FOR PHYSICS**  
 September, 2013



## **Outstanding research groups**

### **“Momentum” Research Groups**

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

### **Wigner Research Groups**

The Wigner Research Groups’ purpose is to provide the best research groups with support for a year. Its primary goal is to retain excellent young researchers who are capable of leading an independent research group in science and in the Research Centre. It aims to energise 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-F. Holographic quantum field theory

“Momentum” group

**Zoltán Bajnok**, János Balog, Francesco Buccheri, Árpád Hegedűs, László Holló, Minkyoo Kim, József Konczer, Gábor Zsolt Tóth

The four fundamental interactions of Nature are electromagnetism, the weak force, the strong force, and gravity. The first two of these, unified by the electro-weak quantum gauge theory, have been tested with high accuracy. The strong interaction is also formulated as a gauge theory, but high precision tests are hampered by its strongly-coupled nature. Additionally, the gravitational interaction does not yet have a satisfactory quantum formulation.

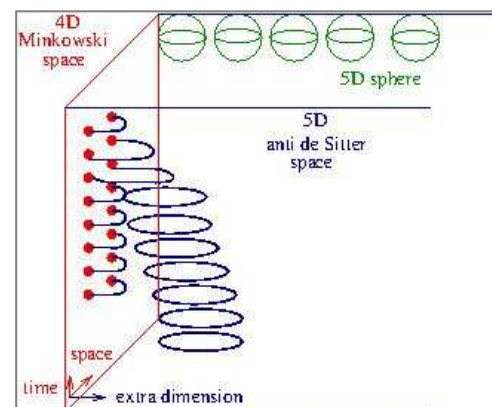
The gauge/gravity duality provides hope for the understanding both the strong interaction and quantum gravity simultaneously, as it connects gauge theories with string theory (including gravity). This conjectured duality relates strongly coupled gauge theories to semi-classical string theory and the deeply quantum string theory (gravity) to perturbative gauge theory.

The 't Hooft limit of the maximally supersymmetric gauge theory provides the best chance to demonstrate the conjectured equivalence of gauge theories and string theory because in this limit the integrability of the two dimensional string theory manifests.

In the holographic description our 4D Minkowski space (indicated in red on Fig. 1), is the holographic boundary of the 5D anti-de Sitter (AdS) space (shown in blue). Above each point a 5D sphere is added (shown in green). The fundamental interactions are communicated by open strings ending at matter particles, while gravity is represented by closed strings that penetrate into the AdS bulk. Absorption of a graviton by a quark-anti-quark pair is stroboscopically shown. The 2D surface swept by the moving strings is called the worldsheet.

In the last twenty years, motivated by particle physics problems, there has been intensive research and relevant progress in two dimensional integrable theories. These theories were solved in the bulk and also with boundaries by determining exactly the spectrum of particles together with their scattering data which were then used to calculate the full spectrum at any finite size.

The objective of our research is to apply these two-dimensional integrable techniques to the holographic duality to describe strongly coupled gauge theories and investigate the quantum domain of string/gravity theory.



**Figure 1.** 4D Minkowski space as the boundary of the 5D anti de Sitter space

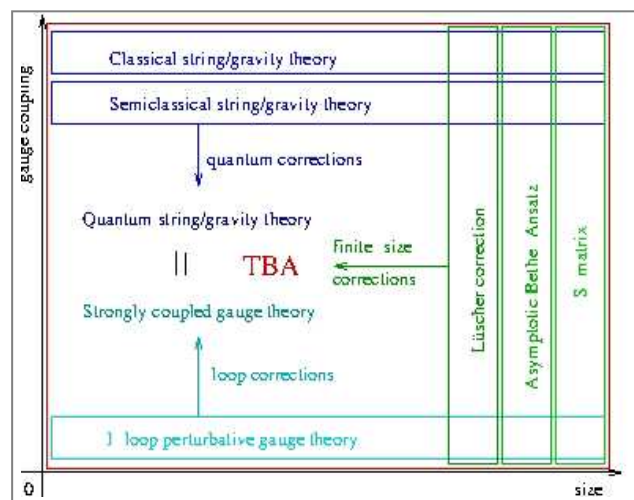
**Spectral problem.** — Heroic efforts have been undertaken to test the holographic conjecture. From the many case studies, the following consistent holographic dictionary has been set up:

The energies of string states are related to the anomalous 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. Due to the high number of symmetries, this effective two-dimensional field theory turned out to be integrable.

Historically, integrability showed up in the weakly-coupled limit of the gauge theory. The anomalous dimension matrix at one loop was mapped to the integrable 1D Heisenberg spin chain, while at higher loops it was related to a long-range spin model. Integrability techniques (such as the Bethe ansatz) were intensively used to determine the spectrum for large sizes (long operators). These results are non-perturbative, that is, valid for any coupling if the size is sufficiently large, but do not contain vacuum polarization effects. We managed to systematically include such finite-size corrections and determined the anomalous dimensions of short operators at high loop orders.

By summing up all finite-size corrections, an exact description can be found that is valid for any finite size and coupling. This “conceptual” solution of the spectral problem takes the form of infinitely-many coupled (Thermodynamic Bethe-Ansatz, TBA) integral equations. Recently, we managed to rewrite these infinitely-many equations in terms of a finite number of unknowns (nonlinear integral equations, NLIE). These results constitute a veritable gold mine, giving an exact interpolating description for all states from weak to strong coupling.

The various methods and their validity ranges are shown on Fig. 2. For weak coupling, perturbative gauge theory is reliable. For large coupling, the string/gravity theory is (semi) classical, allowing a calculative basis. These two validity ranges have no overlap. On the other hand, the holographic correspondence is integrable, thus we can use integrable techniques starting from infinite size and systematically calculate all finite-size corrections. The final solution

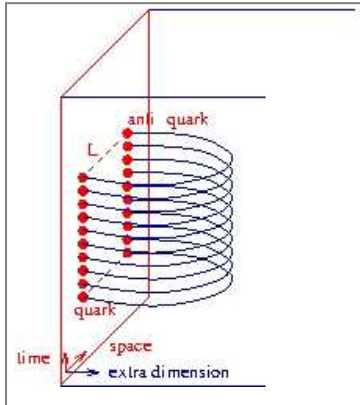


**Figure 2.** Various methods and their validity ranges for the spectral problem

not only solves the spectral problem, but also provides evidence for the holography: gauge theory and string/gravity theory are two equivalent descriptions of the same phenomena.

**Quark anti-quark potential.** — One of the most important quantities in any gauge theory is the quark-anti-quark potential. It encodes the energy of the configuration in which a particle (quark) and its anti-particle (anti-quark) are separated by a given distance. If the interaction energy increases linearly with distance, then the quark and anti-quark pair

cannot be separated: the theory is confining, like QCD. If the interaction energy decreases with distance, then we can observe free quarks. After almost half a century of intensive study, the confinement problem of QCD still remains a mystery. Due to the strongly coupled nature of the gauge theory, there is no analytical method to calculate the potential exactly, and we have to rely on numerical simulations such as lattice QCD. Holography can change this status completely. Using holography, we can map the strongly-coupled gauge theory to semi-classical string theory, over which we have good analytical control.



**Figure 3.** *The quark--anti-quark potential in the holographic picture*

The potential energy of the configuration in the gauge theory is related to the string/gravitational partition function of the 2D surface. For large coupling it is simply the minimal area, while for finite coupling we have to include the quantum fluctuations as well (Fig. 3).

The maximally supersymmetric gauge theory is scale invariant, which forces the quark--anti-quark potential to be proportional to the inverse of the distance, as in quantum electrodynamics. So this theory is not confining; nevertheless, the coefficient (strength) of the potential depends nontrivially on the gauge coupling. Standard perturbative calculations determine this coefficient in terms of a power series giving a good approximation for small coupling. For large coupling, the holographic description can

be used to calculate the string/gravitational partition function on the surface spanning the worldlines of the quark and anti-quark. At leading order, this amounts to evaluating the area of the minimal surface, while for finite coupling the quantum fluctuations must all be included, which is taken into account by a Boundary Thermodynamic Bethe Ansatz (BTBA) equation. We proposed a novel formulation of the BTBA equations, based on real chemical potentials and additional source terms, which allows a systematic weak coupling expansion. We expanded our equations to second (double wrapping) order and tested the results against direct two-loop gauge theory computations. We find complete agreement.

**Tachyons in AdS/CFT (anti-de Sitter/conformal field theory): brane anti-brane system. —**

In most of the applications of the duality conjecture, we gain information on the strongly-coupled gauge theory from the weakly coupled string theory or gravity. Duality enables us to learn about quantum string theory or quantum gravity in a highly curved background. In particular, we can study tachyons in string theory. These are non-perturbative objects that signal instabilities: a brane--anti-brane system is an unstable open-string system. It is believed that the branes annihilate with each other and decay into closed strings. However, there are no non-perturbative results supporting this idea in the literature for curved backgrounds.

Our experience with integrable boundaries together with our insight into the gauge/string duality enabled us to study this important problem. We developed a complete description of the brane--anti-brane system in the context of a gauge theory and as an integrable model.

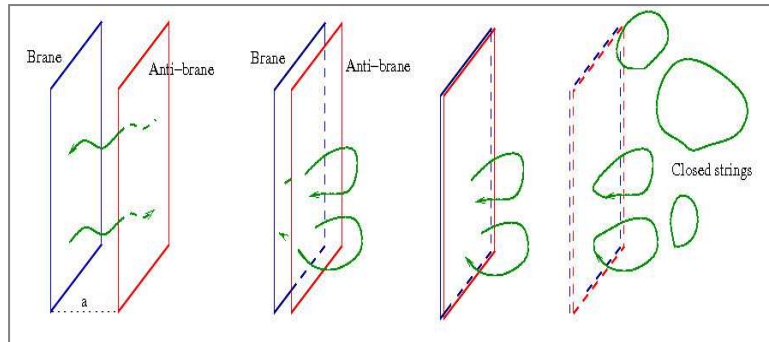


Figure 4. Brane–anti-brane system is an unstable open string system

In particular, we analyzed the spectrum of open strings stretched between a D-brane and an anti-D-brane in planar AdS/CFT using various tools: spin-chain, boundary asymptotic Bethe ansatz and Boundary Thermodynamic Bethe ansatz (BTBA) (Fig. 4.).

We found agreement between a perturbative high order diagrammatic calculation in  $N = 4$  SYM and the leading finite-size boundary Lüscher correction. We studied the ground state energy of the system at finite coupling by deriving and numerically solving a set of BTBA equations. While the numerical calculations give reasonable results at small coupling, they break down at finite coupling when the total energy of the string gets close to zero, possibly indicating that the state turns tachyonic. The location of the breakdown is also predicted analytically.

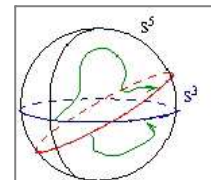


Figure 5. Open strings on the sphere

## Grants and international cooperation

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

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

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

TÉT Hungarian-Japanese bilateral: Integrability in gauge gravity duality and strong coupling dynamics of gauge theory (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 (J. Balog, 2013-2014)

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

## Publications

### Articles

1. Aoki S, Balog J<sup>\*</sup>, Doi T, Inoue T, Weisz P: Short distance repulsion among baryons. *INT. J. MOD. PHYS. E* 22:(5) Paper 1330012. 16 p. (2013)
2. Balog J, Niedermayer F, Weisz P: Symanzik effective actions in the large N limit. *J. HIGH ENERGY PHYS.* 2013:(8) Paper 027. 44 p. (2013)
3. Toth GZs: Projection operator approach to the quantization of higher spin fields. *EUR. PHYS. J. C* 73: Paper 2273. 29 p. (2013)

### Book

4. Samaj L, Bajnok Z: Introduction to the Statistical Physics of Integrable Many-body Systems. Cambridge; New York: Cambridge University Press, 2013. 523 p. (ISBN:978-1107030435)

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\* Underlined authors are members of the Wigner Research Centre for Physics

## R-G. Computational systems neuroscience

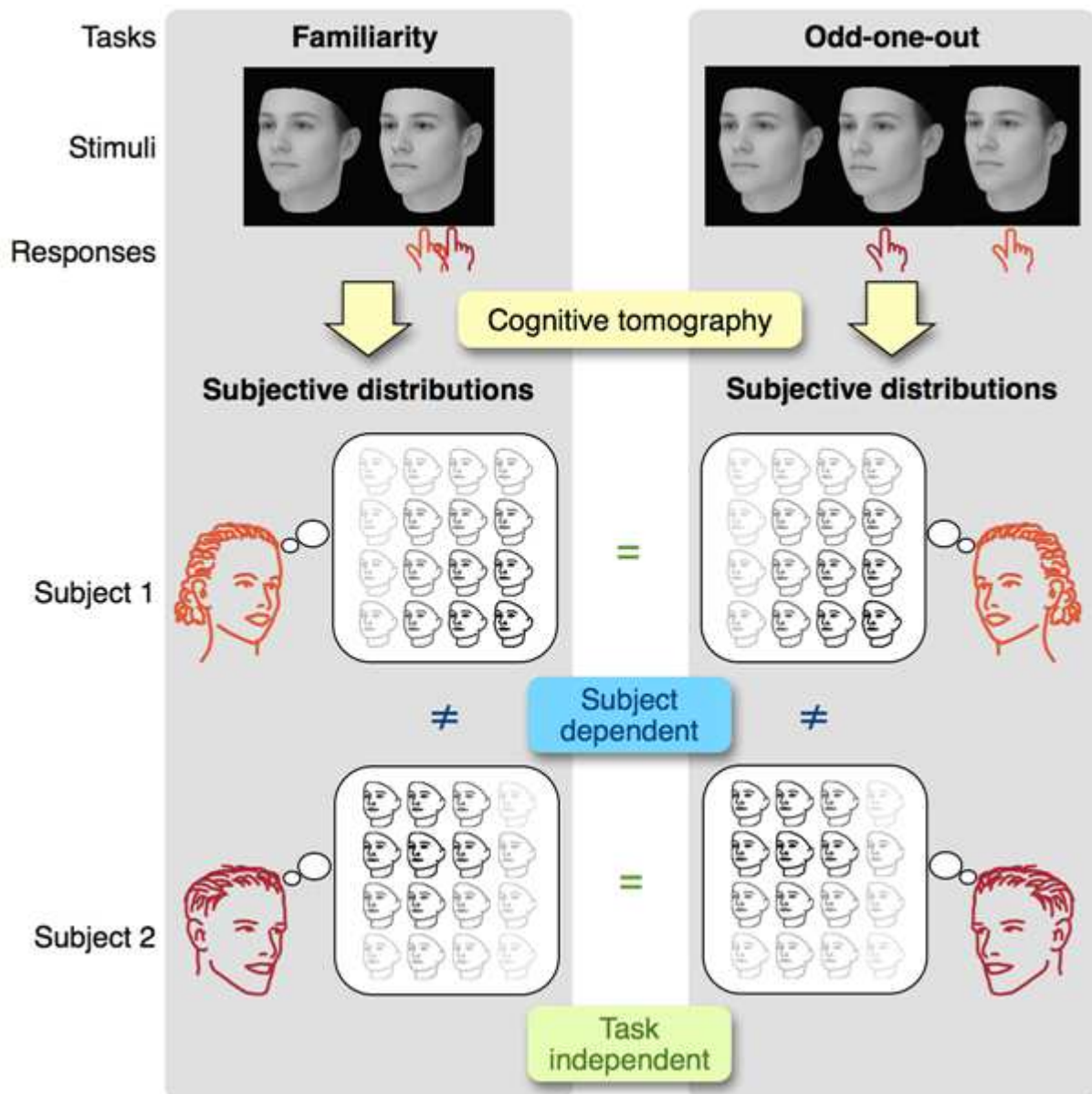
“Momentum” group

**Gergő Orbán**, Mihály Bánay<sup>#</sup>, Előd Gáspár Merse<sup>#</sup>

The nervous system develops rich mental representations that provide support for decisions in the great variety of everyday tasks. However, it has remained unclear whether these representations are specifically tuned for each task or subserve multiple tasks. Mental representations, which are called prior distributions in terms of Bayesian inference, were inaccessible for earlier analysis methods and principled analysis methods to uncover them were lacking. Currently available approaches cannot distinguish between task-specific and task-general mental representations because internal representations obtained by these methods integrate both the model describing the performed task itself and the prior distribution and therefore obtained representations are not comparable. In a collaboration with researchers from the University of Cambridge we developed a method called cognitive tomography that was aimed at tackling the above challenges. Using discrete decisions of humans, cognitive tomography can characterise the features of complex, and high-dimensional mental representations in multiple tasks. Efficiency and predictions of cognitive tomography were tested on a specific stimulus set that was both proven ecologically relevant for humans and everyone has extensive experience with the particular stimuli. As a consequence of extensive experience a strong representation for the particular stimulus set was expected and furthermore since experiences are subjective the specific characteristics of mental representations are expected to change from subject-to-subject. The stimulus set used in our experiments encompassed a wide variety of human faces which varieties could be parametrically controlled in the experimental setup. In order to be able to test the task-dependence of mental representations we used two different tasks to test human subjects: in one, pairs of faces were presented and their familiarity was asked to be assessed by human participants. In the other task participants had to choose from three faces and pick the odd-one-out face. Using cognitive tomography to analyse the responses of human participants measured in the experiments we could demonstrate that prior distributions used to devise decisions are characterised by a complex structure and are varying dramatically across subjects but are invariant across the tasks within each subject. The priors we extract from each task allow us to predict with high precision the behaviour of subjects for novel stimuli and the efficiency of predictions were close to a theoretical upper bound. Furthermore, since cognitive tomography ensures that prior distributions obtained from two tasks are comparable, we could test whether the mental representation that we inferred from the answers given in one task are efficient to predict performance in the other task. This exciting and challenging analysis has shown that the predictions of cognitive tomography hold and human decisions can be predicted across task as well. These results provide the first evidence that naturalistic stimuli are represented using a subjective, high-dimensional and structured mental representations and these representations drive decisions in multiple tasks in a similar manner. These results provide an opportunity to provide independent, behaviour-based regressors for brain imaging technologies for elucidating the neural correlates of complex naturalistic priors.

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<sup>#</sup> Ph.D. student



## Grants and international cooperation

“Momentum” Program of the H.A.S. (G. Orbán, 2012-)

## Publications

### Article

1. Housby NMT, Huszár F, Ghassemi MM, Orbán G, Wolpert DM, Lengyel M: Cognitive Tomography Reveals Complex, Task-Independent Mental Representations. **CURRENT BIOLOGY** 23:(21) pp. 2169-2175. (2013)



## R-H. Hadron physics

Wigner research group

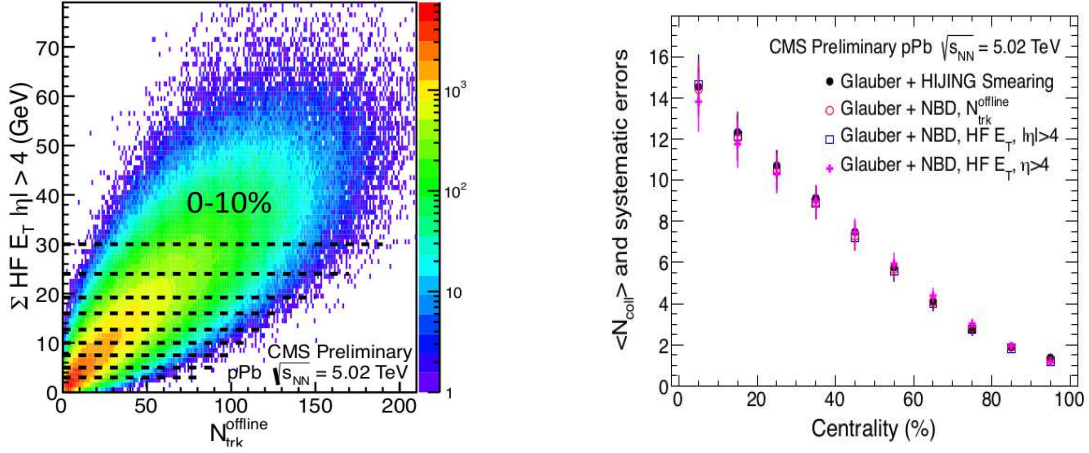
**Ferenc Siklér**, László Boldizsár, Zoltán Fodor, Endre Futó, Sándor Hegyi, Gábor Jancsó, József Kecskeméti, Krisztián Krajczár, András László, Andrew John Lowe, Krisztina Márton, Gabriella Pálla, Sona Pochybová, Zoltán Seres, János Sziklai, Anna Júlia Zsigmond

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

Our research group studies collisions of nucleons and nuclei, performs basic and advanced measurements, and tests theoretical ideas. We participate in several complementary experiments, both in data taking and physics analysis. Hadron-nucleus collisions are important for the interpretation of the properties of nucleus-nucleus collisions and to uncover the partonic structure of nuclear matter at low fractional momenta. Moreover, these collisions are interesting in themselves for answering questions such as: what is the validity of multiple-collision Glauber-model? Can we get a better understanding of the hadronization process? This topic is of particular interest for many theorist colleagues in Hungary and worldwide. The energy range (several TeV) of the LHC enables the use of new and more powerful signals and markers. It is also a region that is relevant for understanding cosmic radiation and atmospheric showers. In the past year several members of our research group participated in data taking and calibration of new pPb data at both the Super Proton Synchrotron (SPS) at CERN and at the LHC: data was collected by the NA61 experiment at the SPS at  $\sqrt{s} = 17$  GeV per nucleon pair, and by the ALICE and CMS experiments at the LHC at  $\sqrt{s} = 5.02$  TeV per nucleon pair. The large amount of collected data allowed us to perform the studies proposed at the beginning of the year.

**Collision centrality.** — To see how much of a heavy ion participates in a collision, a key parameter called centrality must be determined. Centrality is proportional to the number of inelastic proton-nucleon collisions. An estimate of this number is needed when quantities observed in pPb collisions are compared to pp and PbPb results. In the case of heavy-ion collisions, several multiplicity or energy measures are appropriate. They change monotonically with centrality and have a strong correlation due to the high number of particles produced. For pPb collisions, the problem is more complicated: the use of the foregoing methods would result in various biases due to the small number of hadrons created. Our studies show that the number of collisions can be estimated with small bias by

measuring the total energy of the produced particles, that are projected in the direction of the fragmented Pb nucleus. This finding comes from optimizing the weighted sum of the



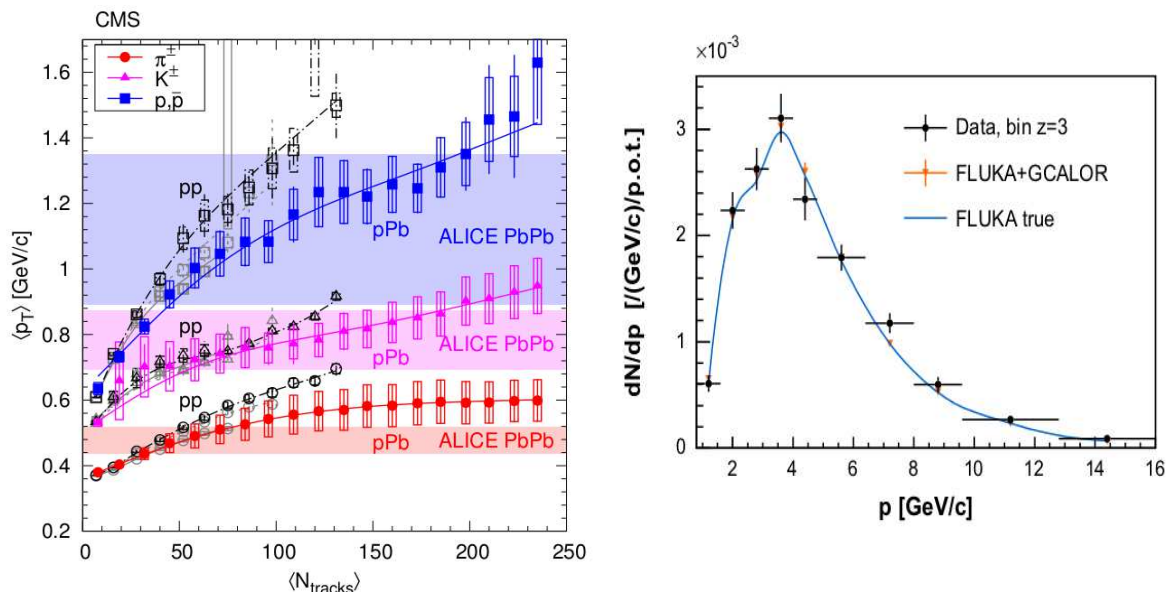
**Figure 1: Left:** The correlation between the number of detected tracks ( $N_{trk}^{offline}$ ) and the energy in the forward calorimeters ( $E_T$ ) in inelastic pPb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV. **Right:** The estimated number of collisions  $\langle N_{coll} \rangle$  and its uncertainty in 10% wide centrality classes. The classifications are based on several measures of centrality.

number of particles produced, where the weights depend on the pseudorapidity of the particle. The best weights are non-zero only for the outer rings of the CMS forward hadronic calorimeter ( $4 < \eta < 5$ ). The corresponding averages and standard deviations were calculated using a Glauber-model (Fig. 1 left).

In the case of NA61 we can directly detect the slow nucleons (protons and nuclei) using a time projection chamber filled with a special gas mixture. It performs simultaneous range and ionization measurements on each charged particle enabling particle identification and momentum measurement at very low momenta. By counting the number of identified protons, the number of collisions can be estimated.

**Momentum distribution of identified particles.** — Charged particles created in collisions of nucleons and nuclei are observed by different kinds of tracking detectors (a gas chamber in NA61 and ALICE; a silicon tracker in CMS). With the help of sophisticated algorithms we can reconstruct their trajectories. Simple measures such as the pseudorapidity density can already be directly compared with those from event generators and theoretical calculations. We have measured the spectra of identified charged hadrons produced in pPb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV using the CMS detector. Charged pions, kaons, and protons were identified from the energy deposited in the silicon tracker and other track information. The yield and spectra of identified hadrons have been studied as a function of the charged particle multiplicity of the event in the range  $|\eta| < 2.4$ . The  $p_T$  spectra are well described by fits with the Tsallis-Pareto parametrization. (This observation stresses the role of non-extensive thermodynamics.) The ratios of the yields of oppositely charged particles are close to unity, as expected at mid-rapidity for collisions at multi-TeV energies. The average  $p_T$  is found to increase with particle mass and with charged particle multiplicity. The EPOS LHC event generator reproduces several features of the measured distributions. This is a significant improvement from the previous version, which is attributed to a new viscous hydrodynamic treatment of the produced particles. Other studied generators (AMPT, HIJING) predict

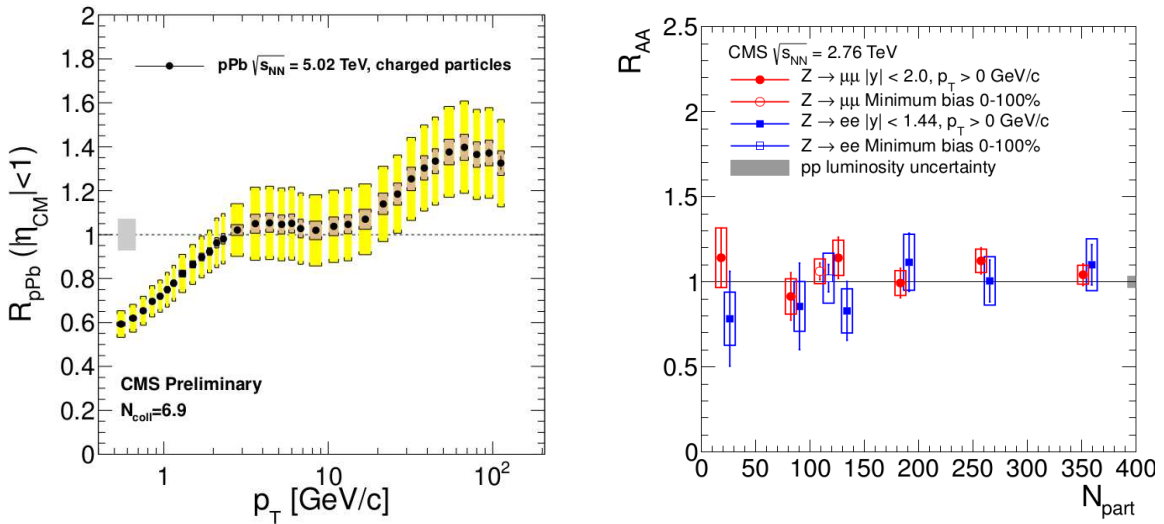
steeper  $p_T$  distributions and much smaller  $p_T$  than found in data, as well as substantial deviations in the  $p/\pi$  ratios. Combined with similar results from pp collisions, the track multiplicity dependence of the average transverse momentum and particle ratios indicate that particle production at LHC energies is strongly correlated with event particle multiplicity in both pp and pPb interactions (Fig. 2). For low track multiplicity, pPb collisions appear similar to pp collisions. At high multiplicities, the average  $p_T$  of particles from pPb collisions with a charged particle multiplicity of  $N_{\text{tracks}}$  (in  $|\eta| < 2.4$ ) is similar to that for pp collisions with  $0.55 \times N_{\text{tracks}}$ . Both the highest-multiplicity pp and pPb interactions yield higher  $p_T$  than seen in central PbPb collisions.



**Figure 2:** *Left:* Average transverse momentum  $\langle p_T \rangle$  of identified charged hadrons (pions, kaons, protons) as a function of the corrected track multiplicity for  $|\eta| < 2.4$ , for pp collisions (open symbols) at several energies, and for pPb collisions (filled symbols) at  $v_{NN} = 5.02$  TeV. Lines are drawn to guide the eye. The ranges of  $\langle p_T \rangle$  values measured by ALICE in various centrality PbPb collisions at  $v_{NN} = 2.76$  TeV are indicated with horizontal bands. **Right:** Spectra of outgoing positively charged pions normalized to the momentum bin size and number of protons on target in the angular interval 40–100 mrad for the central longitudinal bins. Error bars correspond to the sum in quadrature of statistical and systematic uncertainties. Smooth curves show the prediction of the FLUKA simulation.

Data from hadron-nucleus collisions are valuable for other areas such as atmospheric showers, and consequently for neutrino physics. The T2K long-baseline neutrino oscillation experiment in Japan needs precise predictions of the initial neutrino flux. We have shown that the highest precision can be reached based on detailed measurements of hadron emission from the same target as used by T2K exposed to a proton beam of the same kinetic energy of 30 GeV. The corresponding data were recorded by the NA61 experiment using a replica of the graphite target. In the global framework of accelerator-based neutrino oscillation experiments, it has been demonstrated that high quality measurements can be performed with the NA61 setup. They could lead to a significant reduction of systematic uncertainties on the neutrino flux predictions in long-baseline neutrino experiments.

**Momentum distribution at high momenta.** — In the presence of the hot and dense medium created in heavy-ion collisions, the yield of high momentum particles is suppressed compared to independent superpositions of nucleon-nucleon collisions. What is the situation in pPb collisions? Do we also see a suppression, or something else? We have measured the spectra of charged particles and the nuclear modification factor for pPb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV using data taken by the CMS experiment. The results were normalized to a pp reference spectrum derived from a scaled combination of 0.9, 2.76, and 7 TeV pp spectra measured by CMS, as well as 0.63, 1.8, and 1.96 TeV pp spectra measured by CDF. The nuclear modification factor  $R_{pPb}$  shows a steady rise to unity until a  $p_T \approx 4$  GeV/c, is then constant until approximately 20 GeV/c, and then increases at higher  $p_T$  reaching a value around 1.3–1.4 at 70 GeV/c (Fig. 3 left). It is extremely interesting that the rise above unity of  $R_{pPb}$  is in the range of  $p_T$  where parton anti-shadowing is predicted (with momentum fractions of  $x = 0.02$ – $0.2$ ). However, the maximum measured value of  $R_{pPb}$  is significantly larger than the value expected from anti-shadowing in nuclear parton distribution functions (nPDFs) obtained from globally analyzed fits to nuclear hard-process data. The forward-backward asymmetry was also evaluated in various  $\eta$  ranges. Similar anti-shadowing effects are observed in the positive and negative  $\eta$  regions resulting in a ratio close to unity.



**Figure 3: Left:** The nuclear modification factor ( $R_{pPb}$ ) of charged particles measured in  $\sqrt{s_{NN}} = 5.02$  TeV pPb collisions as a function of transverse momentum ( $p_T$ ). **Right:** The nuclear modification factor ( $R_{AA}$ ) for Z bosons measured in  $\sqrt{s_{NN}} = 2.76$  TeV PbPb collisions, from the decay channels  $Z \rightarrow e^+e^-$  (squares) and  $Z \rightarrow \mu^+\mu^-$  (dots) as a function of collision centrality (here, the number of participant nucleons  $N_{part}$ ). The points were shifted for clarity.

**Weak bosons.** — By colliding heavy nuclei we can recreate the Universe as it was some microseconds after the Big Bang. In contrast to hadrons, weakly interacting bosons ( $\gamma$ ,  $W^\pm$ ,  $Z$ ) can escape the hot and dense medium unchanged. Their decay to lepton pairs is clearly seen by the CMS detector, since its capabilities in this field are excellent. We have studied the production of Z bosons in both dimuon and dielectron decay channels in PbPb and pp collisions at  $\sqrt{s_{NN}} = 2.76$  TeV using the CMS detector. The nuclear modification factor  $R_{AA}$  was calculated to study the effect, that the medium formed in PbPb collisions has on Z

production. We find the  $R_{AA}$  for centrality integrated Z-boson production in the dimuon channel to be  $1.06 \pm 0.05(\text{stat}) \pm 0.11(\text{syst})$  and in the dielectron channel to be  $1.02 \pm 0.08(\text{stat}) \pm 0.17(\text{syst})$ . Therefore, the production of Z bosons in both decay channels in PbPb collisions is consistent with scaling of the pp cross section with the number of binary collisions. The scaling is seen to hold in the entire kinematic region studied, as expected for a colorless probe that is unaffected by a deconfined quark-gluon plasma. The ongoing study of the properties and the production of these particles created in pPb collisions will be important in the comparison with PbPb interactions.

## Grants and international cooperation

OTKA NK 106119, „Attometer physics phenomena: experimental and theoretical studies at the CERN LHC ALICE”

OTKA NK 81447, „Hungary in the CMS experiment of the Large Hadron Collider”

OTKA K 81614, „New analysis methods and tests of quantum chromodynamics at the LHC”

OTKA NK 109703 „Consortional main: Hungary in the CMS experiment of the Large Hadron Collider”

EC FP7 C 262025, „Advanced European Infrastructures for Detectors at Accelerators (AIDA)”

„Wigner research group” support

## Publications

### Articles

1. Agócs AG et al. incl. Barnaföldi GG, Bencédi G, Bencze G, Berényi D, Boldizsár L, Futo E, Hamar G, Kovacs L, Lévai P, Molnar L, Varga D [50 authors]: R&D studies of a RICH detector using pressurized  $C_4F_8O$  radiator gas and a CsI-based gaseous photon detector. **NUCL. INSTRUM. METHODS A** 732:(21) pp. 361-365.(2013)
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## CMS collaboration

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1. Chatrchyan S et al. incl. [Bencze G](#), [Hajdu C](#), [Hidas P](#), [Horvath D](#), [Sikler F](#), [Veszpremi V](#), [Vesztergombi G](#) [2197 authors]: Evidence for associated production of a single top quark and W Boson in pp collisions at  $\sqrt{s}=7$  TeV. *PHYS. REV. LETT.* 110:(2) Paper 022003. 25 p. (2013)
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**See also: R-C.2**



## R-I. “Lendület” innovative particle detector development

“Momentum” group

**Gergő Hamar**, Dezső Varga, Gyula Bencédi, Ervin Dénes, Gábor Kiss, Tivadar Kiss, László Oláh, Tamás Tölyhi

The Detector Physics Research Group has undergone considerable restructuring during the summer of 2013, and this is apparent both in the change of the name, and in the shift of the research objectives. During the first half of the year the gravity has been on the consolidation of the results, whereas starting from 15th July, owing to the successfully achieved “Momentum” support from the Hungarian Academy of Sciences, the developments towards more ambitious perspectives have been undertaken.

The key research projects were the following:

- High position resolution, single UV photon scanning system for microstructure gaseous detectors. The system has been developed with the aim of optimization of UV sensitive gaseous detectors. We have obtained the financial support of the CERN RD51 Collaboration for the project (Common Funded Project), and during the year we have built the final prototype.
- Cosmic muon detection for geophysical applications. The Muon Tomograph detector system, built by our group, has been applied for underground measurements at various locations, demonstrating the applicability of the device for soil density measurements. The detector has also been applied to measure cosmic muon background: the angular dependence of the muons, reaching underground to the proposed low-background site in Felsenkeller (Germany) was evaluated.
- Innovative gaseous detector development. We have successfully combined the Thick GEM technology with multi-wire proportional chambers, and proved its applicability for high efficiency Cherenkov radiation detection.
- In the framework of the NA61 Collaboration, we have concentrated on proton-nucleus interactions. In such collision systems the determination of event centrality plays a key role, however this is particularly problematic due to the few number of produced particles. We have earlier built a detector (the LMPD) for the NA61 experiment, which addresses specifically the characterization of event centrality via counting of low momentum protons. This device has been operated in physics data taking of the NA61 proton-lead runs. We have prepared a technical paper on the working principle and commissioning of the pertinent detector.
- The experts of our DAQ team continued to provide software, firmware and hardware support for the operation and continuous development of the Detector Data Link (DDL) system of the ALICE experiment. During the ongoing first long shut-down in 2013-14, the Read-out Receiver Cards (RORC) of several subdetectors will be replaced by a new, much higher performance custom FPGA card, the C-RORC, which will serve as a new common read-out card for the Data Acquisition (DAQ) and the High-Level Trigger Farm (HLT). The integration of this new hardware into the ALICE software environment is completed. The Wigner RCP is the responsible institute of the development of the new Common Read-out Units (CRU) that will be a central element of the new, upgraded read-out system.

The tasks of the newly established “Momentum” research group for the first year include the realization of an internationally competitive lab framework for the development of gaseous detectors. We have refurbished practically all the available laboratory spaces, including two new sites as well. The completed critical infrastructures are the following:

- Gas distribution system, for precision mixing of various high purity gases
- Clean compartment, optimized for microstructure and traditional gaseous detector handling, construction, and maintenance

## Grants and international cooperation

KTIA/OTKA CK77815: Micro-pattern particle detector development in the framework of the CERN RD51 Collaboration

“Momentum” Program of the HAS

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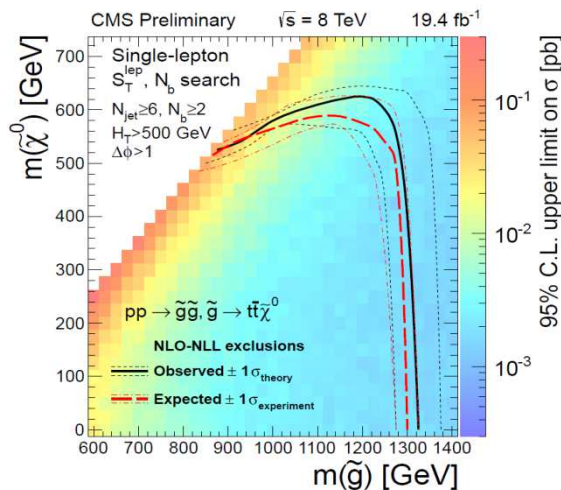
See also: R-H.1

## R-J. Standard model and new physics

Wigner research group

**Viktor Veszprémi**, Dániel Barna, Márton Bartók, Lajos Diósi, Ferenc Glück, Csaba Hajdu, András Házi, Pál Hidas, Dezső Horváth, István Manno, Gabriella Pásztor, József Tóth, Tamás Vámi, György Vesztergombi, István Wágner

During the past few decades the Standard Model (SM) of particle physics has been tested in various experiments to great precision and has been found to be immensely successful in describing particle interactions up to the electroweak scale. Nevertheless, there are arguments for the existence of physics beyond the SM, such as the inability of the model to describe physics at the energy scale at which quantum gravitational effects become important. The Standard Model cannot account for the dark matter that dominates our Universe, it does not predict an exact unification of the fundamental gauge interactions, and it does not explain the matter-antimatter asymmetry. It also suffers from the so-called "hierarchy" problem. By this, we mean that the mass of the Higgs boson acquires quantum corrections that are much larger than the actual mass of the Higgs. The situation worsens if we assume that there is physics beyond the SM. This is because if new physics manifests itself in the form of new particles that couple to the Higgs field, that is to say, they have mass, they must also contribute to the Higgs boson mass. These corrections contribute negatively in the case of bosons, and positive in the case of fermions. Maintaining the existence of a light Higgs boson requires that all these contributions somehow cancel each other. Such a cancellation appears naturally in theories with supersymmetry (SUSY). If SUSY exists, it could provide a dark matter candidate, and it could make the unification of fundamental forces exact at energies from  $10^{14}$  to  $10^{16}$  GeV. It would also mean that the new particle we discovered in 2012 is not exactly the SM Higgs boson, but rather one of the SUSY Higgs bosons which looks very much like it. Our group has set out a goal to investigate these questions from various experimental angles in analyses of high energy proton collision



**Figure 1:** Exclusion limit in the parameter space of the simplified model as a function of the gluino and LSP masses.

events. We also build and maintain detectors and software systems for data-calibration and reconstruction which are used in the measurement of the physical processes that take place in these collisions.

**Physics analyses.** — The Minimal Supersymmetric Standard Model (MSSM) is one of the most promising extensions of the SM that incorporates SUSY. Our group has performed searches with the Compact Muon Solenoid (CMS) experiment at the Large Hadron Collider (LHC) at CERN. We have focused on simplified models in which gluino pairs are produced in proton-proton collisions. Each gluino decays into a top quark and its supersymmetric partner, the scalar top. The scalar tops subsequently decay into tops, yielding four top quarks and

the lightest SUSY particle (LSP), a possible dark-matter candidate, in the final state:

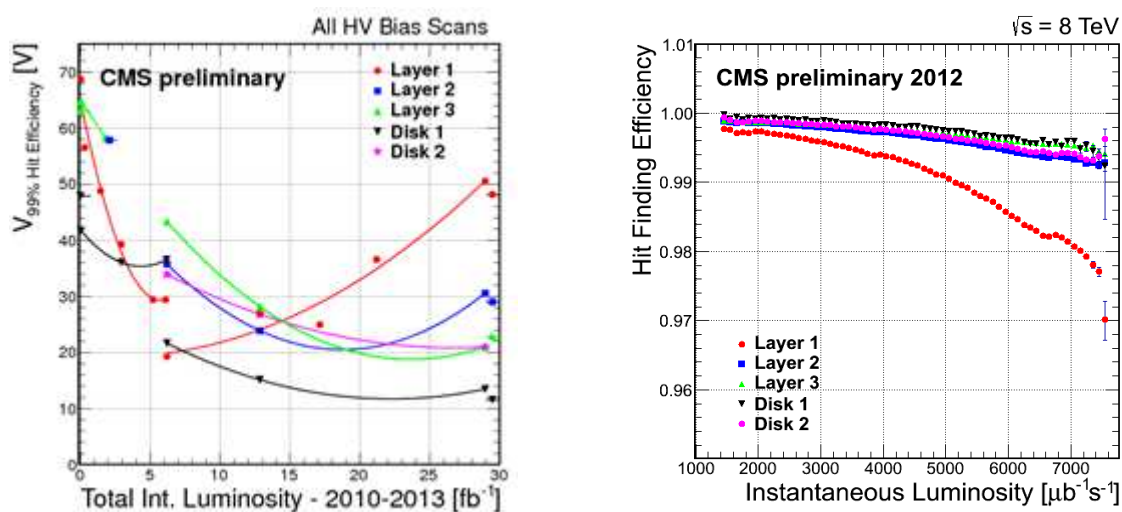
$$pp \rightarrow \tilde{g}\tilde{g} \rightarrow t\bar{t}t\bar{t} \rightarrow t\bar{t}t\bar{t}\chi^0\chi^0$$

Top quarks are identified using a standard analysis method called b-tagging as they decay almost exclusively into b-quarks. We extended the exclusion limits (Fig.1) of this simplified process in events which contain an electron or muon, b-quarks, and multiple jets.

The effect of new particles' appearance on the Higgs boson mass can be turned to our advantage in searching for new physics. Exploring the fundamental properties of the recently discovered Higgs boson can provide a portal to uncharted territories. Any new particle is expected to modify the coupling constants of the Higgs boson to known particles which are easier to detect. Our CMS and ATLAS groups have been making advancements in the study of the Higgs boson properties.

The existence of the asymmetry that is observed in the ratio between the amount of matter and antimatter in the Universe is unexplained by the SM. Despite fundamental theoretical arguments, the properties of matter and antimatter might be different. Two of our group members have been participating in a small experiment, called ASACUSA, at CERN's Antiproton Decelerator (AD), with ground-breaking results on laser spectroscopy of antiprotons trapped by Helium atoms.

**Detector calibration and measurement methods.** — b-quarks are generated in the decays of third generation squarks, and b-production is also the dominant decay mode of the Higgs boson. Their detection is a powerful tool in physics searches; however, it poses the greatest challenge from the instrumentation point of view. The identification (or "tagging") of jets originating from b-quarks depends on high-precision tracking measurements. Hadrons containing b-quarks have a unique feature: they have sufficient lifetime that they travel some distance (typically a few millimetres) before decaying, and consequently the tracks corresponding to their charged decay products intersect at a vertex that is measurably displaced from the collision point.



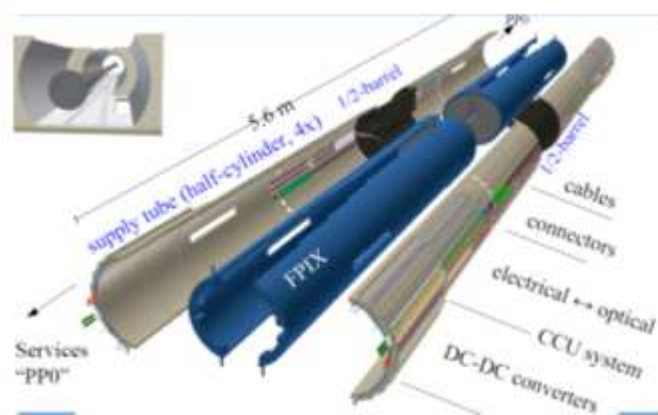
**Figure 2:** *Left:* Pixel measurement efficiency in various tracking layers of the detector as a function of total integrated collision data. *Right:* Instantaneous luminosity

We participate in the running and maintenance of a high-precision charged particle tracking device in CMS, the pixel detector. The pixel detector provides key measurements for purposes additional to b-tagging. It is also used in the reconstruction of primary vertices in the LHC, lepton identification, and data luminosity measurements.

In the last three years our group leader has also been serving as the group leader of the pixel calibration, reconstruction, and simulation (pixel offline) group in CMS. Naturally, we have a strong contribution to the results in pixel offline. We are maintaining the calibration database used in the reconstruction of the data taken by the pixel detector. The pixel detector is the innermost device in CMS. It is situated at a distance of less than 4 cm from the nominal collision point of the LHC beams. Consequently, it is exposed to high level of radiation which cause the physical properties of the pixel sensors to continuously change (Fig. 2 left). The most important role of the pixel offline group is to understand this change and correct for it with proper calibrations. Thorough studies have been performed by our group. A senior member and a graduate student have developed a new method to simulate the efficiency loss of the pixel detector that occurs at high collision rates, as shown in (Fig. 2 right). This effect leads to loss of efficiency and resolution in the reconstruction of charged particles, in the detection of b-quarks, and in the measurement of the amount of collision data delivered by the LHC. Therefore, the proper understanding of this effect is very important in the statistical interpretation of all physics results.

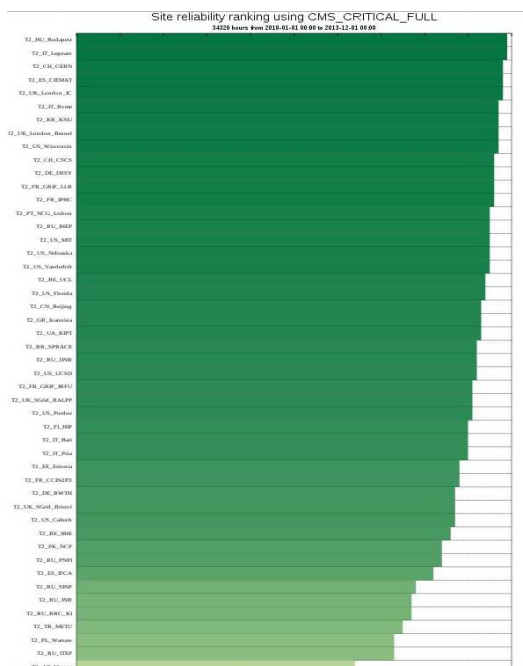
The pixel detector is surrounded by the strip detector, another charged particle tracking device. Both detectors are installed within the CMS magnet, which is the largest superconducting solenoid magnet ever built. The structures of these tracking devices can move and become distorted by various effects, such as changes in temperature within the enclosure or magnet power-cycling. Knowledge of each module's position in three-dimensional space with a precision better than the intrinsic resolution of the tracker detectors is required for track reconstruction when measurement points localised on individual modules are placed into the common frame of CMS. We have played a significant role in the measurement of this information.

**Detector upgrades.** — Due to its position closest to the LHC beams, the pixel detector is exposed to more beam radiation than any other detector in CMS. The continuous increase of the instantaneous luminosity in the LHC will worsen these effects. Radiation-induced damage of sensors and readout electronics degrades the resolution of position measurements to the extent that the detector is rendered unusable. Therefore it will need to be replaced. This will happen in two steps, called phase I and phase II upgrades, in the next couple of



**Figure 3:** Picture of the supply tube mechanics situated on the two sides of the detector barrel. The supply tube holds the control electronics (CCU system and electrical-optical converters.)

decades. Our group has played a leading role in studying radiation effects and we are now also key contributors to the design of the new-generation pixel detector. The new pixel detector can be thought of as a large digital camera without the optical apparatus (Fig. 3). It consists of semiconductor sensors arranged coaxially on a mechanical structure serving as its frame. It receives power from DC-DC converters. The settings of the pixel detector's sensors, the measurement triggers, and the data read-out are regulated by its control electronics. The barrel detector has been developed by multiple institutes, most of which are located in Europe. Countries with participating institutes include Switzerland, Germany, the UK, and Hungary. The sensors are developed at the Paul Scherrer Institute (PSI) in Zurich. Modules are bump-bonded and assembled in various institutions in Germany and in Switzerland. The mechanical structure is built at the University of Zurich. The DC-DC converter boards are constructed at DESY in Germany. The control electronics are designed by our group at Wigner RCP. We presented our results in a CERN-wide peer-review committee last December. Modules closer to the interaction point need to measure a larger flux of particles than those farther away. These measurements also need to be made earlier due to differences in the module-to-interaction point distance. Based on the experience we have acquired with the present system, we designed the new detector electronics so that the data-acquisition time of its modules are aligned according to the time-of-flight of the incoming charged particles. The grouping of the modules in the data read-out is designed so that their read-out bandwidths are balanced equally among read-out units. The solution to the problem of how this latter requirement should be met is based on a realistic simulation of the 2017 LHC accelerator conditions by an undergraduate student in our group as his BSc thesis work.



**Figure 4:** Site availability in the CMS Tier-2 computing network from 2010 to 2013. The Budapest site is at the first place with ~98% efficiency.

**Computing infrastructures.** — The Worldwide LHC Computing Grid (WLCG) is a computing network with sites distributed on five continents. Our group maintains a Tier-2 level site at Wigner RCP. It consists of about 350 CPUs and over 250 TB of storage space. About two-thirds of the site is dedicated to the CMS project, supporting the physics analyses (SUSY and QCD) we perform at Wigner RCP, common CMS data-processing work, and computational tasks required for the calibration of the pixel detector. In 2013, our group members performed a total upgrade of the computing infrastructure: the computers have been moved to a new cooling solution, and their entire software framework system has been upgraded to the new version required at the restart of LHC data-taking which is due within a year. Thanks to continuous efforts in 2013, our Tier-2 site has become the most efficient Tier-2 system in CMS (Fig. 4). Our expert members also provided help to our

colleagues at Debrecen University to make their new Tier-3 site a certified CMS computing center by the end of last year. We have also installed a new multi-CPU user interface computer which is used by many members of our group for interactive analysis work

**Theoretical work.** — Our group is also active in fundamental theoretical work in quantum mechanics, especially in the field of quantum gravity. We have one member working on this: Lajos Diósi. His theoretical work on the spontaneous collapse of the wave function of massive objects has motivated a boom of experiments in Europe and in America. The role he played in the foundation of the theory along with Roger Penrose of Oxford was acclaimed in a recent article in Scientific American.

## Grants and international cooperation

OTKA NK 81447, „Hungary in the CMS experiment of the Large Hadron Collider”

OTKA NK 109703 „Consortional main: Hungary in the CMS experiment of the Large Hadron Collider”

„Wigner research group” support

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### ATLAS collaboration

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## R-K. Femtosecond spectroscopy and X-ray spectroscopy

“Momentum” group

**György Vankó**, Csilla Bogdán, Zoltán Németh, Mátyás Pápai<sup>#</sup>, Emese Rozsályi, András Szabó, Dorottya Szemes

Information technology requires advanced materials with special transport properties and excitation characteristics. *Strongly correlated oxides based on transition metals* play already an important role in innovative technologies. In these compounds the interplay of spin, electron, lattice and valence degrees of freedom leads to special transport properties, such as high-temperature superconductivity or colossal magnetoresistance. Besides oxide or metal-based nano-scaled devices, *switchable molecular compounds* with a transition metal center have great potential as very high-density devices. Switching of such compounds between their (meta)stable states usually proceeds through excited states; the excitation characteristics are determined by the strongly coupled electron, magnetic, and structural dynamics. Understanding the microscopic origin of the behaviour of these materials, and thus motivating developments in the field, is only possible after the fine details of their electronic structure, their valence, spin and magnetic states are revealed. Synchrotron-radiation-based *high-resolution X-ray spectroscopies* can provide element-selective insights into many of the relevant characteristics of the above materials in their different states and during the transitions: these techniques are able to characterize the occupied and unoccupied electronic density of states, the spin state, the valence excitations, the coordination number and local geometry.

Understanding the elementary steps of transitions is an essential goal in the research on these systems. Transformations at the atomic and molecular level take place at time scales ranging from femtoseconds to nanoseconds. In order to address the elementary 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. The pulsed nature of light from synchrotrons and the new free electron lasers offer the opportunity to exploit them as probes to study the electron dynamics with picosecond and femtosecond time resolution, respectively. This allows us to implement and employ hard X-ray techniques to study the intermediates of the switching of molecules. At the same time, this also opens up the opportunity to extend these *time-resolved studies* to a wide range of molecular transformations to unveil the transient species in molecular reactions, phase transitions or biochemical functioning, which are essential for the functioning of molecular storage or switching devices, light-harvesting systems, catalysts, enzymes, to name a few.

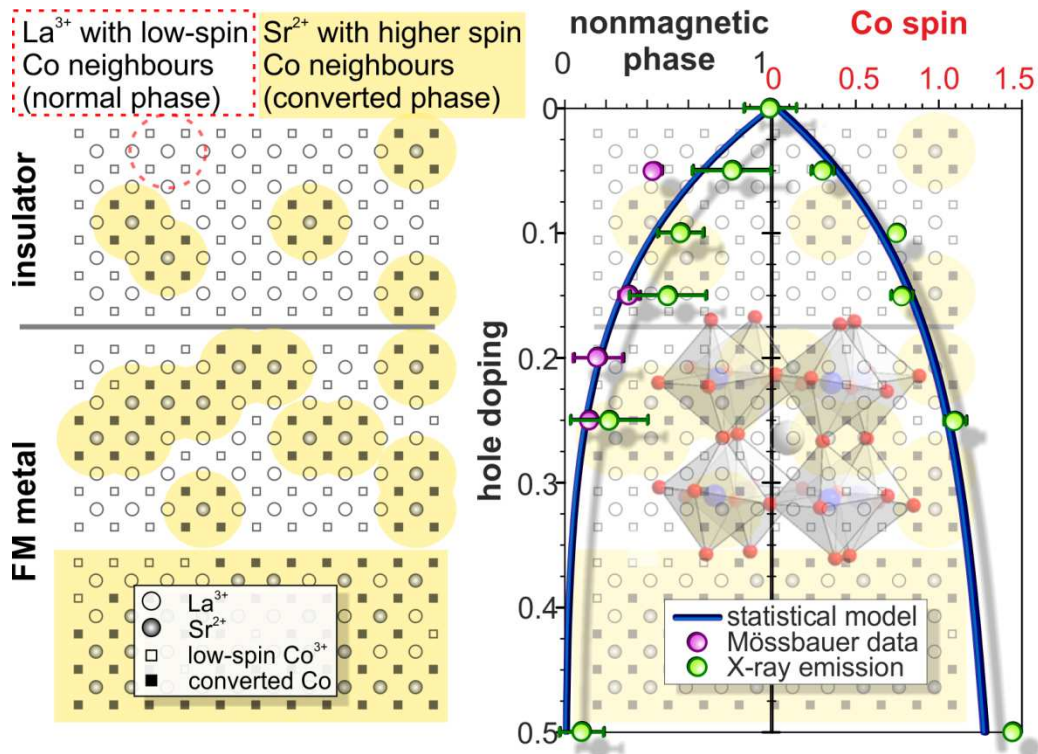
However, it is vital to complement the time-resolved X-ray studies (performed at remote facilities) with an extensive local in-house research programme of *optical pump-probe* investigations. Such experiments can provide essential information on the excitation characteristics, the bleach of the ground state, the formation and decay of transient states, the relevant lifetimes and branching ratios. Therefore, we are in the process of realizing a local optical pump-probe facility, which will allow us to study the ultrafast dynamics on the

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<sup>#</sup> Ph.D. student

fs to ns time scales through the transient absorption spectra in the slightly extended visible region. With our *theory programme* we make strong efforts to describe all molecular states, their energetics, and possibly the branching ratios and the lifetimes, which shall also facilitate the interpretation and even the design of the experiments.

In what follows, recent results related to the above aims are reported.

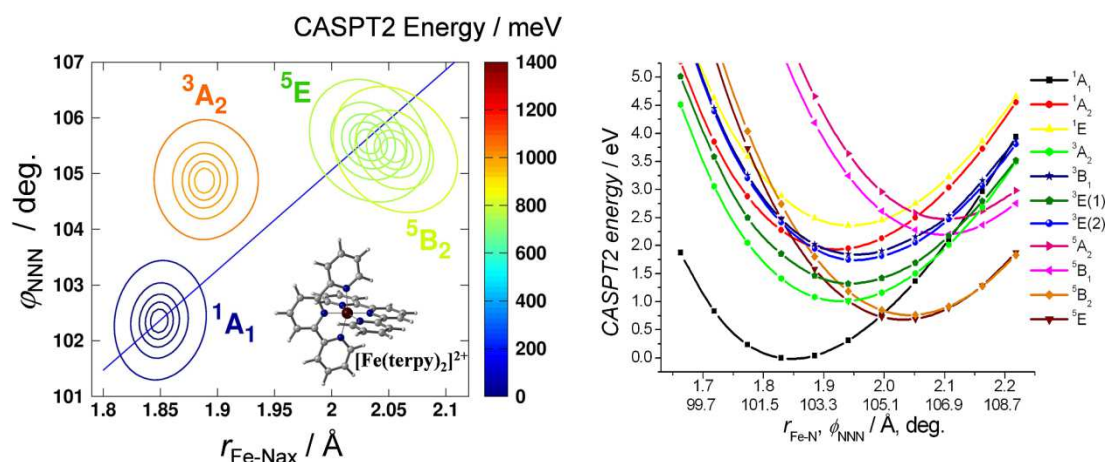


**Figure 1.** *Left:* Illustration of the possible formation of converted magnetic clusters at different hole concentrations in  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$   $0 \leq x \leq 0.5$ . *Right:* Experimental data compared to a statistical model describing the variation of the Co spin momentum as well as the phase fractions as a function of doping (right).

**Microscopic origin of nanometer-scale magneto-electronic phase separation in perovskites.** — In complex oxides that exhibit extraordinary magnetic and transport properties (for instance magnetoresistance (MR), an essential phenomenon in hard disk drives), nanometer-scale magneto-electronic phase separation (MEPS) has long been observed. Curiously, this phenomenon, which is believed to have a major role in the colossal variations in the MR, takes place in a chemically homogeneous phase. Due to the local nature of this phase separation, it is difficult to grasp the coexisting tiny magnetic phases experimentally. Also, despite of its prime importance, the origin of the phenomenon is far from being understood even though relevant research efforts have been conducted in the recent decades.

Utilizing local investigation techniques, we were able to give a direct experimental evidence for the coexistence of the separated nanoscale phases in Sr-doped  $\text{LaCoO}_3$  perovskites. Mössbauer spectroscopy and synchrotron-based hard X-ray spectroscopies provided a local picture of the composition, electronic and spin structure, and relative amount of these nanoscale phases. A simple model describing how the hole doping affects the local spin

momentum and the magnetism are in excellent agreement with the data, and sheds light on the microscopic origin of the nanoscale magneto-electronic phase separation.

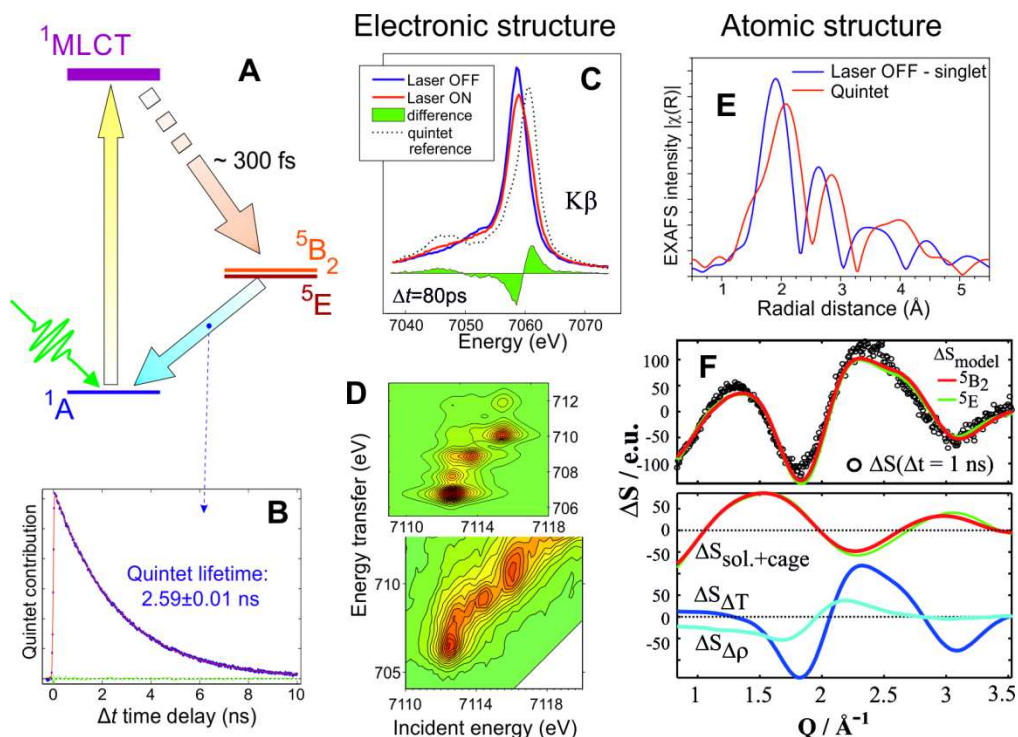


**Figure 2.** *Left:* CASPT2 2D potential energy surfaces of the  $[\text{Fe}(\text{terpy})_2]^{2+}$  complex for the lowest singlet, triplet and quintet states. *Right:* 1D potential energy curves along the combined coordinate connecting the  $^1A_1$  and the  $^5E$  state.

**Molecular transitions and electronic structure: quantum chemical studies.** — Switchable molecular Fe(II) complexes are very promising candidates for high-density magnetic storage and data devices, since their electronic  $\text{Fe-}3d^6$  configuration can be switched back and forth between a low-spin (LS,  $S = 0$ ) singlet and a high-spin (HS,  $S = 2$ ) quintet state. First-principle theoretical modeling of the properties of these materials, including the determination of the potential energy curves of the electronic states involved in the mechanism of the molecular switching can facilitate the interpretation of the experimental data, and lead to a better understanding of the behaviour of these systems. We have carried out a theoretical investigation on the  $[\text{Fe}(\text{tz})_6]^{2+}$ ,  $[\text{Fe}(\text{bipy})_3]^{2+}$  and  $[\text{Fe}(\text{terpy})_2]^{2+}$  complexes, which have been actively studied experimentally, and with their respective mono-, bi-, and tridentate ligands, they constitute a comprehensive set for theoretical case studies. While molecules with mono- and bidentate ligands can be described to vary along a single configuration coordinate based on the Fe–N bond lengths, anomalous lifetimes observed for the  $[\text{Fe}(\text{terpy})_2]^{2+}$  indicated that the latter system requires a more complex description. In this report we describe only findings on this system. Density functional theory (DFT) can provide reliable results for the ground state properties of these relatively large molecular systems with an open  $d$ -shell, excited states require more involved calculations. We have obtained the singlet, triplet and quintet potential energy curves for the investigated compounds obtained with both time-dependent density functional theory (TD-DFT) and multiconfigurational second-order perturbation theory (CASPT2). The results indicate that both methods provide reliable energetics for the experimentally observed singlet-quintet spin-state transition in these molecular Fe systems. In particular, the DFT and CASPT2 LS-HS state splitting energies (which parameter is decisive for the lifetime of the excited HS state) are both in good agreement with the experimentally expected values.

Additionally, the two dimensional (2D) potential energy surfaces above the plane spanned by the two relevant configuration coordinates in  $[\text{Fe}(\text{terpy})_2]^{2+}$  were successfully determined with both DFT and CASPT2. The two modes needed for the description are

associated with the bond length of the middle nitrogen ( $N_{ax}$ ) and the Fe, and with the NNN “bite” angle of the ligands. These 2D surfaces indicate that the singlet-triplet and triplet-quintet states are separated along these different configuration coordinates, i.e. different vibration modes. Our results confirm that in contrast to the case of complexes with mono- and bidentate ligands, the singlet-quintet transitions in  $[Fe(terpy)_2]^{2+}$  cannot be described using a single configuration coordinate.



**Figure 3.** X-ray results on the quintet state of the  $[Fe(terpy)_2]^{2+}$  complex. **A** the excitation and relaxation scheme. **B** X-ray spectral intensity of the quintet state reflecting a lifetime of 2.6 ns. **C**  $K\beta$  XES shows 40% quintet yield 80 ps after the light excitation. **D** The  $1s2p$  RIXS spectra of the transient shows the conversion of the  $d$  electron states to the quintet (top: high-spin  $3d^6$  calculated with multiplet theory, bottom: measured). **E** Structural changes upon transition around the  $Fe^{2+}$  ion as reflected by EXAFS, and the variation of the dynamical structure factor of the molecule and **F** the solvent cage reflected by X-ray diffuse scattering.

Ultrafast molecular transitions: X-ray studies — Unveiling the elementary steps of light-induced molecular switching requires ultrafast pump-probe experiments. The modern X-ray sources provide X-ray light in short pulses, that makes possible picosecond-resolved studies at synchrotrons, and femtosecond-resolved investigations at the emerging free electron lasers, which allows us to introduce new high-performance X-ray probes into structural dynamics research. Our group has been making relevant efforts to implement element-sensitive high-resolution X-ray spectroscopy as probes in ultrafast experiments. Here we report on the detailed characterization of the quintet excited state of a photoswitchable model system,  $[Fe(terpy)_2]^{2+}$  (discussed above in the theoretical results), that is populated on the subpicosecond time scale after light excitation with an ultrashort green laser pulse into the metal-to-ligand charge-transfer (MLCT) states. The nature of the intermediates in this process are debated, and we expect they will soon be unravelled in fs-resolved XFEL experiments. Nevertheless, the long lifetime of the quintet state allowed us to investigate it

in great detail with synchrotron radiation. Scattering and spectroscopy hard X-ray techniques have been joined to characterize the atomic and electronic structure of this state, which is reported in Figure 3. X-ray emission, being sensitive to the occupied electron density of states (DOS) and the total spin momentum of the transition metal, shows an unambiguous transition to a quintet state. The X-ray absorption near edge structure (XANES) maps out the unoccupied electron DOS, which agrees well with the simulated spectra based on the theoretical structures (not shown). The structural techniques, the X-ray diffuse scattering as well as the extended X-ray absorption fine structure (EXAFS) are also in good agreement with the theoretically predicted structures, and they reveal that a variations over a single configuration mode are insufficient, and thus two modes predicted by theory are required at the singlet-to-quintet transition in this system. A more involved experimental technique, 1s2p resonant inelastic X-ray scattering (RIXS) has also been applied for the first time in time-resolved studies with hard X-rays; it reflects the formation of the quintet state; more detailed information on the electronic structure are expected when these structures are compared to quintet states of the simpler molecules.

## Grants and international cooperation

ERC Starting Grant ERC-StG 259709, ✂-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 H.A.S.: Functional molecules caught in the act: Electronic structure – function relationships studied by femtosecond spectroscopy, G. Vankó, 2013 – 2018

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NFÜ TÉT (French-Hungarian bilateral) Investigation of switching mechanisms in Fe molecular complexes by hard X-ray spectroscopies: contribution from experiments and theory, G. Vankó, 2012–2013

*Main cooperations:* Prof. C. Bressler (Hamburg), Prof. F. M. F. de Groot (Utrecht), Dr. A. Juhin (Paris), Dr. K. Knížek (Prague), Prof. M. M. Nielsen (Copenhagen), Prof. F. Renz (Hannover), Dr. S. H. Southworth (Argonne), Prof. V. Sundström (Lund)

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## S-A. Strongly correlated systems

“Momentum” group

Örs Legeza, Gergely Barcza, Imre Hagymási, Kazumasa Itai<sup>A</sup>, Jenő Sólyom, Szilárd Szalay, Edina Szirmai, Máté Tímár, Ferenc Woynarovich<sup>A</sup>

For some years already, strongly correlated systems that can be realized with ultracold atoms loaded into optical lattices are in the focus of interest. One of the most important reasons behind this is the special unique feature of fermionic alkali-earth metal ions. These systems can have extremely high symmetry like  $SU(n)$  where  $2 < n < 10$ . Due to this high symmetry, it is possible to study numerous novel physical phenomena, including those that do not have analogues in condensed matter physics. Moreover, studying these highly symmetric systems gives very important contribution to quantum information theory and quantum computation. Among others, new results can be expected on transition-metal oxides, heavy-fermion systems or spin-liquid states. Transition-metal oxides have highly unique chemical properties that are direct consequences of their complicated electronic structures, increasing relativistic effects, and appearance of different intermediate states in the chemical reactions. Due to these special properties, the investigation of transition-metal compounds is one of the biggest challenge of quantum chemistry. The density-matrix renormalization-group (DMRG) algorithm that involves numerous concepts of quantum information theory provides an adequate theoretical treatment for both research topics, namely  $SU(n)$  symmetric strongly correlated systems and quantum chemistry, respectively. Furthermore, in these days, the computational resources are developing extremely fast, and they allow us to reproduce various interesting experimental results, too. Other promising directions are the tensor-network-state (TNS) based algorithms which reflect more explicitly the so-called entanglement patterns in strongly correlated systems. These methods may help to understand and simulate physical processes in higher dimensions, and opens the possibility e.g. to determine more precisely the properties of poly-diacetylene which plays an important role in nanotechnology, or to describe the different interaction processes in the two-dimensional graphene. Our main aims are to determine the properties of systems described above by different analytical and numerical methods and to develop new numerical renormalization algorithms exploiting various concepts of quantum information theory.

According to our research plan we have studied various strongly correlated magnetic and electronic systems using analytical methods and numerical approaches. Our results have been presented in international conferences and published in high quality journals. Below we briefly summarize our main results:

**Condensed matter physics.** — We studied theoretically poly-diacetylene chains diluted in their monomer matrix. We employed the density-matrix renormalization-group method (DMRG) on finite chains to calculate the ground state and low-lying excitations of the corresponding Peierls–Hubbard–Ohno Hamiltonian which is characterized by the electron transfer amplitude  $t_0$  between nearest neighbours, by the electron-phonon coupling constant  $\alpha$ , by the Hubbard interaction  $U$ , and by the long-range interaction  $V$ . We treated the lattice relaxation in the adiabatic limit, i.e., we calculated the polaronic lattice

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<sup>A</sup> Associate fellow

distortions for each excited state. Using chains with up to 102 lattice sites, we safely performed the extrapolation to the thermodynamic limit for the ground-state energy and conformation, the single-particle gap, and the energies of the singlet exciton, the triplet ground state, and the optical excitation of the triplet ground state. We determined a coherent parameter set ( $t_0^*=2.4$  eV,  $\alpha^*=3.4$  eV/A,  $U^*=6$  eV,  $V^*=3$  eV) from a fit of the experimental gap energies to the theoretical values which we obtained for 81 parameter points in the four dimensional search space ( $t_0$ ,  $\alpha$ ,  $U$ ,  $V$ ). We identified dark in-gap states in the singlet and triplet sectors as seen in experiment.

In the triplet sector we found a linear dispersion of the excitations which contradicts predictions from field theory calculations on systems with local interactions. We, therefore, checked and reproduced numerically the field theory predictions on simple spin and fermionic systems and systematically switched on long-range interaction, lattice distortion and lattice relaxation effects.

We investigated the behavior of the periodic Anderson model in the presence of d-f Coulomb interaction ( $U_{df}$ ) using mean-field theory, variational calculation, and exact diagonalization of finite chains. The variational approach based on the Gutzwiller trial wave function gave a critical value of  $U_{df}$  and two quantum critical points (QCPs), where the valence susceptibility diverges. We derived the critical exponent for the valence susceptibility and investigated how the position of the QCP depends on the other parameters of the Hamiltonian. For larger values of  $U_{df}$ , the Kondo regime is bounded by two first-order transitions. We showed that these first-order transitions merge into a triple point at a certain value of  $U_{df}$ . For even larger  $U_{df}$  valence skipping occurs.

**Quantum chemistry.** — The accurate calculation of the (differential) correlation energy is central to the quantum chemical description of bond-formation and bond-dissociation processes. In order to estimate the quality of single- and multi-reference approaches, various diagnostic tools have been developed. We showed that one- and two-orbital-based entanglement measures provide quantitative means for the assessment and classification of electron correlation effects among molecular orbitals. The dissociation behavior of some prototypical diatomic molecules features all types of correlation effects relevant for chemical bonding. We demonstrated that our entanglement analysis is convenient to dissect these electron correlation effects and to provide a conceptual understanding of bond-forming and bond-breaking processes from the point of view of quantum information theory.

The accurate description of the complexation of the CUO (Carbon-Uranium-Oxygen) molecule by Ne and Ar noble gas matrices represents a challenging task for present-day quantum chemistry. Especially, the accurate prediction of the spin ground state of different CUO--noble-gas complexes remains elusive. We investigated the interaction of the CUO unit with the surrounding noble gas matrices in terms of complexation energies and dissected into its molecular orbital quantum entanglement patterns. Our analysis elucidated the anticipated singlet--triplet ground-state reversal of the CUO molecule diluted in different noble gas matrices and demonstrated that the strongest uranium-noble gas interaction is found for CUOAr<sub>4</sub> in its triplet configuration.

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

**Quantum chemistry and tensor factorization.** — We presented the Coupled Cluster (CC) method and the DMRG method in a unified way, from the perspective of recent developments in tensor product approximation. An introduction into recently developed hierarchical tensor representations was given, in particular tensor trains which are matrix-product states in physics language. The discrete equations of full CI approximation applied to the electronic Schrödinger equation were casted into a tensorial framework using second quantization. A further approximation is performed afterwards by tensor approximation within a hierarchical format or equivalently a tree tensor network. We established the (differential) geometry of low rank hierarchical tensors and applied the Dirac Frenkel principle to reduce the original high-dimensional problem to low dimensions. The DMRG algorithm was established as an optimization method in this format with alternating directional search. We compared this approach in the present discrete formulation with the CC method and its underlying exponential parametrization.

**Algorithmic developments.** — In the numerical analysis of strongly correlated quantum lattice models one of the most useful algorithms developed to balance the size of the effective Hilbert space and the accuracy of the simulation is the DMRG algorithm. Since the most time-consuming step of the diagonalization can be expressed as a list of dense matrix operations, the DMRG is an appealing candidate to fully utilize the computing power residing in novel kilo-processor architectures. We developed a smart hybrid CPU-GPU implementation, which exploits the power of both CPU and GPU and tolerates problems exceeding the GPU memory size. Furthermore, a new CUDA kernel has been designed for asymmetric matrix-vector multiplication to accelerate the rest of the diagonalization. Besides the evaluation of the GPU implementation, the practical limits of an FPGA implementation were also discussed.

We have also improved our DMRG method and calculated some 8000 correlation functions (in a fully parallelized manner) required to construct the two-site mutual information for the SU(5) Hubbard model. This calculation was mandatory to finish our project started in 2011 to prove that in the one-dimensional SU(n) Hubbard model with repulsive Coulomb interaction highly entangled subunits are formed for commensurate,  $p/q$ , fillings as a function of  $n$  for  $q < n$ .

We further developed the momentum space version of our DMRG code. We first studied entanglement diagrams of the one-dimensional Hubbard model and interpreted our results in terms of the  $g$ -ology model.

**Quantum information theory.** — We began to study entanglement in multicomponent systems. Since for more than two subsystems mutual information and entanglement are not uniquely defined we first studied three-site entanglement in simple spin systems and the behavior of the Kullback-Leibler relative entropy and its relations to other quantum entropies.

## Grants and international cooperation

OTKA K100908 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(ERA-Chemistry) “Generalized tensor methods in quantum chemistry” under OTKA NN110360, DFG SCHN 530/9-1 project under Grant No. 10041620 and FWF-E1243-N19

“Momentum” Program of the H.A.S.: Tensor factorization in high-dimensional spaces and applications to ultracold atomic systems and transition metal complexes (Ö. Legeza 2012-2017).

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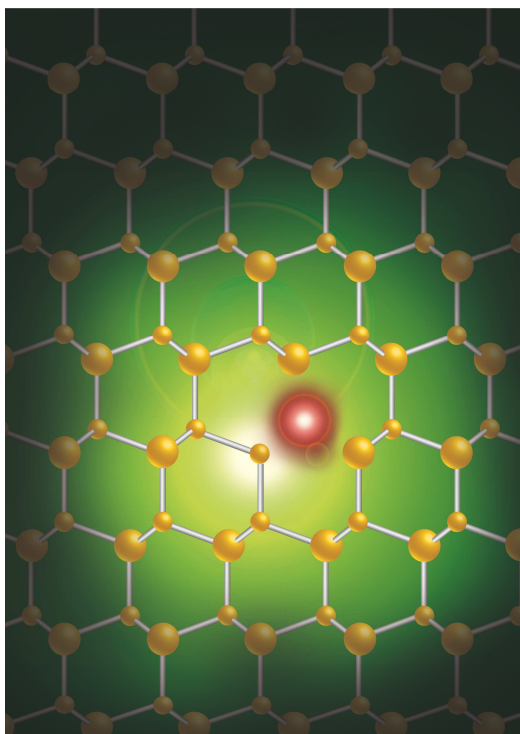
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## S-D. Semiconductor nanostructures

“Momentum” group

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The research team is active in three different fields: the development of new types of biomarkers, spintronics, and 3<sup>rd</sup> generation solar cells.



**Figure 1.** The colour centre, which emits red light, is embedded in 4H-type silicon carbide. It consists of a carbon vacancy (a carbon atom missing from SiC lattice) and a neighbouring silicon atom substituted with carbon. Silicon and carbon atoms are represented by large and small balls, respectively.

We found and identified silicon carbide as a colour centre, that can act as a single-photon source (Figure 1). This result, which was achieved in an international collaboration with partners from Australia and Japan was published in *Nature Materials*.

Colour centres are crystal point defects that emit light in the visible range. This emission occurs when the colour centre is exposed to light of a particular wavelength. The emitted light can be extremely bright if the incoming light has the appropriate wavelength. If the locations and distribution of colour centres are well-engineered within the embedding material, these centres can be used as efficient single-photon sources. Controlled production of single photons is of great importance in quantum metrology. Single colour centres like these could be used to map the three-dimensional structure of proteins and determine their physical properties. Single-photon sources could also be used as fundamental components for an entirely new generation of computers: quantum computers.

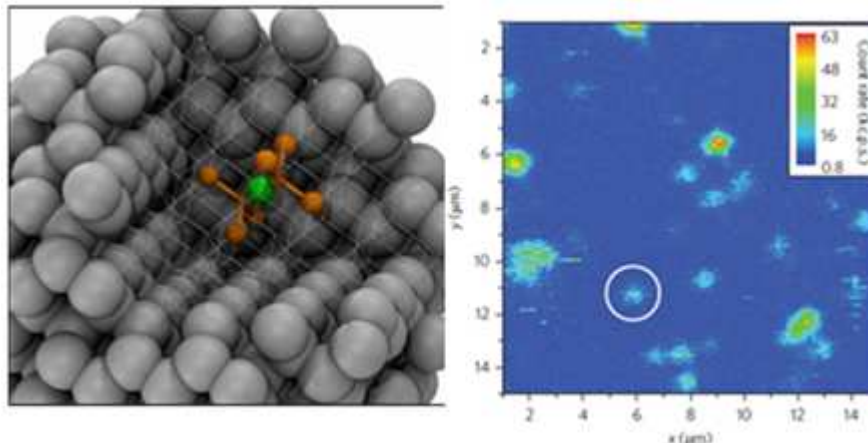
We have achieved a significant result in the development of diamond-based fluorescent biomarkers. We showed with simulations that a particular near-infrared colour centre remains

stable if embedded in a molecule-sized nanodiamond, where its emission wavelength is blue-shifted with respect to bulk diamond. Working in a broad international cooperation with German and Russian physicists, we proved the theoretical result experimentally in diamond particles discovered in meteorites (Figure 2). The most striking aspect of this finding is the tiny size of nanodiamonds which contain these stable, bright colour centres, and thus fulfil the stringent criteria of *in vivo* biomarkers. These stable biomarkers form the

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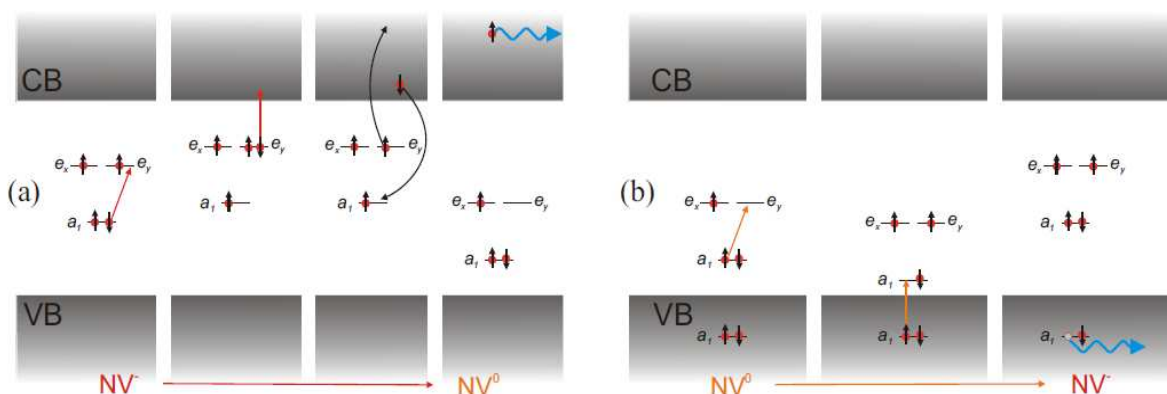
<sup>#</sup> Ph.D student

basis of the development of biomarker systems which will be usable in, for example, DNA research or for studying the human brain.



**Figure 2.** The molecule-sized nanodiamond and the embedded SiV colour centre (a pair formed from a substitutational silicon atom and a vacancy). The spots in the false-colour confocal microscope image shows the locations of such nanodiamonds, red middle regions correspond to brighter areas.

Biologists, and especially neurologists, urgently need biomarker systems which trace (for example) cancer cells in the blood stream. Systems to do this have already been developed, but most are either unstable or toxic, and consequently are not suitable for therapy. In contrast, we are seeking biomarker systems that can be applied *in vivo*. Diamond-based structures, consisting of carbon atoms, are good candidates. By using molecular size markers, it will become possible to monitor processes in living organisms. Our members have performed computational simulations in both of the aforementioned research projects our international partners carried out the experimental studies.

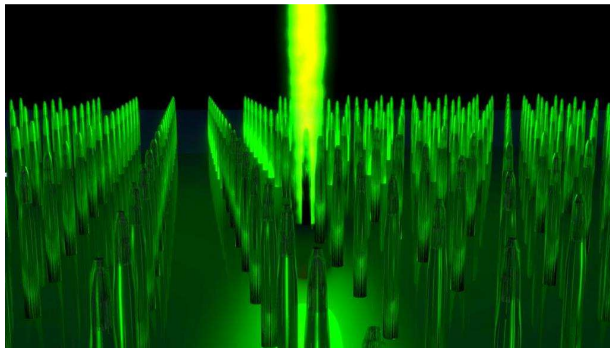


**Figure 3.** Schematic picture of ionization (a), and re-ionization (b) processes of the nitrogen-vacancy (NV) centre. VB: valence band, CB: conduction band;  $a_1$ ,  $e_x$ ,  $e_y$  are electronic states in the band gap and the valence band. (a) The negatively charged NV center is first excited by absorbing a photon, and the second photon pushes the excited electron up to the valence band. Next, the NV centre gets ionized via an Auger process. (b) The neutral NV centre is excited by the first photon, while the second excites an electron from a defect state resonant with the valence band. Finally, the resulting high-energy hole leaves the NV centre, thus re-ionizing it.



Significant results have been achieved in the research of solid-state quantum bits, which may be the building blocks of a future implementation of a quantum computer. In collaboration with German physicists, it has been shown that the famous nitrogen-vacancy centre in diamond ionizes when excited in the usual confocal microscope setup, due to an Auger process following two-photon absorption. Moreover, it has been explained why the re-ionization process has high probability even with low-intensity excitation (Figure 3).

So far, the most successful solid-state quantum bit is the nitrogen-vacancy centre in diamond, which has the outstanding feature that it can be manipulated at room temperature. Research for new, more efficient implementations is in progress, however. The newly discovered ST1 centre seems to be a defect of this kind. It can be manipulated individually with optical methods at room temperature. The quantum bit properties are realized in ST1 by electrons and their interaction with possible neighbouring carbon-13 nuclei.



**Figure 4.** An artist's rendering of ST1 centre manipulation. Diamond nanowires are excited with a green laser to access quantum bits in ST1 centres in them.

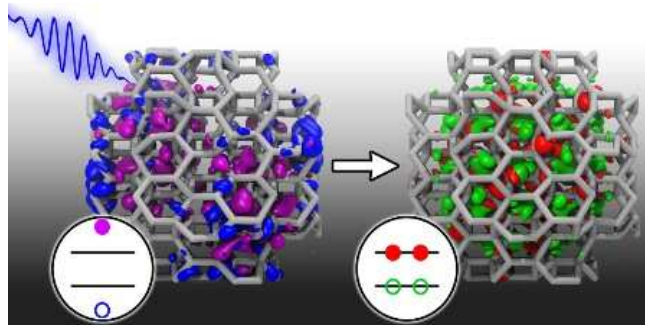
The greatest advantage of the new colour centre is that it stores quantum information magnitudes for a longer time than the NV centre. In this project, a sample containing diamond nanowires with a diameter of 200 nm and a length of 100  $\mu\text{m}$  was produced by physicists at Harvard University; the colour centres were examined by their partners in a Stuttgart-based laboratory that provided instruments to access these colour centres individually. We analyzed the experimental results based on the symmetry properties of the new colour centre, together with Australian

colleagues from Australian National University in Canberra. It has been proved that manipulations of this centre do indeed perform quantum bit operations.

Finally, in an international cooperation, we developed a computer software to investigate whether solar cells can be made more efficient by using nanocrystals that is to say nanometer-sized pieces of crystals. The answer is clear: yes, calculations show that a less-studied form of silicon — the body-centred cubic variant — is not only more efficient in absorbing light, but also more efficient in absorbing impact ionization, by which we mean the situation in which multiple low-energy charge carriers are produced by a high-energy one (Figure 5). Although nanocrystals of this kind have been produced earlier, there has never been an attempt to use them to enhance photovoltaic properties.

Efficiency of current, relatively cheap state-of-art photovoltaics is theoretically limited to approximately 32%, even allowing for future enhancements. The ubiquitous polysilicon solar cells seen on roofs of buildings have an even lower efficiency; up to about the half of the above limit. This means that at least 68 percent of light energy is wasted in heating the solar cells.

A solution to the solar cell inefficiency problem might be based on impact ionization by directing more energy in the electronic sector. One high-energy photon absorbed by the solar cell creates here not only one, but two or three charge carriers. This results in a higher current,



**Figure 5.** BC8 body-centered cubic silicon nanocrystal. A high-energy (blue) photon produces a high-energy electron-hole pair, which very efficiently decays to two pairs of lower energy holes and electrons thereafter. Distributions of probabilities of finding the electrons and holes are shown with clouds of their respective schematic colours.

which improves power efficiency. Note that in this very demanding field of research, any percentage point improvement in efficiency is regarded as a breakthrough. Intensive research have been carried out for a considerably long time to find materials where impact ionization is efficient, in contrast to the poor results of bulk silicon. Such systems are silicon nanocrystals which consist of a few thousand atoms, and provide higher impact ionization efficiency through quantum effects. Furthermore, manufacturing silicon nanocrystals is easier than manufacturing bulk silicon for contemporary solar cells, because the former is far less sensitive to the quality of the material. Thus, the new type of solar cells based on our research results could be more efficient and less expensive to produce than traditional solar cells.

## Grants and international cooperation

EU FP7 No. 270197: DIAMANT-Diamond based atomic nanotechnologies (A. Gali, 2011-2014)

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

OTKA K106114: Development of novel silicon carbide nanomarkers and more effective glutamate and GABA uncaging materials for measurement of neuronal network activity and dendritic integration with three-dimensional real-time two-photon microscopy (A. Gali, 2013)

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## S-J. Gas Discharge Physics

Wigner research group

**Péter Hartmann**, Aranka Derzsi, Zoltán Donkó, Ihor Korolov, Anikó Zsuzsa Kovács<sup>#</sup>, Kinga Kutasi, Pál Mezei, Károly Rózsa

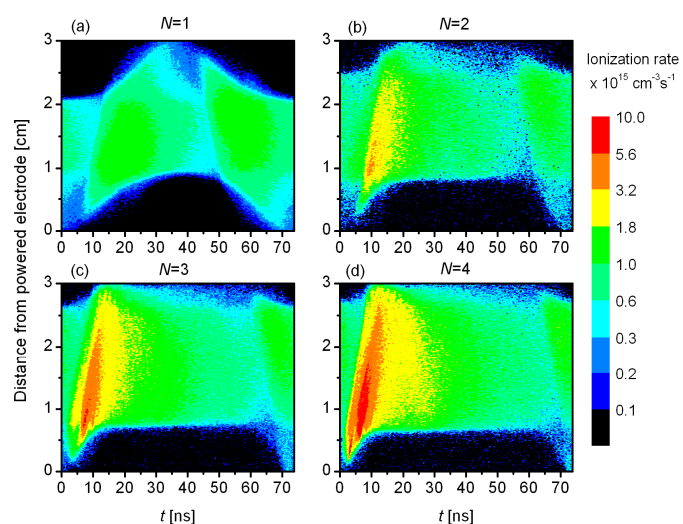
Our research focuses on the scientific challenges related to fundamental processes in gas discharges and their future emerging applications. Our ongoing activities cover a broad range of sub-fields, such as the study of collective phenomena in many-particle systems in plasma environments, and the investigation of biomedical, nanotechnological and environmental protection applications of gas discharge plasmas. A common aspect of these studies is the bottom-up approach that we follow, by which we mean that we seek an understanding and description of the observed macroscopic phenomena at the most fundamental level, often down to the scale of atoms and their elementary interactions. For the majority of the studies we combine experiments with advanced numerical or analytical methods to obtain the most complete and detailed physical picture. In the following we briefly introduce some of our recent achievements in our four main research areas.

### Physics of electric discharges.

— Gas discharges are non-equilibrium systems of unbound electrons and ions in low-pressure gas backgrounds. An electric field is induced in the discharge volume by an external electric circuit and drives, through the acceleration of charged particles, the elementary collisions in the plasma. Discharge properties strongly depend on the composition of the gas and the characteristics of the driving voltage. Gas

discharges are utilized in a wide range of consumer and industrial high-tech applications, such as lighting sources, display panels, microlithography, surface treatment, material synthesis, and so forth. Our mission is to attain a fundamental understanding of the microscopic mechanisms involved in gas discharges. This could pave the way for the improvement of current technologies and the development of new applications.

One of our approaches to address this topic is use a theoretical description of discharge systems. A self-consistent, first-principle theoretical description of a complete gas discharge can only be solved numerically. Over the last decades, several simulation methods and codes have been developed. In order to achieve realistic results a verification of the numerical simulations is necessary. An ideal way to do this would be to compare results



**Figure 1.** Spatio-temporal plots of the ionization rate for different number of applied harmonics,  $N$ .

<sup>#</sup> Ph.D student

from the numerical simulations with experimental results. However, these experiments often lack the level of reproducibility required for them to serve as reference standards, due to the sensitivity to small impurities. Based on particle-in-cell simulations, and in partnership with four other collaborating research groups using independent simulation codes, we have established rigorous benchmarks that can be used as a basis for evaluating the accuracy and efficiency of various numerical approaches developed for the description of low-pressure capacitively coupled radio frequency discharges.

Using experiments, simulations, and analytical models we have explored the possibility of controlling the transport of dust particles by changing the applied voltage waveform in dual-frequency discharges.

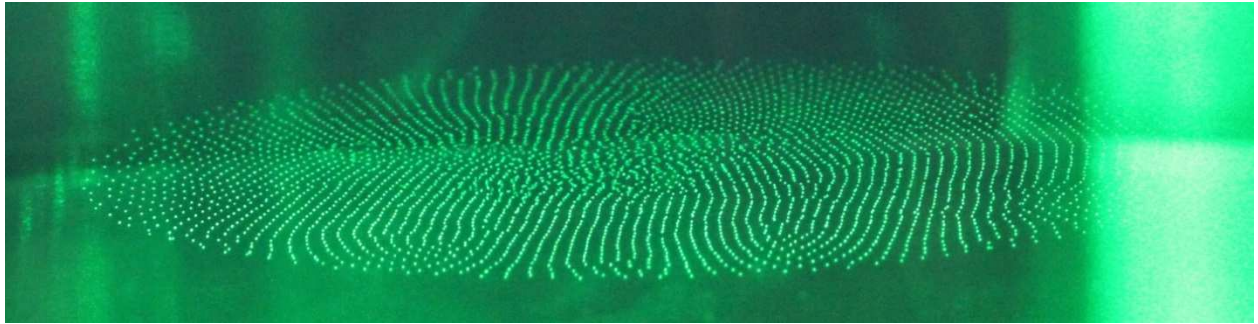
Using different kinetic models, we have analyzed the dynamics of plasma boundary sheaths in the intermediate radio frequency regime and found temporal asymmetry of the sheath charge-voltage relation due to ion inertia.

We have performed particle-in-cell simulations to reveal the influence of the secondary electron induced asymmetry on the electrical asymmetry effect in capacitively-coupled plasmas. We have found that the superposition of these effects is non-linear and significantly influences the range over which the control of the mean ion energy at the electrodes can be realized.

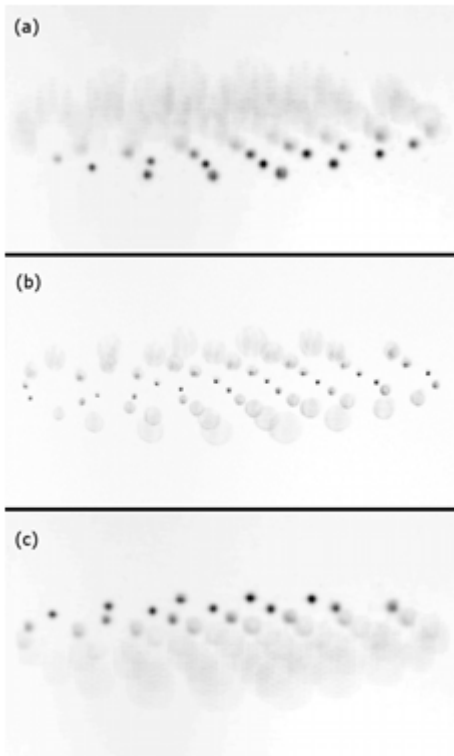
We have identified the coupling mechanisms of the driving frequencies in electronegative capacitive plasmas operated at two substantially different frequencies and clarified their effect on the discharge operation and plasma parameters.

As a result of a systematic particle-in-cell simulation of capacitive discharges driven by customized voltage waveforms, we have demonstrated the impact of applying multiple consecutive harmonics on the electron heating dynamics and on the quality of the control of ion properties (Figure 1).

**Strongly coupled plasma research.** — In contrast to gas discharges, strongly coupled plasmas are systems of charged particles, in which the long-range electrostatic interaction between charges dominates the dynamics over the thermal motion of the particles. Such plasmas are found in dense astrophysical objects, cold ion traps, charged colloidal suspensions, and, our system of interest, dusty plasmas. Dusty plasmas are gas discharges with micron-sized solid grains immersed in them. In this case, the grains become charged in the discharge plasma and become trapped in the electric field present in the discharge. As the dynamics of the dust grains and the gas discharge have very different characteristic time scales, the ensemble of charged dust grains can be treated independently of the discharge. The dust component can be approximated well with the one-component plasma model featuring screened Coulomb (Yukawa) inter-particle interactions. The dust grains tend to form crystalline solid or liquid structures, resulting in an exemplary system that is ideal for studying classical phenomena in condensed matter at the particle level (Figure 2). We conduct both experimental and numerical investigations on these systems, and are involved in the development of new diagnostic tools and procedures.



**Figure 2.** Image of a single layer dust cloud levitating in a gas discharge



**Figure 3.** Digitally refocused images from the single light field image of the dust cloud.

A completely new 3D particle imaging method was developed and benchmarked, which is based on the principle of light-field photography and utilizes a single camera with a single exposure to obtain all spatial coordinates (Figure 3).

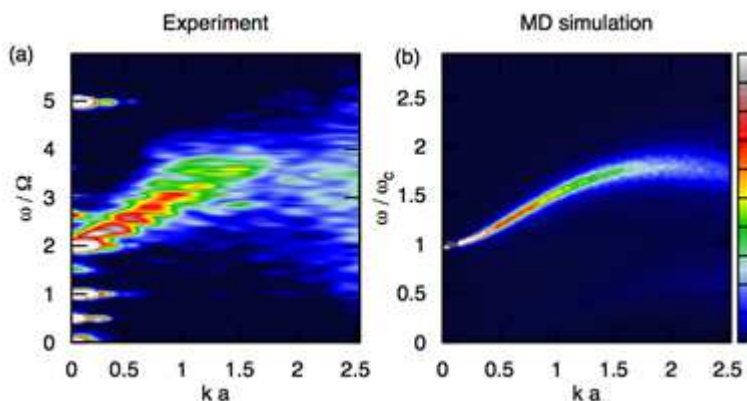
By applying a fast rotation to a single-layer dusty plasma crystal, an equivalent magnetic induction in the range of 3000 Tesla could be reached. The appearance of magneto-plasmon wave dispersion was observed in the longitudinal fluctuation spectra and compared to numerical results (Figure 4).

Using a molecular dynamics simulation of binary Yukawa systems and quasi-localized charge approximation (QLCA) calculations, we found that the low-frequency acoustic excitations are governed by the oscillation frequency of the average atom, while the high-frequency optic excitation frequencies are related to the Einstein frequencies of the systems.

**High-frequency discharge systems for biomedicine and nanostructuring.** —

In addition to analysis of the fundamental properties of gas discharges and the characterization of strongly coupled plasmas, we also

contribute to the development and optimization of future emerging plasma technologies. In the field of biomedicine plasmas have been proposed for the sterilization of sensitive



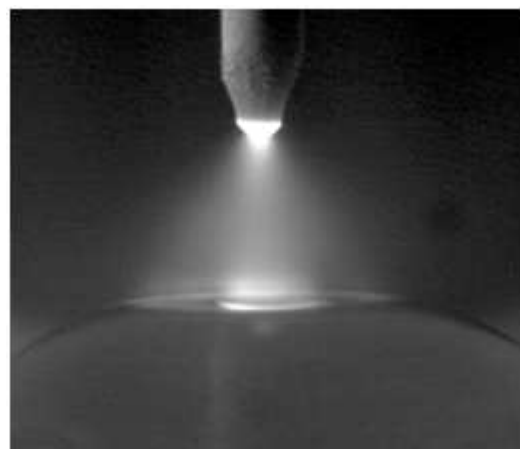
**Figure 4.** Experimental and numerical current fluctuation spectra of the highly (quasi) magnetized 2D dusty plasma.

medical devices and for direct wound treatment to assist the natural healing process. In case of nanotechnology, similar high-frequency driven plasmas in the medium to atmospheric pressure range were shown to have potential for synthesizing new materials with well-controlled structures at the nanometer scale. Recently we have extended our work in these areas: in addition to our theoretical work we now also conduct experimental research. Accordingly, we have built several high-frequency (surface wave microwave, inductively-coupled radio-frequency and kHz dielectric barrier) discharge and afterglow systems (Figure 5). We have started to test their applicability for sterilization of medical tools, surface treatment and functionalization, and synthesis of nano-structures. Moreover, a modeling tool has been used to determine the density of active species in the processing area to understand the role of active species in surface functionalization, and their interaction with bacteria and proteins during the sterilization process.



**Figure 5.** Microwave surface-wave excited plasma (left, bright part), and reactive streaming afterglow (right, large volume part)

**Electrolyte cathode atmospheric pressure glow discharge (ELCAD).** — The most powerful multi-purpose material analysis techniques are based on light emission spectra. Each element and molecule has a unique emission spectrum. The ELCAD technique is useful for analyzing liquid samples, because the cathode of the atmospheric glow discharge is the liquid itself (Figure 6). The sample enters the discharge region as a result of sputtering and evaporation of the liquid. In the discharge region, the excitation due to electron collisions drives the emission of light. High-resolution spectral analysis enables the detection and identification of trace elements down to the ppm level. This is possible even in an industrial environment, including that of waste-water monitoring. The understanding of the mutual interplay of liquid and gas phase processes is critical for further advancing this technique.



**Figure 6.** ELCAD atmospheric discharge between a tungsten anode tip and an electrolyte (liquid) cathode.

The emission spectra of ELCAD plasma was analyzed to detect exotic elements, particularly those relevant to research involving advanced materials that are used for environmental monitoring and in the field of non-linear optics at extreme high laser intensities. Under optimized conditions, high signal intensities of indium, rhodium and tellurium have been observed in aqueous solutions. Several resonant transition lines have been identified for



indium, rhodium, platinum and tellurium. The most important transition lines were found in the visible spectral range. Thus, a new analytical technique has been proposed and demonstrated for the analysis and development of modern optical materials. These results can also be used for analytical monitoring purposes in natural and waste-water samples.

## Grants and international cooperation

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

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)

TÉT\_10-1-2011-0717: Study of Ar-O<sub>2</sub> surface-wave microwave discharges and their post-discharges (Hungarian-French bilateral, K. Kutasi 2011-2013)

COST Action MP1101: Biomedical Applications of Atmospheric Pressure Plasma Technology (Manager 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)

„Wigner research group” support

Cooperations: Boston College, Ruhr Universität Bochum, Baylor University Texas, Institute of Physics Belgrade, Instituto Superior Técnico Lisbon, Technical University Porto, Josef Stefan Institute Ljubljana, Institut Jean Lamour Ecole des Mines Nancy, Gabriel Lippmann Centre Luxembourg, Université de Montréal Quebec

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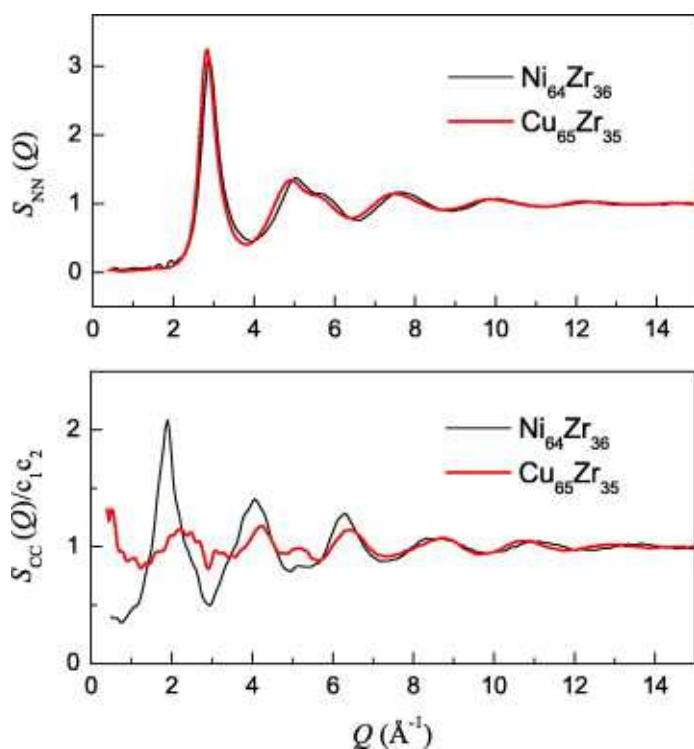
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## S-K. Liquid Structure

Wigner research group

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The main activity of our research group is the investigation of the microscopic structure of liquids, amorphous materials and disordered crystals. We combine experimental data, such as total scattering structure factors (TSSF) from X-ray and neutron diffraction (XRD and ND, respectively) and EXAFS spectra, with computer modeling tools, such as Reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations. As a result of such an approach, large sets (containing tens of thousands) of atomic coordinates ('particle configurations') in simulation boxes are provided that are consistent (within errors) with experimental data. These configurations are then subjected to various geometrical analyses, so that specific questions concerning the structure of a material may be answered. Below we provide some selected results from the year of 2013.



**Figure 1.** Comparison of the Bhatia-Thornton number-number (**upper panel**) and composition-composition (**lower panel**) partial structure factors of  $\text{Ni}_{64}\text{Zr}_{36}$  and  $\text{Cu}_{65}\text{Zr}_{35}$ .

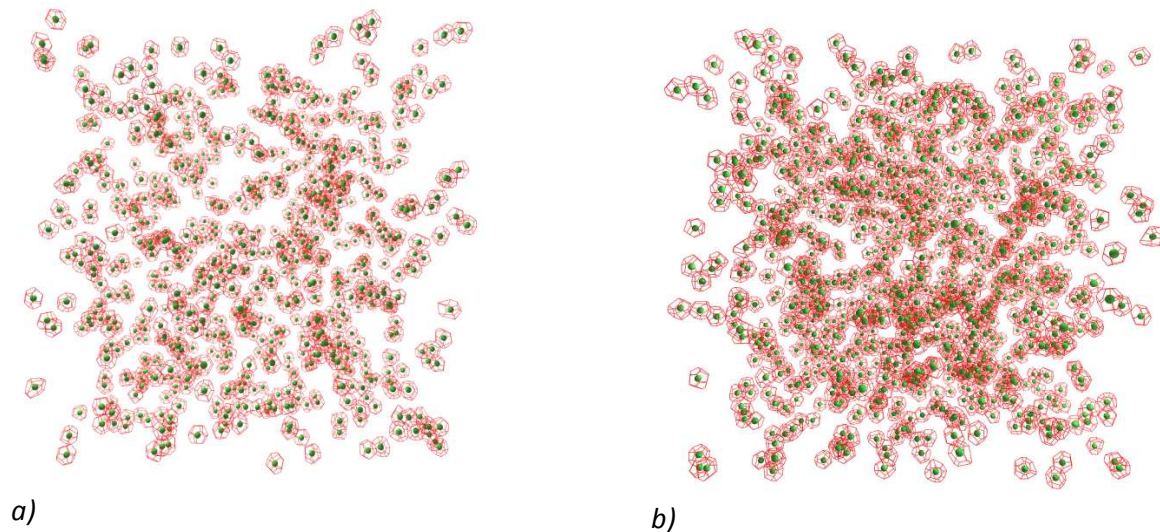
1, lower panel). While several strong peaks are present in  $S_{CC}(Q)$  for the  $\text{Ni}_{64}\text{Zr}_{36}$  glass, the oscillations are relatively weak over the whole  $Q$ -range for the  $\text{Cu}_{65}\text{Zr}_{35}$  glass. It can thus be concluded that the  $\text{Ni}_{64}\text{Zr}_{36}$  glass is characterized by pronounced topological and chemical

**Metallic glasses.** — X-ray diffraction, neutron diffraction with isotopic substitution, EXAFS and computational methods such as reverse Monte-Carlo simulation, molecular dynamics modelling, Voronoi analysis) were applied to elucidate the atomic structure of *Ni-Zr and Cu-Zr alloys* in glassy and crystalline states and to explain differences in the glass-forming abilities of the  $\text{Ni}_{64}\text{Zr}_{36}$  and  $\text{Cu}_{65}\text{Zr}_{35}$  compositions. The  $S_{CC}(Q)$  and  $S_{NN}(Q)$  Bhatia-Thornton structure factors for the  $\text{Ni}_{64}\text{Zr}_{36}$  and  $\text{Cu}_{65}\text{Zr}_{35}$  glasses calculated from the Faber-Ziman structure factors are compared below. Almost the same number density correlations up to high  $Q$ -values are observed in the  $S_{NN}(Q)$  curves (Fig. 1, upper panel) for both the  $\text{Ni}_{64}\text{Zr}_{36}$  and  $\text{Cu}_{65}\text{Zr}_{35}$  glasses. However, notable differences are observed for the concentration-concentration structure factors (Fig.

<sup>A</sup> Associate fellow

ordering, while the  $\text{Cu}_{65}\text{Zr}_{35}$  glass is topologically ordered and chemically relatively disordered.

The short-range atomic order and topology in the glassy and crystalline structures are remarkably different, and these differences are presumed to hinder crystal nucleation and growth, hence promoting glass formation upon fast cooling of the  $\text{Ni}_{64}\text{Zr}_{36}$  and  $\text{Cu}_{65}\text{Zr}_{35}$  liquid alloys. The Voronoi analysis of the glass configurations revealed that both glasses are characterized by a large number of ideal or distorted icosahedra. The distribution of ideal icosahedra and their networking are shown in Fig. 2. It is remarkable that the number of ideal icosahedra and the degree of their connectivity are both higher in  $\text{Cu}_{65}\text{Zr}_{35}$ .



**Figure 2.** Networks of ideal icosahedra in the RMC model configurations for the  $\text{Ni}_{64}\text{Zr}_{36}$  (a) and  $\text{Cu}_{65}\text{Zr}_{35}$  (b) metallic glasses.

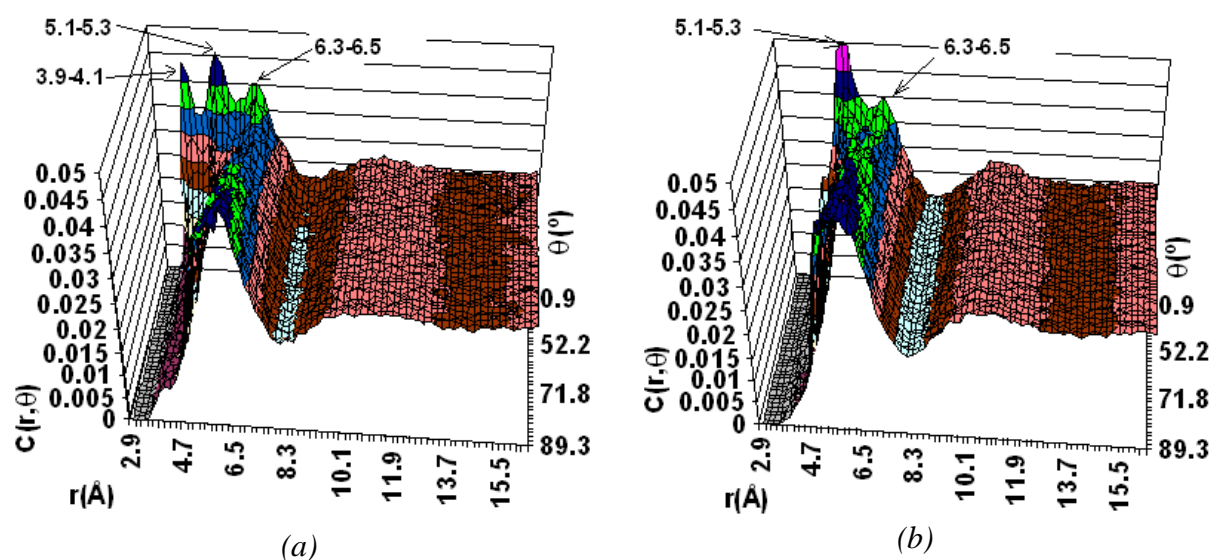
Our results show that chemical ordering alone cannot guarantee the good glass forming ability of an alloy. Other factors, such as topological ordering and differences between the glassy and crystalline structures should also be taken into account.

**Chalcogenide glasses.** — Due to its low production cost and high scalability, phase change random access memory (PCRAM) is a promising non-volatile memory. PCRAM is operated by Joule heating to induce phase transition between a high-resistance amorphous state (reset state) and a crystalline state with a low resistance (set state) of a phase change material (PCM).  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST) has been intensively studied for PCRAM applications because of its fast phase-change speed and good reversibility between amorphous and crystalline states. However, the melting point of GST is over  $600\text{ }^\circ\text{C}$ , which means a high power consumption is required for its reset operation, while its crystallization temperature is about  $150\text{ }^\circ\text{C}$ , which limits its data retention capability. Therefore, PCRAM requires an advanced PCM to lower its power consumption and enhance its data retention. Very recently, it has been found that amorphous  $\text{GeCu}_2\text{Te}_3$  (GCT) can be obtained by sputter deposition. The crystallization temperature of GCT is over  $200\text{ }^\circ\text{C}$ , while its melting point is around  $500\text{ }^\circ\text{C}$ . Thus, amorphous GCT shows a higher thermal stability than amorphous GST. Moreover, it has been demonstrated that the GCT memory device shows memory switching behavior and exhibited a 10% lower power consumption for the reset operation than the GST memory device. Further, the thickness change in a GCT film upon crystallization is as

low as +2%, while that of GST films is around -6%. These results indicate that GCT is promising for PCRAM application.

Amorphous  $GeCu_2Te_3$  was investigated by X-ray diffraction and extended X-ray absorption fine structure (EXAFS) measurements at the Ge, Cu and Te K-edges. Structural models were obtained by fitting the four experimental datasets simultaneously by Reverse Monte Carlo (RMC) structural modeling. It was found that Ge-Ge and Cu-Cu bonding are both significant. The average coordination numbers of Cu and Te, as well as Ge, are close to four. The high average coordination number of the network was found to contribute to the enhanced thermal stability of amorphous  $GeCu_2Te_3$ .

**Molecular liquids.** — Molecules with a planar geometry have resisted RMC modeling for more than two decades, due to difficulties with efficient movement schemes in previous versions of the RMC code. Following the appearance of RMC\_POT, it is intramolecular interaction potentials that keep flexible molecules in their proper geometry and this way, planar molecules should not be a problem any longer.

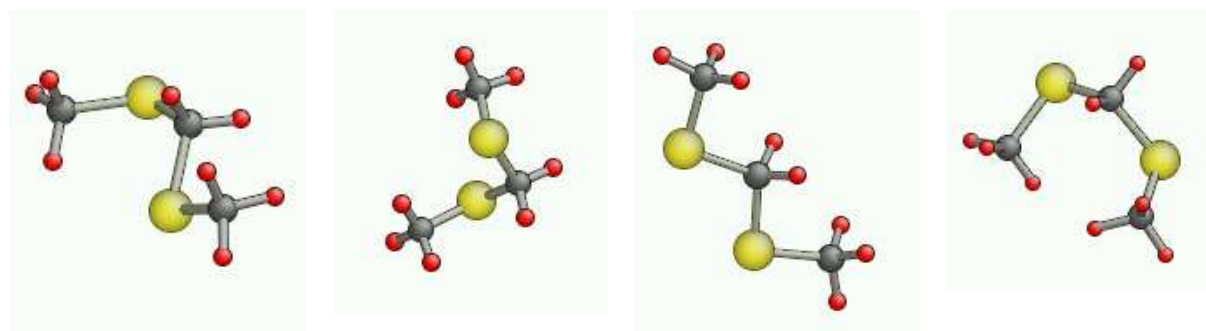


**Figure 3.** Angular distributions depending on the angle between molecular axes and on the distance between molecular centers for (a) the most successful 'ED\_MID' and (b) the least fortunate 'ED\_CI' models. For both structures, the dominance of angles around 0 degrees, characteristic to the parallel arrangement of the molecular axes, is apparent. (Numbers in the pictures are in Å, indicating the position of the maxima.)

As the first demonstration, the liquid structure of *tetrachloroethene* has been investigated on the basis of measured neutron and X-ray scattering structure factors, applying molecular dynamics simulations and reverse Monte Carlo (RMC) modeling with flexible molecules and interatomic potentials. As no complete all-atom force field parameter set could be found for this planar molecule, the closest matching OPLS-AA intra-molecular parameter set was improved by bond length and angle values coming from electron diffraction experiments. In addition, four different intra-molecular charge distribution sets were tested, so in total, eight different molecular dynamics simulations were performed. The best parameter set proved to be the one that uses the electron diffraction based intra-molecular parameters and the charge set  $q_C = 0.1$  and  $q_{Cl} = -0.05$ . The structure was further successfully refined by

applying RMC computer modeling with flexible molecules that were kept together by interatomic potentials. Correlation functions concerning the orientation of molecular axes and planes were determined. They reveal that the molecules closest to each other exclusively prefer the parallel orientation of both the molecular axes and planes, as it is exemplified by Fig. 3.

As another example of the application of the RMC\_POT software, this time, for detailed conformational analyses of liquid *bis(methylthio)methane* and *diethyl sulfide*, series of flexible molecule Reverse Monte Carlo calculations (FMP-RMC), using bonding and non-bonding interatomic potential functions, were performed. During RMC modeling, the experimental X-ray total scattering structure factor was approached. The room temperature liquid structure of bis(methylthio)methane is excellently described by the FMP-RMC simulation that applied the EncadS force field parameters. The main conformer was found to be AG, followed by the G+G+(G-G-) and AA structures (see Fig. 4). The stability of the G+G+(G-G-) conformer is most probably caused by the anomer effect. The liquid structure of diethyl sulfide can be best described by applying the OPLS-AA force field parameters during FMP-RMC simulation. Here the two main conformers are AG and AA. In addition to findings on the actual real systems, a fairly detailed comparison between traditional RMC and FMP RMC methodology was provided.

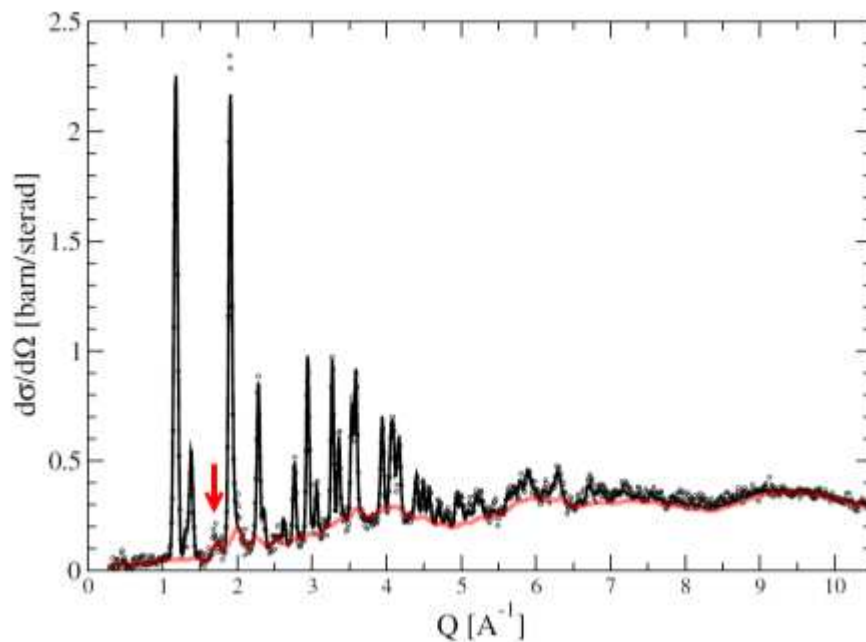


**Figure 4.** From left to right: the AG, G+G+, AA and G+G- conformers of *bis(methylthio)methane* (large yellow spheres: sulphur atoms; medium size grey spheres: carbon atoms; small red balls: hydrogen atoms).

**Disorder in molecular crystals.** —In many cases, the powder diffraction pattern of a crystalline material contains not only Bragg-peaks, that are characteristic to the infinite translational symmetry of the perfect crystal, but also a 'diffuse' contribution underneath the Bragg-peaks (see Fig. 5) that is (generally thought to be) the footprint of local (dis)order. Tetrahedral molecules, such as the CX<sub>4</sub> family (X: Cl, Br, I), are well-known examples of such powder patterns: during the past year, carbon-tetraiodide was scrutinized by our research group.

Total scattering neutron powder diffraction measurements were performed on the tetragonal phase of *carbon-tetraiodide*, Cl<sub>4</sub>. The experiments were followed by Reverse Monte Carlo (for POWder diffraction (RMCPOW)) modeling. Detailed analyses of the resulting particle configurations revealed that the observed diffuse scattering originates from the libration of the molecules. By examining the partial radial distribution functions a distinct carbon-iodine peak at 4.5 Å is found, which appears as a consequence of corner-to-

face mutual alignment of two molecules. The occurrence of edge-to-edge alignments is also significant within the first carbon-carbon coordination shell.



**Figure 5.** Experimental and simulated neutron powder diffraction patterns of tetragonal  $Cl_4$ . Circles: measured differential cross section; black solid line: RMCPOW; red solid line: the separated diffuse contribution. The red arrow indicates the strongest parasitic Bragg-peak, most probably from iodine.

### Grants:

OTKA K083529: Investigations concerning the structure of complex liquids (L. Pusztai, 2011-2014)

TÉT\_10-1-2011-0004 (Hungarian-Japanese bilateral): Investigations of structural disorder in liquids, as well as in amorphous and crystalline solids, via combining diffraction and EXAFS experiments with Reverse Monte Carlo modelling (L. Pusztai, 2012-2013)

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)

„Wigner research group” support

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**See also: S-F.7**

## S-S. Quantum Optics and Quantum Informatics

“Momentum” group

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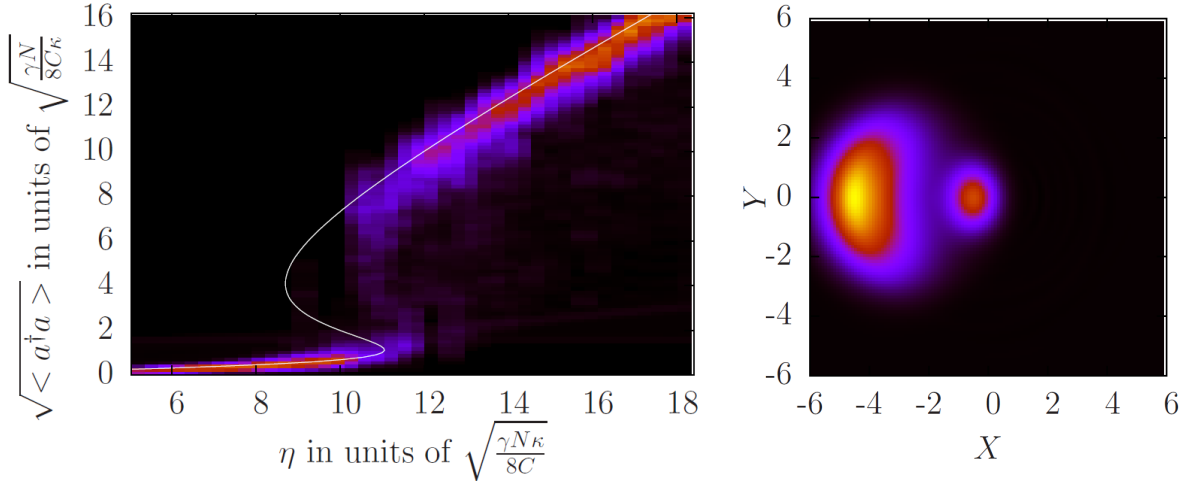
**Cavity quantum electrodynamics, Bose-Einstein condensates, and many-body physics with ultracold atoms.** — Optical bistability is an experimentally accessible and controllable example of a non-equilibrium phase transition in a damped–driven open system. The output intensity of a driven cavity containing an ensemble of atoms exhibits bistability and hysteresis in a given range of driving strength and detuning, an effect that has been observed for many decades. The advent of the strong-coupling regime of optical cavity QED opened a route for studying the interplay of quantum fluctuations and nonlinear atom–light coupling at low intracavity photon number. Today, cavity QED also enables the controlled variation of the size of the atomic medium with single atom resolution. It is thus a suitable platform for exploring quantum corrections in a finite-size system to the semiclassical mean-field results, which is a particularly exciting opportunity in the vicinity of a critical point.

We have explored the transition between the quantum and the semiclassical regimes of optical bistability. The quantum model in the few atom regime has been described by means of a numerically-exact quantum trajectory method. We have observed the formation of the familiar semiclassical bistability curve as the atom number is gradually increased from  $N = 2$  to 8. Surprisingly, even such a low atom number is sufficient to resolve the two semiclassical attractors in steady-state. The analysis of linearized quantum fluctuations in the steady-state reveals non-trivial quantum correlations between the atomic and radiation degrees of freedom. This theoretical analysis supports the hypothesis that experimentally-achievable few-atom cavity QED systems can be suitable devices for ultra-low intensity quantum signal processing: for optical switches, for example. These results were reported in a paper [Dombi et al., J. Phys. B 46, 224010] that was included in the “Highlight of 2013” selection of papers published in Journal of Physics B.

The dispersive interaction of a Bose-Einstein condensate with a single mode of a high-finesse optical cavity realizes the radiation pressure coupling Hamiltonian. In this system the role of the mechanical oscillator is played by a single condensate excitation mode that is selected by the cavity mode function. We studied the effect of atomic s-wave collisions and showed that it merely renormalizes the parameters of the usual optomechanical interaction. Moreover, we showed that even in the case of strong harmonic confinement – which invalidates the use of Bloch states – a single excitation mode of the Bose-Einstein condensate couples significantly to the light field; that is to say the simplified picture of a single “mechanical” oscillator mode remains valid.

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<sup>#</sup> Ph.D student



**Figure 1.** *Left:* The familiar S-shaped curve of the intracavity steady state field amplitude in the semiclassical model (white), superimposed on the color coded histogram over the mean amplitude of the fluctuating quantum state of the system, both as a function of the driving field amplitude  $\eta$  ( $N$  is the atom number,  $C$  is the cooperativity parameter,  $\kappa$  is the cavity mode linewidth, and  $\gamma$  is the atomic spontaneous emission rate). *Right:* The Wigner function of the steady-state cavity field shows bimodal distribution in phase space, which corresponds to the mixture of the semiclassical attractors in the bistable domain.

We studied spin liquid phases of spin-5/2 alkaline earth atoms on a honeycomb lattice at finite temperatures. Our analysis was based on a Gutzwiller projection variational approach recast to a path-integral formalism. In the framework of a saddle-point approximation we determined spin liquid phases with lowest free energy and studied their temperature dependence. We identified a critical temperature, where all the spin liquid phases melt and the system transitions to the paramagnetic phase. We also studied the stability of the saddle-point solutions and showed that a time-reversal symmetry breaking state, a so called chiral spin liquid phase is realized even at finite temperatures. We also determined the spin structure factor, which (in principle) is an experimentally measurable quantity and is the basic tool to map the spectrum of elementary excitations of the system.

**Quantum information processing, quantum walks, and chaotic dynamics of entangled qubits.** — Discrete-time quantum walks (DTQW) have topological phases that are richer than those of time-independent lattice Hamiltonians. Even the basic symmetries, on which the standard classification of topological insulators hinges, have not yet been properly defined for quantum walks. We introduced the key tool of time frames, that is to say, we describe a DTQW by the ensemble of time-shifted unitary time-step operators belonging to the walk. This gave us a way to consistently define chiral symmetry (CS) for DTQW's. We showed that CS can be ensured by using an “inversion symmetric” pulse sequence. For one-dimensional DTQW's with CS, we identified the bulk  $\mathbb{Z} \times \mathbb{Z}$  topological invariant that controls the number of topologically-protected 0 and  $\pi$  energy edge states at the interfaces between different domains, and gave simple formulas for these invariants. We illustrated this bulk-boundary correspondence for DTQW's with the example of the “4-step quantum walk”, where tuning CS and particle-hole symmetry realizes edge states in various symmetry classes.

**Molecule dynamics.** — We explained why the generalized discrete variable representation is variational neither with respect to the size (truncation) of the basis set nor with respect to the selection of grid points.

## Grants:

“Momentum” Program of the H.A.S.: Quantum Measurement Theory in Hybrid Mesoscopic Couplers and Networks (P. Domokos 2011-2015)

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

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

NKTH ERC\_HU\_09 OPTOMECH: Optomechanical coupling: extending Cavity Quantum Electrodynamics (P. Domokos 2010-2014)

EU FP7 Initial Training Network: CCQED Circuit and Cavity Quantum Electro-Dynamics (P. Domokos 2011-2014)

TÉT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-11/2009): Quantifying non-classicality in quantum walks and quantum optical networks (T. Kiss, 2010-2012)

MÖB-DAAD: Quantum measurement in the hybrid system of coupled Bose-Einstein condensate and carbon nanotubes (P. Domokos, MÖB/18-1/2012)

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**Institute for Particle and Nuclear Physics**

## R-A. Field theory

**Gyula Fodor**, Gabriella Böhm, Viktor Czinner<sup>A</sup>, László Fehér, Péter Forgács, Andor Frenkel<sup>A</sup>, Tamás Herpay, Gyula Kluge<sup>A</sup>, Árpád Lukács, Balázs Mikóczi, Júlia Nyiri<sup>A</sup>, László Szabados, Kornél Szlachányi, Kálmán Tóth<sup>A</sup>, Péter Vecsernyés

**Total mass of closed universes.** — In the last year we suggested a definition of the total mass of closed universes, and we showed that it coincides with the first eigenvalue of the Sen-Witten operator, and its vanishing is equivalent to the existence of non-trivial solutions of Witten's gauge condition, and also to the flatness of the spacetime with toroidal spatial topology. In 2013 we generalized these results: The total mass is equivalent to the holonomic triviality of the spacetime, in which case the number of the linearly independent solutions of Witten's equation is even; and in the presence of a positive cosmological constant the cosmological constant is a sharp lower bound for the total mass, and the mass takes this minimal value if and only if the spacetime is locally isometric to the de Sitter spacetime, which is just the asymptotic final state of one aeon of the 'conformally cyclic cosmological model' of Penrose.

**(Weak) Hopf algebras in duoidal categories.** — Duoidal categories generalize braided monoidal categories by allowing for two different but compatible monoidal structures. The definition of a bialgebra relies on both monoidal structures in a symmetric way. We compared the possible definitions of Hopf algebra - that all become equivalent in the category of vector spaces, but that are conceptually different. In suitable duoidal categories we proved the fundamental theorem of Hopf modules. We defined weak bialgebras in duoidal categories. We investigated the structure of the base algebras and proved also here the fundamental theorem of Hopf modules.

**Weak multiplier bialgebras.** — Defining weak multiplier bialgebras we showed that the base algebra is a subalgebra of the multiplier algebra that carries a coseparable co-Frobenius coalgebra structure. We proved the expected behavior of (appropriate) representations: they constitute a monoidal category via the tensor product over the base algebra. We defined the antipode describing thereby the relation to Van Daele and Wang's weak multiplier Hopf algebra. We proved the monoidality of the category of (appropriately defined) comodules. Comparing the centers of the categories of modules and of comodules, we proposed a definition of Yetter-Drinfeld module. We proved that they constitute a monoidal category as well.

**Integrable many-body systems.** — We continued the studies of integrable many-body systems started earlier, whose principal aim is to develop a group-theoretic understanding of the duality relations of models of Calogero-Sutherland and Toda type. These models describe arbitrary number of particles moving in one dimension. Duality between two systems requires a canonical transformation between their phase spaces, whereby the action variables of one system turn into particle coordinates of the other, and vice versa. A new group-theoretic interpretation was given for the duality property of the open Toda lattice, which was found originally by Ruijsenaars using a direct method. The role of the  $SL(2, \mathbb{Z})$  group was surveyed from a novel perspective, and new spin-extensions of Sutherland models were derived.

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<sup>A</sup> Associate fellow



**Plane waves as tractor beams.** — We have shown that in a large class of systems, plane waves act as tractor beams: i.e., an incident plane wave can exert a pulling force on the scatterer. The underlying physical mechanism for the pulling force is due to the sufficiently strong scattering of the incoming wave into another mode carrying more momentum, in which case excess momentum is created behind the scatterer. This tractor beam or negative radiation pressure (NRP) effect is found to be generic in systems with multiple scattering channels. In a birefringent medium, electromagnetic plane waves incident on a thin plate exert NRP of the same order of magnitude as optical radiation pressure, while in artificial dielectrics (metamaterials), the magnitude of NRP can even be macroscopic. In two dimensions, we study various scattering situations on vortices, and NRP is shown to occur by the scattering of heavy baryons into light leptons off cosmic strings, and by neutron scattering off vortices in the XY model.

**Gravitational waveforms of compact binaries.** — We have computed the eccentric gravitational waveforms of the compact binaries based on the gravitational radiation formula up to first post-Newtonian order, then we have given the full explicit time depending of the all quantities with help of the Hansen expansion. We have shown that the quantities with the general true anomaly parameterization are simpler than type of the Damour-Deruelle orbital parameterization. We have analyzed the perturbed two body problem with quaternions which is well-known in celestial mechanics. In terms of perturbation we have computed the equations for the gravitational radiation reaction and the pure relativistic leading-order correction of Kepler problem using the quaternion algebra. Due to the gauge depending of the acceleration for radiation reaction we have given the new gauge transformation which is necessary carrying out regularization but that transformation is different from the case of no regularization in literature.

**Skew-monoidal categories.** — Generalizing the notion of modules over quantum groupoids I studied the structure of modules over a skew-monoidal category. Under mild exactness conditions I have proved that there is an intrinsic tensor product of modules without having any underlying category that would play the role of the bimodule category of quantum groupoids. Requiring stronger exactness properties a strong monoidal forgetful functor to an appropriate underlying category is also shown to exist.

**Common causes and Bell inequalities.** — Bell inequalities can be understood as constraints between classical conditional probabilities, and can be derived from assumptions representing a joint common causal explanation of classical correlations. We have shown that Bell inequalities used in quantum theories can be derived only from commuting common causes. In the noncommuting case just the opposite is true: a joint noncommuting common causal explanation can be given for a set of correlations even if they violate the Bell inequalities, i.e. if the corresponding state is entangled. Namely, one can reproduce the EPR-Bohm scenario in the AQFT setting with locally finite degrees of freedom and a joint noncommuting common cause can be constructed for the set of spacelike separated correlating events violating maximally the Clauser--Horne inequality.

## **Grants and international cooperation**

OTKA K108384 Investigation of quantum symmetries by category theory (G. Böhm, 2013-2017)

OTKA K101709 Nonlinear interactions of waves and particles in field theories, and their physical consequences in astrophysics and cosmology (P. Forgács, 2012-2015)

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13. Fehér L, Klimcik C: The Ruijsenaars self-duality map as a mapping class symplectomorphism. In: Dobrev V (ed.): IX. International Workshop: Lie Theory and Its Applications in Physics. 500 p. (Varna, Bulgaria, 2011.06.20-2011.06.26.) Sofia: Bulgarian Academy of Sciences, 2013. pp. 423-437. (Springer Proceedings in Mathematics & Statistics; 36.) (ISBN:978-4-431-54269-8)
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**See also: R-B.2**

## R-B. Heavy-ion physics

**Gergely Gábor Barnaföldi**, Dániel Berényi<sup>#</sup>, Tamás Sándor Biró, Tamás Fülöp, Péter Lévai, Szilveszter Miklós Harangozó<sup>#</sup>, Miklós Horváth<sup>#</sup>, Péter Kovács, Károly Ürmösy<sup>#</sup>, Péter Ván, György Wolf, Miklós Zétényi

High-energy heavy-ion physics is connected to a large variety of physics disciplines by its nature. Our researches probe fundamental concepts of classical and modern thermodynamics, hydrodynamics, and quantum theory. Therefore, we have several theoretical and practical topical research directions in a wide spectrum, such as: thermodynamics, perturbative and non-perturbative QCD, high-energy nuclear effects, hadronization, hadron phenomenology, and gravity/cosmology too. Our studies are strongly motivated by the requests of several large-scale facilities, like collaborations at LHC (CERN, Switzerland) and RHIC (BNL, USA), as well as, future experiments at FAIR (GSI, Germany) and NICA (Dubna, Russia). In 2013 we started new investigations in many new directions of high-energy physics phenomenology connected to the existing and future state-of-the-art detectors. We present these below in details.

**Improvements on thermodynamics.** — Non-relativistic continuum thermodynamics is a theoretical framework for classical continua, including continuum mechanics or electrodynamics. In this year we have derived the equations of motion for non-dissipative and dissipative generalized continua of Cosserat–Eringen–Suhubi–Mindlin type from thermodynamic principles. The importance of this result is that the derivation does not refer to usual mechanical notions like variational principles or momentum balance (Newton equation).

We have also investigated the role of heat capacity in entropy formulas. Analyzing the classical, non-relativistic ideal gas we have proved that the zero mutual information approach between subsystems delivers the Rényi and Tsallis entropy formulas, with the  $q$  parameter uniquely determined by heat capacities of the bath and the whole system.

This points out the importance of the physical modeling of the finite heat bath in high energy particle physics calculations. By introducing the Universal Thermostat Independence principle we have generalized this result to energy or entropy dependent heat capacities and demonstrated differences between constant volume and adiabatically expanding systems of quark matter in this respect.

**Hadronization.** — We focused on the power-law tail behavior of transverse momentum spectra in electron-positron collisions by fitting the results of our statistical model to earlier measurements. As a novelty, recent pp, AuAu and PbPb collision data in RHIC and LHC experiments have been successfully described. In order to test the new Tsallis-Pareto-like distributions and their extension to a microcanonical treatment a jet-fragmentation function fitter program has been developed and applied. This program provides best fit values for all quark-hadron channels for any kind of fragmentation function ansatz via calculating inclusive hadron spectra and minimizing the squared deviation sum automatically. The code, developed by our group, has been recently tested for the pion production and soon will be ready for further hadron species. By now three different types of  $x$ -distributions are implemented as choices: polynomial, Tsallis–Pareto, and microcanonical Tsallis (i.e. cut

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<sup>#</sup> Ph.D student

power-law of  $-\ln(1-x)$ ). The latter – most promising – ansatz received theoretical background.

**Perturbative & non-perturbative QCD.** — We achieved progress on the application of perturbative and non-perturbative QCD methods to nuclear phenomena. Concerning nuclear modifications in high-energy collisions the pQCD improved parton model calculations were updated. The new code includes recent shadowing functions while predicting hadron spectra measured in pPb collisions at LHC energies. We have predicted the size of the shadowing effect in pPb collisions applying DGLAP evolution in the nuclear shadowing function. Recent data from CERN LHC pPb experiments at 5.02 TeV energy validate our theoretical calculation and prove the existence of jet energy loss in hot dense deconfined matter in heavy ion collisions.

A new non-perturbative QCD method has been developed and published in a research book on “The Mass Gap and Its Application”. In this book we do not only consider the familiar idea of a mass gap, but prove its existence in quantum gauge field theory and provide recipes for applications, e.g. in obtaining the equation of state of non-perturbative QCD matter.

**Hadrons at low energy.** — In 2013 our most important results include some important steps in describing the low energy hadronic sector by an  $SU(3)\times SU(3)$  symmetric linear sigma model. We described the meson masses and widths for the (pseudo) scalar octets and (axial) vector octets. Our results shows that the  $(A^0(1450), K^0(1430), f^0(1370), f^0(1710))$  scalar octet is the chiral partner of the low energy pseudoscalar (Goldstone-boson) octet. The lower mass scalars are probably tetraquark or meson molecule states. We also showed that our results are independent of the special choice of the  $U_A(1)$  breaking anomaly term. We incorporated baryons, too, and obtained a very good description for the lowest lying baryon octet and decuplet masses, as well as a reasonable description for the decuplet decays.

Furthermore, calculating the dilepton production in pion induced reactions, we developed a gauge invariant description for both photon and dilepton production. We predicted the invariant mass spectra for energies available at GSI for the HADES collaboration.

**Applications in curved space-time.** — AdS/CFT phenomenology of particle spectra were tested using the Rényi entropy formula and the Hawking–Bekenstein correspondence for event horizon entropy: we pointed out an equivalence between the radial temperature profiles in Anti-de-Sitter scenarios with the classical Boltzmann–Gibbs entropy formula and in the pure Schwarzschild metrics with the  $q$ -entropy formula promoted by Rényi and Tsallis. We noticed that the simplest geometric picture requires  $q = 1 + 2/\pi^2$ , a value surprisingly close to the one observed at RHIC in cut power-law particle transverse momentum spectra re-calculated on the quark level.

From the special and general relativistic extensions of the action principle behind the Schrödinger equation we identify the conformal content of the above and obtain classical gravitation for massive particles, but with a cosmological term representing off-mass-shell contribution to the energy-momentum tensor. In this scenario the - on the Planck scale surprisingly small - cosmological constant stems from quantum binding with a Bohr radius ' $a$ ' as being  $3/a^2$ . This is the same relation as for the de Sitter cosmological horizon.

## Grants and international cooperation

OTKA NK 77816: Theoretical and experimental investigation of high energy particle production in the CERN LHC ALICE experiment (P. Lévai, 2009-2013)

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

OTKA K71989: Nuclear matter in extreme condition at the FAIR (GSI Darmstadt) accelerator (Gy. Wolf, 2008-2013)

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

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

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

Hungarian-South-African TÉT Grant No-10-1-2012-0061: MAG Zrt. Tender for Innovation, (Hungarian leader: T.S. Biró, South-African leader: A. Muronga, 2011-2013)

TÉT Chinese-Hungarian Grant No TET\_12\_CN\_D0524D1E (P. Lévai, 2013-2015).

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

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

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

CompStar ESF project, G.G. Barnaföldi, (Steering Committee Member, 2009-2013)

NewCompStar EU COST MP1304 action, (Hungarian Representatives: G.G. Barnaföldi, M. Vasúth, 2013-2017)

## Long term visitor

N. Mitsui, Research Center for Seismology, Volcanology and Disaster Mitigation, Graduate School of Environmental Studies, Nagoya University, Nagoya University, Japan, August 3, 2012-December 31, 2013 (host:P. Ván)

## Publications

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7. Gogokhia V, Barnaföldi GG: The Mass Gap and Its Applications. Singapore: World Scientific Publishing Co., 2013. 252 p. (ISBN:978-981-4440-70-7)

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

### ALICE Collaboration

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## R-C. Gravitational Physics

**Gergely Debreczeni**, István Rácz, Mátyás Vasúth, Dániel Barta<sup>#</sup>, Balázs Kacs Kovics<sup>#</sup>

The Gravitational Physics Group of RMI is involved in both experimental and theoretical studies of Einstein's theory of gravity. The principal part of our research interest is devoted to gravitational wave physics. Our group is involved in the Virgo Scientific Collaboration operating the Virgo detector, the European gravitational wave observatory. The related issues do also motivate many of our theoretical investigations.

The most important research results of our group members are as follows:

- Within the generic null characteristic initial value problem István Rácz has deduced a reduced set of the evolution equations, from the coupled Newman–Penrose and Maxwell equations for smooth four-dimensional electrovacuum spacetimes allowing a non-zero cosmological constant. He showed that these reduced equations make up a first-order symmetric hyperbolic system of evolution equations, and also that the solutions to this reduced system are also solutions to the full set of the Newman–Penrose and Maxwell equations provided that the inner equations hold on the initial data surfaces.
- An innovative noise reduction technique has been developed and will be applied to the measurement data of the Virgo detector to increase signal detection sensitivity..
- Playing leading role in designing, creating and coordinating the data transfer, processing and framework of the of the Virgo experiment. Gergely Debreczeni has been nominated as the Computing Coordinator of the Virgo Collaboration.
- We have done major contributions to the data analysis pipeline developed within the LIGO - Virgo Collaboration which targets the detection of gravitational waves emitted by spinning binary neutron stars. As a result of the work it will be feasible to look for such signal in the measurement data of the advanced detectors, as such increasing the probability of the first direct detection.
- Developing the numerical packages GridRipper and CBwaves aiming to provide accurate waveforms for data analyzing activities. With the help of the CBwaves simulation packages we study the important differences caused by the inclusion or neglect of various post-Newtonian contributions to the approximate waveform equations which affects detection and parameter estimation sensitivity.
- The adaptation of GPU technology in data analysis activities and development of new search algorithms to analyze the noisy data of the LIGO and Virgo detectors. The GWTools algorithm packages has been developed and used for various data analysis algorithms resulting a significant increase in speed and sensitivity.

### Grants and international cooperation

AKTION Österreich-Ungarn Wissenschafts- und Erziehungskooperation Projektantrag Beim Ausfüllen des Formulars ist das Merkblatt 2013 zu beachten: PHYSIK SCHWARZER LÖCHER (I. Rácz)

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<sup>#</sup> Ph.D. student

A2-SZJ-TOK-13 János Szentágothai Grant for experienced researchers kategória (I. Rácz, 2013)

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3. Nagy-Egri MF, Rácz I, Debreczeni G: Evolution of non-linear dynamics using Graphical Processing Units. **ASTRON. NACHR.** 334:(9) pp. 1036-1038. (2013)

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1. Adrian-Martinez S et al. incl. Debreczeni G, Endroczi G, Gaspar ME, Racz I, Vasuth M [960 authors]: A first search for coincident gravitational waves and high energy neutrinos using LIGO, Virgo and ANTARES data from 2007. **J. COSMOL. ASTROPART. P.** (6) Paper 008. 40 p. (2013)
2. Degallaix J et al. incl. Debreczeni G, Endroczi G, Gaspar ME, Racz I, Vasuth M [183 authors]: Advanced Virgo Status. **ASTR. SOC. P.** 467: pp. 151-160. (2013)
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gravitational-wave detector network. *PHYS. REV. D* 88: Paper 062001. 24 p. (2013)

8. Aasi J et al. incl. Debreczeni G, Endroczi G, Gaspar ME, Racz I, Vasuth M [801 authors]: Search for gravitational waves from binary black hole inspiral, merger, and ringdown in LIGO-Virgo data from 2009-2010. *PHYS. REV. D* 87:(2) Paper 022002. 15 p. (2013)
9. Aasi J et al. incl. Debreczeni G, Endrőczi G, Ráczi I [877 authors]: Search for long-lived gravitational-wave transients coincident with long gamma-ray bursts. *PHYS. REV. D* 88:(12) Paper 122004. 13 p. (2013)

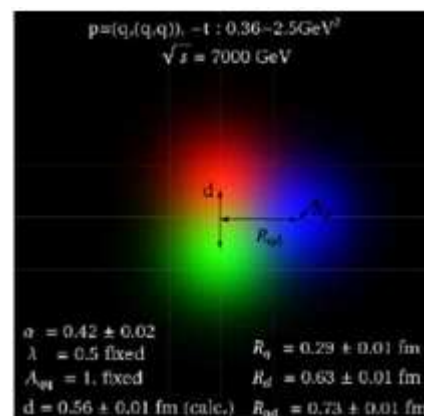
## R-D. Femtoscopy

Tamás Csörgő, László P. Csernai<sup>A</sup>, László Jenkovszky<sup>A</sup>, Béla Lukács<sup>A</sup>, Frigyes Nemes<sup>#</sup>, András Ster, Márton Vargyas<sup>#</sup>, Róbert Vértési

The Femtoscopy research group successfully conducted both theoretical and experimental physics research in the recently established research area of femtoscopy, that investigates the space-time evolution of strongly interacting elementary particle and heavy ion reactions on the femtometer length and femtometer/c time scales. Our experimental studies were performed and in the TOTEM experiment at the LHC accelerator at CERN and in the PHENIX experiment at the RHIC accelerator at the Brookhaven National Laboratory, US.

During 2013 our main contribution to the success of the **TOTEM Collaboration** was the calibration of the LHC optics from TOTEM data. The Hungarian group played a larger role in TOTEM as compared to the ratio of Hungarian participants in TOTEM: we not only provided a major contribution to TOTEM data taking of pPb collisions, but by reducing significantly the errors coming from the parameters of the LHC optics we contributed significantly to the reduction of the error of the total cross-section measurement of pp collisions. We have successfully reached one of the major goals of the TOTEM experiment, namely the measurement of the LHC absolute luminosity and, at the same time, the measurement of the total cross-section of proton-proton scattering with the luminosity-independent method, at both 7 and 8 TeV colliding energies. Our results at 7 TeV were highlighted as „**Editor’s Choice**” paper in Europhysics Letters, while our measurement at 8 TeV was published in one of the leading journals of our field, in the Physical Review Letters. At the end of 2013, our group leader got appointed as a new member of the Editorial Board of the TOTEM Collaboration.

Our group played a significant role in the **theoretical interpretation** of these measurements: we have discovered and published a simple relationship, the observation that the **product of the total cross section and the  $|t|$  value of the dip is a constant**, which is different from the same constant in the black disc limit. We have also interpreted the differential cross-section of elastic proton-proton collisions at 7 TeV, and our results were reported by invited talks at international conferences specializing in forward physics and diffraction. We have **generalized the Bialas-Bzdak model** of elastic proton-proton scattering by adding a small real part to the forward scattering amplitude which resulted in an improved description of differential cross-section data at ISR and LHC energies. We found that for a full description, a non-perturbative contribution has to be taken into account, for which the unitarization of the Bialas-Bzdak model provides a realistic opportunity. In a collaboration with Harvard University we have tested **the Glauber-Velasco model** for the



**Figure 1.** Valence quarks in the proton, a femto-scopic picture from TOTEM data, utilizing the generalized Bialas - Bzdak model.

<sup>A</sup> Associate fellow  
<sup>#</sup> Ph.D student



interpretation of the elastic scattering data in the dip region, and found that this model **provides a statistically acceptable interpretation** of the differential cross-section of elastic proton-proton scattering at 7 TeV in the dip region.

From a first analysis of the **PHENIX dilepton** spectra in 200 GeV Au+Au collisions at RHIC and its comparison with an earlier femtoscopic analysis we determined that  $m^*(\eta')$ , the mass of the in-medium modified  $\eta'$  meson, that propagates in hot and dense hadronic matter, is in the range of  $400 < m^*(\eta') < 757$  MeV. We had to replace our PHENIX simulation cluster, due to an explicit request from the Computer Network Center of Wigner RCP, and this change significantly drained our manpower and financial resources, but we successfully completed the transition with the help of software experts from Brookhaven National Laboratory.

Let us highlight three **invited conference talks**, that were given by members of the group during 2013. We presented the results of the Bialas-Bzdak and the Glauber-Velasco model analysis of elastic proton-proton scattering data at the Low-X 2013 conference in Eilat, Israel, gave an invited review talk about the comparison of PHENIX and STAR kaon femtoscopy in the WPCF 2013 conference in Acireale, Italy, and gave an invited TOTEM talk at the 7th Joint International Hadron Structure 2013 conference in Slovakia.

In December 2013, we organized our annual **Zimányi Winter School on Heavy Ion Physics**, the 13th in a row, in a Wigner-ELTE collaboration. The main organizer was Máté Csanád (ELTE) with T. Csörgő, who acted as the honorary chair of this meeting. This School is broadly recognized as the most significant annual scientific event at the RMI Institute for Particle and Nuclear Physics at Wigner RCP, it attracted participants from several countries including leading scientists from Japan and the US. It was a honor to host three former spokespersons of the PHENIX experiment: Shoji Nagamiya (RIKEN, Japan), the founding spokesperson of the PHENIX experiment, William A. Zajc (Columbia University), the second, and Barbara Jacak (Department of Physics, State University of New York at Stony Brook, NY, USA), the third Spokesperson of the PHENIX experiment. B. Jacak (PHENIX) presented the most recent PHENIX results in an Ortvy Colloquium about the collective behaviour found in d+Au collisions, interpreted as the appearance of a small volume perfect fluid of quarks, which changed the earlier interpretation of d+Au results as cold nuclear matter effects. T. Csörgő summarized the most significant achievements of first 10 years of Hungarian groups of Wigner RCP, ELTE and Debrecen in PHENIX, noted that from 2014, the University of Debrecen opted to discontinue its participation in PHENIX-Hungary and announced his stepping down, after 10 years, as the principal investigator of PHENIX-Hungary. From 2014, M. Csanád is the new coordination of the PHENIX-Hungary sub-collaboration, he will lead this Wigner-ELTE collaboration to the future of PHENIX, in particular to the era of superPHENIX.

## **Grants and international cooperation**

OTKA NK101438 (Principal Investigator T. Csörgő, 2012-2015)

Cooperation in theoretical femtoscopy with Harvard University (T. Csörgő, R.J. Glauber, F. Nemes)

Cooperation in theoretical femtoscopy with Lund University (T. Csörgő, A. Ster, L. Lönnblad, G. Gustafson)

Collaboration with the PHENIX experiment at RHIC accelerator, Brookhaven National Laboratory, USA (Hungarian Principal Investigator: T. Csörgő, participants from Wigner: J. Sziklai, R. Vértési)

Collaboration with the TOTEM experiment at LHC accelerator, CERN (Hungarian Principal Investigator T. Csörgő, participants from Wigner: F. Nemes, J. Sziklai).

## Publications

### Articles

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2. Yan YL, Cheng Y, Zhou DM, Dong BG, Cai X, Sa BH, Csernai LP: HYDRO-PACIAE, a hydrodynamic and transport hybrid model for ultra-relativistic heavy ion collisions. *J. PHYS. G* 40:(2) Paper 025102. 15 p. (2013)

### Conference proceedings

3. Fiore R, Jenkovszky L, Lavorini A, Sali A: Reggeometry of lepton- and hadron-induced reactions. *AIP CONF. PROC.* 1523:(1) pp. 83-86. (2013)
4. Jenkovszky L, Orava R, Sali A: Diffraction dissociation at the LHC. *AIP CONF. PROC.* 1523:(1) pp. 13-16. (2013)

### Others (accessible online only)

5. Csanad M, Csorgo T: Initial energy density of p+p collisions at the LHC. In: 15th conference on Elastic and Diffractive scattering, EDS Blois 2013., Saariselka, Finnország (2013.09.09-2013.09.13.), 2013, Tuula Maki (ed.) p. 4., Paper 53 (2013)
6. Csorgo T: Higgs Boson -- on Your Own. <http://arxiv.org/abs/arXiv:1303.2732> (2013)
7. Csörgő J, Török Cs, Csörgő T: Memory of Quark Matter Card Game <http://arxiv.org/abs/arXiv:1303.2798> p. 4 (2013)
8. Csörgő T, Nagy MI: A new family of exact and rotating solutions of fireball hydrodynamics. <http://arxiv.org/abs/1309.4390>, p. 15. Dedicated to T. Kodama on the occasion of his 70th birthday (2013)
9. Csörgő T, Nemes F: Elastic scattering of protons from  $\sqrt{s}=23.5$  GeV to 7 TeV from a generalized Bialas-Bzdak model. <http://arxiv.org/abs/1306.4217> p. 36 (2013)

## Phenix collaboration 2013

Due to the vast number of publications of the large collaborations in which the research group participated in 2013, here we list only a short selection of appearances in journals with the highest impact factor.

1. Adare A et al. incl. Csörgő T, Sziklai J, Vértési R [384 authors]: Azimuthal anisotropy of  $\pi^0$  and  $\eta$  mesons in Au + Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. C* 88:(6) Paper 064910. 10 p. (2013)
2. Adare A et al. incl. Csörgő T, Hidas P, Nagy MI, Ster A, Sziklai J, Vértési R [548 authors]: Direct photon production in d+Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. C* 87:(5) Paper 054907. 8 p. (2013)
3. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértési R [385 authors]: Double-spin asymmetry of electrons from heavy-flavor decays in p+p collisions at  $\sqrt{s}=200$  GeV. *PHYS. REV. D* 87:(1) Paper 012011. 17 p. (2013)
4. Adare A et al. incl. Csörgő T, Ster A, Sziklai J [383 authors]: Inclusive cross section and single transverse spin asymmetry for very forward neutron production in polarized p plus p collisions at  $\sqrt{s}=200$  GeV. *PHYS. REV. D* 88:(3) Paper 032006. 17 p. (2013)
5. Adare A et al. incl. Csörgő T, Nagy MI, Ster A, Sziklai J, Vértési R, Zimányi J [561 authors]: Medium modification of jet fragmentation in Au+Au collisions at  $\sqrt{s_{NN}}=200$  GeV measured in direct photon-hadron correlations. *PHYS. REV. LETT.* 111:(3) Paper 032301. 8 p. (2013)
6. Adare A et al. incl. Csörgő T, Sziklai J, Vértési R [385 authors]: Neutral pion production with respect to centrality and reaction plane in Au+Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. C* 87:(3) Paper 034911. 19 p. (2013)
7. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértési R, [376 authors]: Nuclear modification of  $\psi'$ ,  $\chi_c$ , and  $J/\psi$  production in d+Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. LETT.* 111:(20) Paper 202301. 7 p. (2013)
8. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértési R, [376 authors]: Quadrupole Anisotropy in Dihadron Azimuthal Correlations in Central d plus Au Collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. LETT.* 111:(21) Paper 212301. 7 p. (2013)
9. Adare A et al. incl. Csörgő T, Nagy MI, Sziklai J, Vértési R, [415 authors]: Spectra and ratios of identified particles in Au plus Au and d plus Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. C* 88:(2) Paper 024906. 16 p. (2013)

10. Adare A et al incl. [Csörgő T](#), [Nagy MI](#), [Novak T](#), [Ster A](#), [Sziklai J](#), [Vértési R](#), [Zimányi J](#), [636 authors]: The PHENIX Collaboration. *NUCL. PHYS. A* 904: pp. 1083-1087. (2013)
11. Adare A et al. incl. [Csörgő T](#), [Sziklai J](#), [Vértési R](#), [384 authors]: Transverse-momentum dependence of the  $J/\psi$  nuclear modification in d+Au collisions at  $\sqrt{s_{NN}}=200$  GeV. *PHYS. REV. C* 87:(3) Paper 034904. 22 p. (2013)
12. Adare A et al. incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Vértési R](#), [498 authors]:  $\Upsilon(1S+2S+3S)$  production in d+Au and p+p collisions at  $\sqrt{s_{NN}}=200$  GeV and cold-nuclear-matter effects. *PHYS. REV. C* 87:(4) Paper 044909. 13 p. (2013)
13. Atomssa ET, for the PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Zimányi J](#)): Dielectron measurements by PHENIX using the HBD. *NUCL. PHYS. A* 904: pp. 561C-564C. (2013)
14. Barish KN, PHENIX collaboration: PHENIX spin program: Recent results and prospects. *AIP CONF. PROC.* 1523:(1) pp. 182-187. (2013)
15. Drees A, PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Vértési R](#), [Zimányi J](#)): Thermal Radiation Mapping the Space-Time Evolution. *NUCL. PHYS. A* 910: pp. 179-184. (2013)
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17. Frawley AD, PHENIX collaboration (incl. [Csörgő T](#), [Ster A](#), [Sziklai J](#)): Cold Nuclear Matter Effects and Heavy Quark Production in PHENIX. *NUCL. PHYS. A* 910: pp. 123-130. (2013)
18. Gu Y, PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Zimányi J](#)): PHENIX Measurements of Higher-order Flow Harmonics for Identified Charged Hadrons in Au plus Au collisions at  $\sqrt{s_{NN}}=39-200$  GeV. *NUCL. PHYS. A* 904: pp. 353C-356C. (2013)
19. Haggerty JS, PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Zimányi J](#)): The sPHENIX Barrel Upgrade: Jet Physics and Beyond. *NUCL. PHYS. A* 904: pp. 925C-928C. (2013)
20. Hollis RS, PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Zimányi J](#)): Forward/backward  $J/\psi$  production and hadron  $v(n)$  in Cu+Au collisions in PHENIX. *NUCL. PHYS. A* 904: pp. 507C-510C. (2013)

21. Huang SL, PHENIX collaboration (incl. [Csörgő T](#), [Nagy MI](#), [Ster A](#), [Sziklai J](#), [Zimányi J](#)): Measurements of identified particle anisotropic flow in Cu plus Au and U plus U collisions by PHENIX experiment. **NUCL. PHYS. A** 904: pp. 417C-420C. (2013)
22. Kurosawa M, PHENIX collaboration: Higher harmonics flow measurement of charged hadrons and electrons in wide kinematic range with PHENIX VTX tracker. **NUCL. PHYS. A** 904: pp. 397C-400C. (2013)
23. McCumber MP, PHENIX collaboration: High  $p(T)$ : Energy Loss Physics at PHENIX. **NUCL. PHYS. A** 904: pp. 154C-161C. (2013)
24. McGlinchey D, PHENIX collaboration: Recent Heavy Quarkonia Results from PHENIX. **NUCL. PHYS. A** 904: pp. 603C-606C. (2013)
25. Mitchell JT, PHENIX collaboration: The RHIC Beam Energy Scan Program: Results from the PHENIX Experiment. **NUCL. PHYS. A** 904: pp. 903-906. (2013)

## R-E. Theoretical neuroscience and complex systems

Fülöp Bazsó, Dorottya Cserpán<sup>#</sup>, Péter Érdi, László Négyessy, Zoltán, Somogyvári, László Zalányi, Krisztina Szalisznyó<sup>A</sup>

**Structural correlates of brain functions.** — We found that neighbouring distal finger pad representations are connected to each other, and therefore this mutual connectivity could form the first steps of cortical processing resulting in global haptic perception. We found that transmission of information between somatosensory cortical areas are mostly restricted to the given distal finger pad representations. Most importantly, our results suggest that the anatomical pattern of connectivity determines the resting state (or intrinsic spontaneous) functional connectivity at the level of cortical functional modules. We found that tissue nonspecific alkaline phosphatase (TNAP), an enzyme vital for brain functions among others, exhibits specific laminar pattern of activity in the vertebrate retina. Furthermore, TNAP activity is localized in specific synaptic sub-layers of the retina, which suggest a distinctive role for this enzyme in processing visual information.

**Microelectric imaging techniques.** — We have shown, that it is possible to determine cellular and synaptic layers in the hippocampus and in the neocortex, based on extracellular multi-electrode potential measurement. High density silicon probes provided the basis for high-frequency power map, which clearly marked the pyramidal layer and the dentate-hilar area in the hippocampus. We have calculated the gamma-band coherence between all channels, and clustered them based on the resulted coherence values. The specific laminar distribution of the efferent hippocampal pathways enables identification of the anatomical layers in the dendritic area based on the coherence. This method reliably determined the different anatomical layers not only in the hippocampus, but identified three separate layers, corresponding to the superficial (II/III), middle (IV) and deep (V/VI) layers in the neocortex as well. Finally the temporal dynamics of the local field potentials and current source density in hippocampal layers were examined, showing the spatio-temporal distribution of synaptic events leading to action potentials in pyramidal and interneurons during theta oscillation and sharp-wave ripple periods.

**Dynamics of budgeting process.** — We developed a more general theory of budgetary politics and examined its implications on a new dataset on US government expenditures from 1791 to 2010. We used three major approaches to budgeting: the decision-making theories, primarily incrementalism and serial processing; the policy process models, and path dependency. We showed that the incrementalist budget model is recursive, and its solution is exponential growth, and isolated three periods in which it operates in pure form. The equilibrium periods are separated by critical junctures, associated with wars or economic collapse. Our theory is composed of three major ascertainments: exponential incrementalism is fundamental to a theory of budgeting. Within equilibrium periods the budgeting system follows stochastic exponential growth. Next, disjoint shifts in the level of spendings caused only by critical events and finally temporally localized policy dynamics can cause bends in the exponential path, longer returns to the exponential path within budgetary eras, and annual punctuations in budget changes.

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<sup>#</sup> Ph.D student

<sup>A</sup> Associate fellow

## International cooperations

Hannu Reittu, VTT Technical Research Centre of Finland, Espoo, Finland

Dragana Bajić, Faculty of Technical Sciences, University of Novi Sad, Serbia

Bryan Jones, University of Texas at Austin, USA

György Buzsáki, NYU Neuroscience Institute, New York University, USA

Caroline Fonta, Centre de Recherche Cerveau & Cognition – UMR5549, Toulouse, Franciaország

Anna Wang Roe, Vanderbilt Vision Research Center, Vanderbilt University, Nashville TN, USA

Vaibhav Diwadkar, School of Medicine, Wayne State University, Detroit, USA

## Publications

### Articles

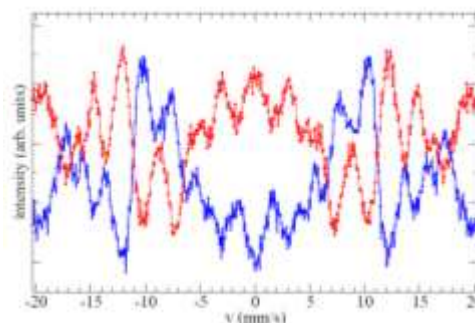
1. Érdi P, Makovi K, Somogyvári Z, Strandburg K, Tobochnik J, Volf P, Zalányi L: Prediction of emerging technologies based on analysis of the US patent citation network. **SCIENTOMETRICS** 95:(1) pp. 225-242. (2013)
2. Lendvai D, Morawski M, Négyessy L, Gáti G, Jäger C, Baksa G, Glasz T, Attems J, Tanila H, Arendt T, Harkany T, Alpár A: Neurochemical mapping of the human hippocampus reveals perisynaptic matrix around functional synapses in Alzheimer's disease. **ACTA NEUROPATHOL.** 125:(2) pp. 215-229. (2013)
3. Négyessy L, Palfi E, Ashaber M, Palmer C, Jakli B, Friedman RM, Chen LM, Roe AW: Intrinsic horizontal connections process global tactile features in the primary somatosensory cortex: Neuroanatomical evidence. **J COMP. NEUROL.** 521:(12) pp. 2798-2817. (2013)
4. Szalisznyo K, Silverstein DN, Duffau H, Smits A: Pathological Neural Attractor Dynamics in Slowly Growing Gliomas Supports an Optimal Time Frame for White Matter Plasticity. **PLOS ONE** 8:(7) Paper e69798. (2013)
5. Wang Z, Chen LM, Négyessy L, Friedman RM, Mishra A, Gore JC, Roe AW: The Relationship of Anatomical and Functional Connectivity to Resting-State Connectivity in Primate Somatosensory Cortex. **NEURON** 78:(6) pp. 1116-1126. (2013)

## R-L. Functional nanostructures

László Bottyán, László Deák, István Dézsi, Miklós Dolgos<sup>#</sup>, Márton Major, Dániel Géza Merkel, Béla Nagy<sup>#</sup>, Dénes Lajos Nagy, Szilárd Sajti

The Functional Nanostructures Research Group focuses research on physical properties of magnetic nanostructures and biological/biomimetic membranes. Activities include experimental studies of these systems by nuclear solid state spectroscopies, primarily by neutron reflectometry and synchrotron-based reflectometries. Development of the theory and the techniques of the applied methods is a particular strength of the group.

**Reciprocity violation in the phase of a scattered wave.** — We recently predicted a new type of violation of the reciprocity principle, which, however, is hidden in experiments detecting only the intensity of the scattered waves. This special case (called *pseudo-reciprocity* or *magnitude reciprocity*) was demonstrated by the group members in a magneto-optical x-ray scattering experiment evidencing violation of reciprocity in the phase of nuclear resonant scattering of synchrotron radiation (Figure 1).



**Figure 1.** Experimental demonstration of magnitude reciprocity by stroboscopic detection of nuclear resonant forward scattering of synchrotron radiation. Experiment at DESY, PETRA III August 2013.

**High-entropy alloys.** — The atomic and magnetic structure of nanotechnologically synthesized and mechanically treated stainless steels and of FeCrNiCoCuTi<sub>x</sub> high-entropy alloy (HEA) was determined. The atomic configuration of mechanically treated HEAs proved to be extremely stable as compared to stainless steels.

**Inverse proximity effect in superconductor/ferromagnet bilayers.** — Inverse (magnetic) proximity effects can be detected by polarized neutron reflectometry *in a single superconductor/ferromagnet bilayer* [MR.1]. Experiments on a V(40 nm)/Fe (1 nm) bilayer have shown that spin asymmetry measured at  $T = 0.5 T_C$  is shifted towards higher momentum transfer values compared to the spin asymmetry measured at  $T = 1.5 T_C$ . Such a shift is ascribed to the appearance of magnetic sublayer in superconducting vanadium with a thickness of 7 nm and a magnetization of +0.8 kG.

**The GINA neutron reflectometer: further development [MR.2].** — A new 4-bounce Fe-Co/Si/glass polarizer/neutron filter was designed and constructed (Figure 3). The polarization degree of the new device is about 99.997% and is an available option of the GINA polarized reflectometer making possible special experiments requiring extremely high degree of polarization. A new biomembrane option (Figure 2) was added opening new of functionality of the neutron reflectometer in biomembrane studies.

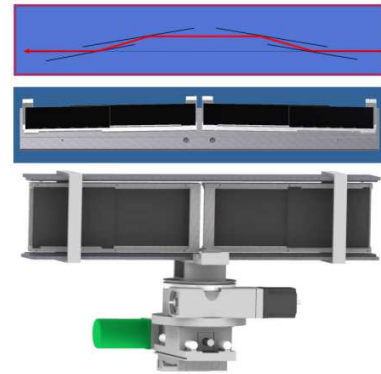
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<sup>#</sup> Ph.D student





**Figure 2.** The new biomembrane option for the GINA neutron reflectometer



**Figure 3.** The design (top) and implementation (bottom) of the installed new neutron polarizer of the GINA reflectometer

## Grants and international cooperation

Taiwan\_MTA\_SNK-69\_2013 MTA-Taiwan NSRC bilateral project: Studying exchange bias effects in ferromagnetic / antiferromagnetic thin films by polarized neutron reflectometry (L. Bottyán, 2013-2014)

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

## Long-term visitor

- Olaf Leupold, DESY, Germany, from 1 September to 22 December, 2013, (host: L. Bottyán)

## Publications

### Articles

1. Bottyán L, Merkel D G, Nagy B, Fuzi J, Sajti Sz, Deak L, Endróczy G, Petrenko AV, Major J: GINA---A polarized neutron reflectometer at the Budapest Neutron Centre. **REV. SCI.C INSTRUM.** 84:(1) Paper 015112. 8 p. (2013)
2. Hildebrandt S, Komissinskiy P, Major M, Donner W, Alff L: Epitaxial growth and control of the sodium content in  $\text{Na}_x\text{CoO}_2$  thin films. **THIN SOLID FILMS** 545: pp. 291-295. (2013)
3. Khaydukov YN, Nagy B, Kim J-H, Keller T, Rühm A, Nikitenko YV, Zhernenkov KN, Stahn J, Kiss LF, Csik A, Bottyán L, Aksenov VL: On the feasibility to study inverse proximity effect in a single S/F bilayer by Polarized Neutron Reflectometry. **JETP LETTERS** 98:(2) pp. 107-

110. (2013)

4. Merkel DG, Nagy B, Sajti Sz, Szilágyi E, Kovács-Mezei R, Bottyán L: Higher harmonics suppression in Fe/Si polarizing neutron monochromators. **NUCL. INSTRUM. METHODS A** 704: pp. 92-97. (2013)
5. Nagy B, Khaydukov YN, Kiss LF, Sajti S, Merkel DG, Tanczikó F, Vasenko AS, Tsaregorodsev RO, Rühm A, Keller T, Bottyán L: Controlling Exchange Coupling Strength in Ni<sub>x</sub>Cu<sub>1-x</sub> Thin Films. **J. SUPERCOND. NOV. MAGN.** 26:(5) pp. 1957-1961. (2013)

#### **Others**

6. Bottyán L, Merkel DG, Nagy B: GINA - neutron reflectometer with polarization option. In: Baranyai R, Makai M, Pálffy H, Rosta L (eds.): Progress Report on the activities at the Budapest Research Reactor: Budapest Neutron Centre 2010-2012. Budapest: KFKI, p. 204-205 (2013).
7. Merkel DG, Sajti Sz, Rühm A, Major J, Ruffer R, Bottyán L: FE Self-diffusion in FEPD revealed by reflectometry. In: Baranyai R, Makai M, Pálffy H, Rosta L (eds.): Progress Report on the activities at the Budapest Research Reactor: Budapest Neutron Centre 2010-2012. Budapest: KFKI, 2013. pp. 29-30.

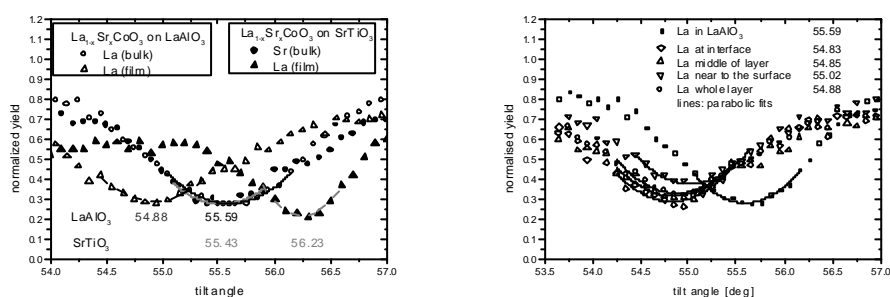
**See also: R-K.4, S-E.1, S-L.19**

## R-M. Ion beam physics

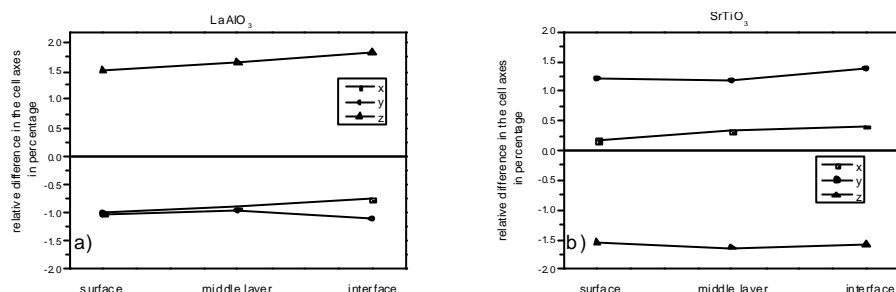
Edit Szilágyi, Pál Kostka, Endre Kótai, Imre Kovács, Attila Németh, Zoltán Szőkefalvi-Nagy

**Strain determination (in cooperation with the X-ray spectroscopy group).** — The cobalt oxide system  $\text{LaCoO}_3$  and its Sr-doped child compounds have been intensively studied for decades due to their intriguing magnetic and electronic properties. Preparing thin  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$  (LSCO) films on different substrates allows for studies with a new type of perturbation, as the films are subject to substrate-dependent epitaxial strain. By choosing a proper substrate for a thin film grow, not only compressing but also tensile strain can be applied. The consequences for the fundamental physical properties are dramatic: while compressed films are metallic, as the bulk material, films under tensile strain become insulating. The goal of this work is to determine the strain tensor in LSCO films prepared on  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  substrates by pulsed laser deposition using RBS/channelling methods.

The strain tensors were determined from angular scans around  $\langle 111 \rangle$ ,  $\langle \bar{1}11 \rangle$ ,  $\langle 011 \rangle$ ,  $\langle 0\bar{1}1 \rangle$ ,  $\langle 101 \rangle$ ,  $\langle \bar{1}01 \rangle$  directions through the corresponding planes. The components of the strain tensor for cubic crystal can be deduced using the relations between changes in angles of channelling crystal directions.



**Figure 1.** *Left:* Normalized yields around  $\langle \bar{1}11 \rangle$  direction. A significant angle difference can be observed between LSCO films grown on  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  substrates due to the different lattice mismatch induced stresses (compressive on  $\text{LaAlO}_3$  and tensile stress on  $\text{SrTiO}_3$  substrates). *Right:* Depth dependence of the angular scan around  $\langle \bar{1}11 \rangle$  direction for LSCO film on  $\text{LaAlO}_3$  substrate. La integral of the film is divided to three parts (interface, middle and surface region).



**Figure 2.** Relative differences in the cell axes of LSCO films grown on a)  $\text{LaAlO}_3$  and b)  $\text{SrTiO}_3$  substrates are plotted in percentage as a function of depth.

Apart from the composition and defect structure of the samples, the depth dependence of the strain tensor, the cell parameters, and the volume of the unit cell are also determined. Asymmetric behaviour of the strained cell parameters is found on both substrates. This asymmetry is rather weak in the case of LSCO film grown on  $\text{LaAlO}_3$ , while stronger on  $\text{SrTiO}_3$  substrate. The strain is more effective at the interface, some relaxation can be observed near to the surface.

**CHARISMA.** — The external proton beam PIXE setup at the the Van de Graaff accelerator of Wigner is an important measuring facility of the BNC platform of the Fixlab of the CHARISMA (Cultural Heritage Advanced Research Infrastructures: Synergy for a multidisciplinary approach to conservation/restoration) EU FP7 Programme. Precise and reproducible aiming by the proton beam at the precious art or archaeological objects is a very essential step of the elemental analysis. As a further improvement of the setup a three axis computer-controlled device allowing fine positioning steps as short as  $2.5 \mu\text{m}$  in x,y and z direction was installed.



**Figure 3.** Ancient silver coins fixed to the positioning device. The beam pipe- detector arrangement and the mechanical aiming tool of the external beam PIXE set-up can also be seen.

Seven foreign groups from England, Germany, Greece, Italy, Poland and Portugal applied successfully for the access of this infrastructure and joint PIXE analyses were made on different cultural heritage objects as lapis lazuli, obsidians, silver coins, sword, crucibles and ancient textiles. It was shown among others that the raw material of Transylvanian Neolithic obsidian tools have a Slovak Tokaj Mountains provenance. This conclusion based on the measured correlation of the Ti to Mn and Rb to Zr ratios (Fig. 3).

## Grant

CHARISMA Grant Agreement No. 228330 (2009-2014)

## Publications

### Articles

1. Mödlinger M, Piccardo P, Kasztovszky Z, [Kovács I](#), [Szokefalvi-Nagy Z](#), [Káli G](#), Szilágyi V: Archaeometallurgical characterization of the earliest European metal helmets. **MATER. CHARACTER.** 79: pp. 22-36. (2013)

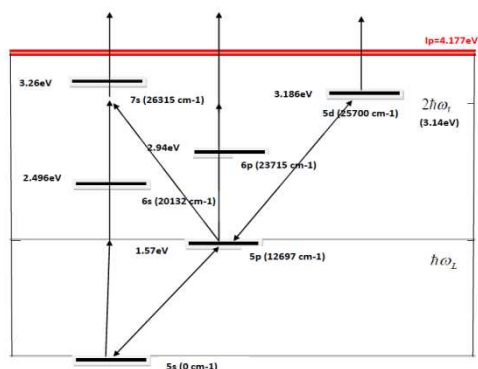
See also R-L.4, S-L.14

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

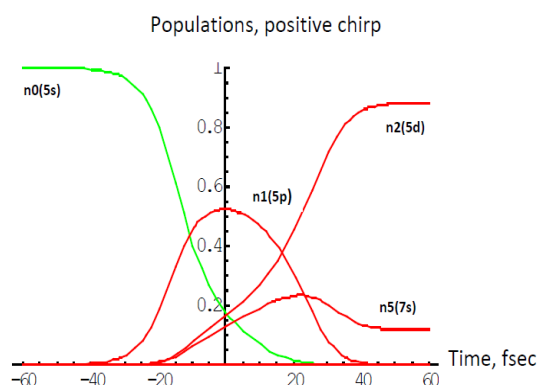
**Gagik Dzsotjan**, József Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós Kedves, Béla Ráczkevi, Nóra Sándor, Zsuzsanna Sörlei

Adiabatic control of atomic and molecular inner and translational degrees of freedom by laser radiation has found immensely rich applications in different fields of contemporary science and technologies. We have proposed and analyzed different novel schemes of coherent adiabatic control using short frequency chirped laser pulses including schemes of robust creation of coherence between ground atomic quantum states in optically thick media for enhancing different resonant nonlinear optical frequency mixing processes, high fidelity photon-echo based schemes for storage and retrieval of quantum information, pre-excitation of alkali atoms by frequency chirped ultra-short laser pulses for generation of highly-homogeneous laser plasma. For experimental verification of this process, an experimental setup has been constructed in order to study the ionization of Rb atoms induced by radiation from a Ti:Sa laser.

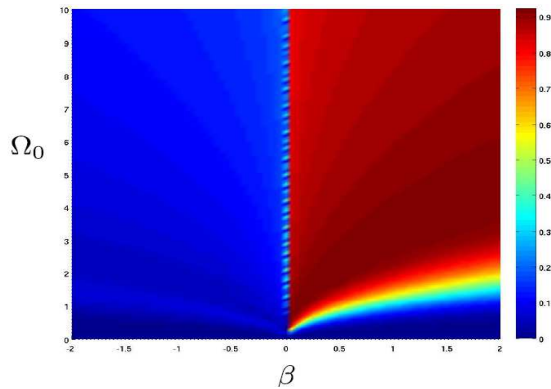
When considering generation of laser plasma with high homogeneity using multi-photon or over-the-barrier ionization, it is advantageous to find ways for decreasing the threshold conditions for the ionization, especially when generation of spatially extended plasma is the main goal. One of the ways to decrease the threshold is to transfer atomic population from its ground state to its excited states before the ionization process, thus significantly decreasing the ionization potential. We have demonstrated that such pre-excitation performed by ultra-short (with duration of tens of femto-seconds) frequency chirped (FC) strong laser pulses, (see Fig.1,2) is extremely robust against the variation of the laser pulse parameters including duration, shape, fluctuations in pulse intensity, phase, etc, see Fig 3.



**Figure 1.** The relevant energy levels of Rb atom along with the excitation and ionization scheme.



**Figure 2.** Excitation of Rb atom to states 5d and 7s by a Gaussian FC laser pulse of 30 fsec duration and positive frequency chirp. The pulse peak intensity is equal to  $3 \times 10^{12} \text{ W/cm}^2$ , the speed of the linear chirp is  $0.3 \text{ fs}^{-2}$ .



**Figure 3.** Dependence of the final population of the state 5d of the Rb atom on peak Rabi frequency  $\Omega_0$  of the laser pulse (in units of  $\text{fsec}^{-1}$ ) and chirp speed  $\beta$  (in the units of  $\text{fsec}^{-2}$ ).

## Grants and international cooperation

OTKA NN 78112. Light slowing down by frequency chirped laser pulses ( G. Dzsotjan, 2010-2013)

Hungarian National Development Agency: ELI-09-1-2010-0010, „HELIOS” grant (G. Dzsotjan, 2010-2013)

Polish-Hungarian Academic Bilateral with the Institute of Physics of the Jagellonian University, Krakow, Poland (G. Dzsotjan, 2010-2013)

TÉT\_12\_FR-1-2013-0019 French-Hungarian Bilateral with the University de Bourgogne, Dijon, France (G. Dzsotjan, 2013-2014)

## Publications

### Articles

1. Demeter G: Solving the Maxwell-Bloch equations for resonant nonlinear optics using GPUs. *COMPUT. PHYS. COMMUN.* 184: pp. 1203-1210. (2013)
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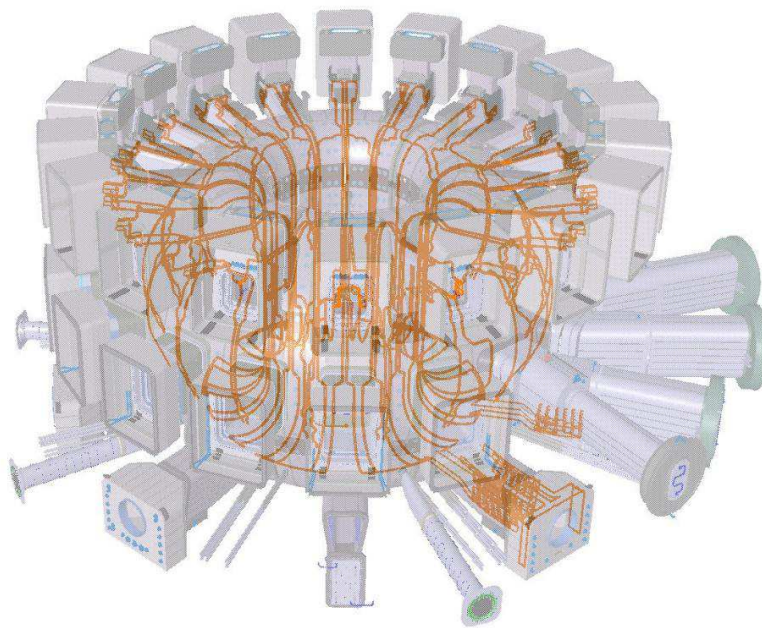
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See also: S-S.5

## R-O. ITER and fusion diagnostic development

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

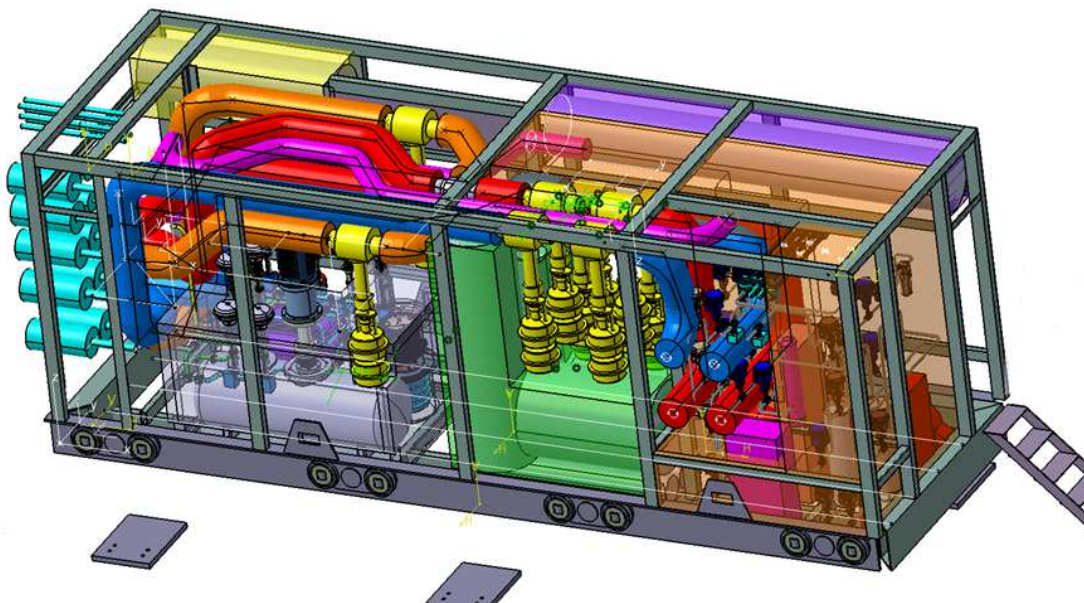
The TSD (Tokamak Services for Diagnostics) consortium is responsible for the development of the ITER diagnostic infrastructure. The consortium consists of four members: MTA Wigner RCP, which conducts the leading role via the "ITER and fusion diagnostics development group", MTA EK and CCFE from UK. The objective of the infrastructure is the appropriate electrical transmission of diagnostic signals outside vacuum vessel. The time frame of the task is about four years, which began in early 2013. The main components to be developed are: cables, looms, cable trays, electrical connectors (robotic and traditional), feedthroughs, cable bridges. In the first year, the consortium analysed the existing proposals of necessary components and determined the approximate number and location of thousands of parts. In addition, we reviewed the boundary conditions: the main problems associated with the components are high temperature, neutron radiation and vacuum. In the case of electrical signals, the source of noise may be the temperature fluctuations, uneven neutron load or thermal load, connectors and magnetic field. Getting to know the boundary conditions, and after extensive market research, we found that due to the special circumstances of ITER, in most cases industrial solutions are not sufficient, therefore R & D activities should be carried out in collaboration with industry. In some cases (looms, feedthroughs) prototypes have also been manufactured. In the case of cable-harnesses the consortium proposed a complex testing which is about to begin.



**Figure 1.** Component of TSD project (cables, cable trays, feedthroughs, connectors)

The research group is in successful collaboration with the TBM (Test Blanket Module) consortium for many years now via Fusion for Energy grants. The main objective of the collaboration is the development of the ITER tritium breeding blanket. Activities in the year 2013 were carried out in two parallel grants. Our main tasks included the development and integration of auxiliary systems of breeding blanket in ITER port cell and development,

specification of sensors and instrumentation of the breeding blankets. We developed the helium cooling circuit, the lithium circulation system and tritium transport system layout in port cell in the framework of OMF-331, taking into account the special requirements of ITER. We investigated the possibilities of maintenance operations of these sub-systems, and developed an universal transport frame, which allows the installation and removal of the auxiliary systems as one unit into or from the port cell. Within the FPA-380 framework partnership we worked in close collaboration with the consortium members and developed partly the specification of the blanket sensors and instrumentations, taking into account the thermo-hydraulic and thermo-mechanical behaviour of breeding blankets. We have also developed a central database and have collected the required instrumentation and the main information of specifications for the next phase of the project, when the available products of potential manufacturer will take place via a wide range of market research.



*Figure 2. Layout of TBM auxiliary systems in the port cell*

## Grants and international cooperation

European Communities under the contract of Association between EURATOM and the Hungarian Academy of Sciences. (S. Zoletnik, 1999-)

Hungarian-Korean Joint Laboratory Program in Science and Technology: Joint fusion laboratory. (S. Zoletnik, 2011-2013)

Fusion for Energy, F4E-FPA-328, (G. Veres 2012-2016)

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**See also: R-Q.1, R-Q.6, R-Q.9**

## R-P. Laser plasma

István B. Földes, Márk Aladi, Angéla Barna, Imre Ferenc Barna

High harmonics of Ti-sapphire laser were generated in gas jet targets. The highest obtained harmonics was 45th time the frequency of the laser, higher than expected from the quasiclassical 3-step model. Modifying the gases and their pressure a regime was found where noble-gas clusters were generated. The conversion efficiency of harmonics was higher in clusters than in atomic gases, nevertheless the highest obtainable intensity is still limited by ionization effects. Varying pressure and laser intensity the wavelengths of harmonics could be shifted, thus providing a continuously tunable coherent light source in the 20-40 nm EUV spectral range. It was shown that the phase and thus the wavelength of harmonics is affected by the free electrons in the interaction range and that of the nanoplasmas generated inside the clusters.

Directional stabilization of the KrF laser of the HILL laboratory of the University of Szeged, Department of Experimental Physics was successfully improved. The here developed feedback system allows a long term stability better than  $10^{-2}$  rad. It means that when focusing the beam using off-axis parabolic mirror the focal diameter can be kept below  $1 \mu\text{m}$ , which allows the availability of intensities as high as  $10^{18} \text{ W/cm}^2$ . Plasma mirror method was investigated for improving the temporal contrast of the short pulse, with which the intensity of pedestals can be decreased by more than an order of magnitude. The obtained  $\sim 50\%$  efficiency significantly improves our previous results which was 40-45%.

We participated in joint experiments in the Max-Planck-Institut für Quantenoptik in Garching. In the experiments we observed the first time harmonics with the relativistically oscillating mirror mechanism when using laser pulses shorter than 5 fs, i.e. with 1.5 cycle laser pulses. According to the expectations these harmonics can be the sources of isolated attosecond pulses. Our group investigates the conversion efficiency into these harmonics. In the preliminary experimental series broadened high harmonics were observed according to the expectations. The reproducibility of the experimental results is under progress.

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## Book chapter

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## R-Q. Beam emission spectroscopy

Dániel Dunai, Gábor Anda, Sándor Bató, Attila Bencze, Sándor Kálvin, Tibor Krizsanóczy, Máté Lampert, Gábor Petravich, Dániel Réfy, Balázs Tál, Sándor Zoletnik

**BES measurements on MAST spherical tokamak.** — A Beam Emission Spectroscopy (BES) diagnostic has been installed on MAST spherical tokamak in 2011. This cutting edge technology diagnostic was developed in cooperation with CCFE, but was mostly operated by the Wigner BES research group. The M9 measurement campaign was 5 months long in 2013, and the BES diagnostic was operational through the entire campaign. The BES diagnostic was a key diagnostic in some of the major physics programs of the campaign. The Wigner BES physics program was focused on the ELM instabilities and detailed study of L-H transitions. Due to the continuous optimization of the optical system and the high sensitivity of the applied avalanche photo diode camera outstanding measurement results were gained. From the measured BES data we identified phenomenon, which can be responsible for triggering the ELM edge plasma instability. The understanding of ELMs is one of the still opened key issues, which is primarily important for ITER and for the future reactors. We also studied the ELM evolution as the process of energy loss during this impulsive edge instability is also not known. The MAST tokamak was shut down in September 2013 for two years. In these two years several major components will be upgraded and other developments are also planned. The BES diagnostic has been dismantled at the beginning of the shutdown and the design and the development of the new diagnostic for MAST-U has already been started.

**Li-beam diagnostics on Compass tokamak.** — In 2013 the components of the Li-beam diagnostic system have been improved and tested. The Li-beam system consists of four components, namely: 1.) the accelerated atomic beam, 2.) the slow (100Hz) CCD camera detection system, 3.) the fast (1MHz) avalanche photodiode detector system and 4.) the atomic beam probe detector (ABP). Due to the multiple improvements of the system, the 40 keV accelerated Li-beam have established a stable operation at 2 mA extracted current. More than 50% of the extracted current has been observed at the end of the flight tube, just before the plasma volume. The spatial calibration of the APD system has been performed by an installed calibration rod. In order to improve the spatial resolution of the ABP measurement a new cylindrical reducer has been designed, manufactured and installed. The field of view of the slow observation system has been increased by means of a newly installed entrance tube. It was also found that during boronization and glow discharge a massive layer is formed on the entrance vacuum window of the CCD optics, therefore a protecting shutter has to be installed. Using the slow observation system the first light profiles have been recorded in various plasmas and the density reconstruction code is under benchmarking. The fast APD camera has been installed and tested in plasma shots. From the recorded signals it was found that the beam is not properly aligned, so adjustment is needed. The analog and digital electronics of the ABP have been tested and installed together with the test detector and is ready for measurements.

**BES measurements on Korean KSTAR tokamak.** — Our research group performs beam emission spectroscopy measurements in every year since 2010 under the Joint Hungarian - Korean research laboratory cooperation on the KSTAR tokamak located in Daejeon, South Korea. We've made developments prior the 2013 measurement campaign in order to have a

more reliable system, furthermore to achieve a higher light intensity and also lower background. These quantities describe best the quality of the measured BES data. During the analysis of the measured data, new physical phenomena was found, which are passing off at the plasma edge region and they are responsible for the plasma confinement. To explore the physical phenomena, the information of the exact measurement position is essential. Hence a method was developed, which can determine the measurement position within 1% error. The method was validated with measurement data, as well. In 2014 BES measurements will be performed by the Wigner BES research group. The Wigner BES physics program will concentrate on the study of plasma edge electron density fluctuations and the changes of electron density profiles.

**Further European BES developments.** — The Wigner BES group upgraded the observation systems of the two most important Lithium BES diagnostics in Europe. A 32 channels ultrafast avalanche photodiode based camera system was installed into both, which was developed and manufactured in Hungary. The primary aim of these measurements is the study of the fusion plasma edge turbulence and the fast transient events, which were not accessible prior these developments. At JET tokamak (UK) the spatial structure of the M-mode was resolved, which is a periodic plasma oscillation in the plasma edge. The trial measurements on ASDEX Upgrade (Germany) proved that, the new detector exhibits two times higher signal to noise ratio with the same applied measurement bandwidth compared to the existing system. Based on these results the final observation system, which is to be completed in 2014, will apply this camera unit.

## Grants and international cooperation

EUROFUSION Consortium tenders

Korean-Hungarian joint laboratory program of Korea Research Council of Fundamental Science and Technology

EAST Diagnostic Li-beam BES contract

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**See also: R-O.7**

## **JET EFDA Contributions**

Due to the vast number of publications of the large collaborations in which the research group participated in 2013, here we list only a short selection of appearances in journals with the highest impact factor. Wigner scientists participating in this collaboration are Cseh G, Dunai D, Gál K, Kálvin S, Kocsis G, Mészáros B, Petravich G, Réfy D, Szabolics T, Szepesi T, Zoletnik S.

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**See also: R-R: ASDEX Upgrade Team: 2**

## R-R. Pellet and video diagnostics

Tamás Szepesi, Gábor Cseh<sup>#</sup>, Gábor Kocsis, Ádám Kovács, Tamás Szabolcs

**Pellet cloud drift investigations at ASDEX Upgrade.** — Although several explanatory models have been published about pellet ablation, basic questions such as the origin of the fluctuation in the light emitted by both cryogenic and impurity pellet clouds are still not well understood. Recently fast framing movies (up to 600 kHz frame rate) recorded during cryogenic pellet ablation clearly show that from time to time cloudlets are erupted from the main pellet cloud. The erupted cloudlets emit visible light for a while and therefore also contribute to the visible radiation. The radiation of the main cloud and the released drifting cloud was separated by applying the 'flux tube approach' revealing that the appearance of the drifting clouds play an important role in the intensity fluctuation. Considering the separated main cloud radiation only, its total radiation still fluctuates therefore we can conclude that substantial amount of the main cloud particles are erupted by the drift process.

**Pellet cloud database analysis at ASDEX Upgrade.** — Cryogenic pellet injection is one of the most successful ways to fuel fusion plasmas and to control instabilities appearing at the plasma edge (Edge Localized Modes – ELMs). To develop the most efficient techniques for the aforementioned applications, substantial understanding of the pellet ablation is necessary. To achieve this goal a pellet cloud database was created. It contains images about the pellet clouds recorded with ultra-high speed fast framing cameras and other pellet- and plasma related parameters needed to analyse the shape of the cloud at given conditions. In this year – after a substantial upgrade of the database – a scaling was made, which aimed to reveal the connection between the width of the pellet cloud and the pellet velocity, pellet volume, plasma temperature and density and the applied magnetic field. It appears that the magnetic field does not have a high influence to the pellet cloud width. However, it is inversely proportional with the pellet velocity and the pellet volume, and it is proportional to the electron temperature. The role of the electron density is not fully understood yet.

**ELM triggering studies with pellets at JET.** — Pellet ELM pacing and triggering was investigated at JET by using small size pellets. The key diagnostics of these investigations is the fast framing camera system operated by HAS. Despite technical limitations, injecting outboard small size pellets resulted in a transient enhancement of the initial ELM frequency up to a factor 4.5.

It was recognized in experiments with the ITER like wall that not all pellets can trigger an ELM, therefore small size pellets were also used to investigate the ELM trigger threshold. It was observed that for outboard pellet launch the ELM triggering probability increases with the time elapsed after the previous ELM, the pellet mass and the pellet speed. Inboard launched pellets - penetrating deeper into the plasma - showed a higher trigger capability than pellets launched from the outboard, where the asymmetric shielding of the pellet resulted in a shallower penetration.

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<sup>#</sup> Ph.D. student

**Video diagnostics development at Wendelstein 7-X stellarator.** — The video diagnostic developed by our group will be located in the AEQ port in all 10 half modules of W7-X, and will enable the observation of almost all of the plasma facing first wall. In 2013 the main emphasis was put on the development and testing of the intelligent camera firmware and software. With the new firmware the camera can already record movies of different ROIs with different readout frequency at the same time. Real-time event processing in EDICAM has been also updated by re-defining some points in the basic specifications and by removing bugs spoiling the logic chain connected to events. Now the logic works reliably and as a result, the real-time processing function of finding the min/max of the ROI or calculating the sum of all pixels, and comparing it to a threshold, is now ready to use. Demonstration tests are ongoing. A new software interface for camera controls was also developed, featuring a console and a GUI application as well.

**Development of a portable pellet injector (TATOP).** — In early 2013 the TATOP was transported to ASDEX Upgrade (AUG) tokamak in Germany. The transport could be carried out using a normal car, demonstrating that the injector is indeed "portable". At AUG we had the possibility to test the device in a real fusion experiment environment, and the TATOP was working normally during the whole test. The injector was also successfully connected to the tokamak vacuum system, under the supervision of the AUG vacuum group. Based on these tests, further steps in the development of the device could be determined, such as: minor modifications to the controlling program code, as well as the usage of more vacuum compatible materials. Using the results of the tests, hardware improvements were also suggested, in order to produce a second prototype of the injector, featuring additional functions. Implementation shall start in 2014.

## Grants and International cooperation

IPP Garching, IPP Greifswald, CCFE, JAEA

## Publications

### Articles

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### Book chapters

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**See also: R-O.7**

### ASDEX Upgrade Team

Due to the vast number of publications of the large collaborations in which the research group participated in 2013, here we list only a short selection of appearances in journals with the highest impact factor. Wigner scientists participating in this collaboration are G l-Hobirk K, K lvin S, Kocsis G, Szepesi T.

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3. Sertoli M et al. [ASDEX Upgrade team]: Characterization of saturated MHD instabilities through 2D electron temperature profile reconstruction from 1D ECE measurements. **NUCL. FUSION** 53:(5) Paper 053015. 14 p. (2013)
4. Salewski M et al. [ASDEX Upgrade team]: Combination of fast-ion diagnostics in velocity-space tomographies. **NUCL. FUSION** 53:(6) Paper 063019. 10 p. (2013)
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## R-S. Space Physics

Zoltán Németh, Zsófia Bebesi, Géza Erdős, Lajos Földy, Antal Juhász, Károly Kecskeméty, Péter Király<sup>A</sup>, Katalin Lukács<sup>#</sup>, Károly Szegő, Mariella Tátrallyay<sup>A</sup>

### Interplanetary Space

**Uniform distribution of the magnetic flux in the heliosphere.** — The magnetic flux in the heliosphere is characterized by the radial component of the magnetic field vector BR. The distribution of that component is a complex function of the solar wind velocity, of the location in the heliosphere and of the epoch of the sunspot cycle. Investigation of the two-dimensional distribution of the radial and tangential component of the magnetic field has proved that this large complexity is due to fluctuations of the magnetic field around its average value. A new method has been developed to reduce the effect of fluctuations.

**The effect of a solar storm on the magnetosphere of Venus.** — We studied the effect of the solar storm that hit Venus on 25 May 2007 using data of the Venus Express mission. We found that the polarity of the induced magnetosphere reversed after the impact.

**Space Weather.** — The strongest source of high energy electrons in the interplanetary space is Jupiter, rather than the Sun, so that the electron flux is higher near interplanetary magnetic field lines connecting it to the observer. Using numerical simulation we pointed out that during the extremely weak solar activity in 2007-2008 a magnetic trap was formed and the recurring flux peaks observed during unfavorable magnetic connection are formed when electrons are trapped in this structure.

### Planets and Magnetospheres

**Plasma structures in the magnetosphere of Saturn.** — The magnetodisk is the key to the understanding of the structure of the Kronian magnetosphere. This complex magnetized plasma phenomenon influences almost every properties of the magnetosphere of Saturn. We developed a new magnetodisk model, which is able to describe the variations of the shape of this complex plasma structure using only one parameter. We have also performed numerical simulations based on a simple centrifugal potential model, and found that the model is able to explain many recently discovered properties of the magnetodisk plasma.

**Energetic electron interaction at Titan.** — The electrons gyrate around Saturn's magnetic field lines, which - due to co-rotation - drape around Titan's ionosphere. The flapping of the magnetodisk often causes the field lines to tilt near Titan, as an additional effect. The incoming electrons are either absorbed in the atmosphere, or are reflected at the strong magnetic gradients of the magnetic pileup boundary.

We studied the nature of the electron loss regions, their altitudes and spatial distribution near Titan. We found, that a significant percentage of the electrons are lost in the exo-ionospheric region. In the dusk-midnight-dawn section of its orbit around Saturn, Titan was found embedded in higher flux plasma during the Cassini flybys, relative to the dayside. This

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<sup>#</sup> Ph.D. student



is due to the bowl shaped magnetodisk - in which the plasma density is higher compared to the lobes - which is more flattened out on the nightside, than on the dayside.

**Modeling the distribution of small trapped Phoebe dust particles in Saturn's magnetosphere.** — We applied our dust model to Phoebe dust particles and found that (independently of the size) about half of the particles are on retrograde orbits and the other half of trapped Phoebe particles are moving around Saturn on prograde orbits. This is true for larger – non trapped – particles too (in the size range of  $0.15 < r_g < 0.35$  micron). The cause of the change in the orientation of the orbits is the radiation pressure. Also, the radiation pressure is responsible for quickly driving dust particles into the inner magnetosphere of Saturn where they can be trapped due to charging effects.

We have also developed a new dust model, which is able to explain the spatial and temporal variations of the nanodust observed in the inner magnetosphere by the STEREO A/B space probes. The model can be applied to cometary nanodust as well. Our model serves as the theoretical background for a new dust detector developed in the LASP (Boulder, Colorado, USA).

## Grants and international cooperation

EU-FP7-CPS CSA Number 228319 „Europlanet RI” (K. Szegő, 2008-2012)

PECS Experimental Arrangement No. 98077 “Cluster Data Exploitation” (M. Tátrallyay, 2008-2012)

PECS Experimental Arrangement No. 98080 “Participation in the development of the Rosetta Consortium Experiment on board Orbiter RPC” (S. Szalai, 2008-2013)

Hungarian space research development URKUT\_10-1-2011-0006 “Participation in the NASA STEREO space mission” (K. Kecskeméty, 2013-2014)

Hungarian space research development URKUT\_10-1-2011-0011 “Participation in the NASA Cassini space mission” (Z. Németh, 2013-2014)

Participation in current and upcoming international space and planetary exploration missions: Bepi Colombo, Cluster, Cassini, JUICE, Rosetta, SoHO, Solar Orbiter, Stereo, Venus Express

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## R-T. Space Technology

János Nagy, ...

The main goal of **Plasma Wave Complex (PWC)** experiment is to study dynamic processes in the magnetosphere and ionosphere accompanied by a variety of electromagnetic phenomena by means of a permanent long-term observation site onboard the International Space Station (ISS). The PWC designers are from institutions of Bulgaria, England, Hungary, Poland, Russia and Ukraine. The control and data acquisition computer system of PWC has been developed by our engineers. It is a distributed intelligence system working in its own local network of three processors. The flight model was delivered to the ISS on a board of a Soyuz Progress spacecraft on the 12<sup>th</sup> of February 2013. It was put in operation on the 12<sup>th</sup> of April 2013 during a 6 hour duration spacewalk of astronauts. Since April it has been working continuously. Since the telemetry capacity is limited, only small part of data is transmitted to Earth. Measurement data will be transported to Earth by delivery the onboard storage unit in May 2014.

Engineers of our group have completed the flight model of the power supply unit for the **Planetary Ion Camera (PICAM)** of ESA's Bepi-Colombo mission to be launched to Mercury in 2016. PICAM is an ion mass spectrometer operating as a Planetary Ion camera for charged particles to study the chain of processes by which neutrals are ejected from the soil, eventually ionized and transported through the environment of Mercury. PICAM will provide the mass composition, energy and angular distribution of low energy ions up to 3 keV in the environment of Mercury. We delivered the flight model in IWF Graz (Space Research Institute Graz) for further integration.

Launched in 2004, **ESA's Rosetta spacecraft** will be the first to undertake the long-term exploration of a comet. It comprises a large orbiter, designed to operate at large distances from the Sun, and a small lander. Each of these carries a large complement of scientific experiments designed to complete the most detailed study of a comet ever attempted. The Rosetta-Philae space probe pair of the European Space Agency is targeted to comet Churyumov-Gerasimenko; Philae is scheduled to land on the surface of the comet nucleus in November 2014.

Our group has participated in the development of the Command and Data Management Subsystem (CDMS) for Philae lander. The in-flight corrections of the parameters referring to the instruments and to the comet require continuous fine-tuning of the software of the CDMS. Our scientists as software developers of the central computer of Philae are actively participating in this procedure. A new software version

The **JUICE (JUper ICy moon Explorer)** was chosen in 2012 by the Science Programme Committee of ESA as the first large-class interplanetary mission. The icy moons of Jupiter are in the focus of this science mission; it investigates the Jupiter system. One of the objectives is the quest for evidence of life in the Solar System; this requires the understanding of what makes a planet habitable. JUICE will be launched in 2022, the end of mission is foreseen around 2032. Our job in the mission is the development DC/DC power supply unit of PEP experiment containing four DPUs and six sensors. System plans were made of DC/DC power supply unit. During the preparatory phase, ESA requested a lot of documents about the PEP experiment (e.g. interface definition, radiation model, electronic,

mechanical parts list, etc.). We have prepared DC/DC converter sections of these documents. The PEP experiment has been redesigned several times to meet JUICE mission because of limitation requirements in weight and energy usage. Our unit was also redesigned following these changes in order to insure reliable operation by implementing redundancy in power supply unit, minimizing weight and volume and maximizing the efficiency will be uploaded to the Lander in 2014 before landing.

**Institute for Solid State Physics and Optics**

## S-B. Complex Systems

Ferenc Iglói<sup>A</sup>, Róbert Juhász, István Kovács, Gergely Roósz, Attila Virosztek, András Sütő, Péter Szépfalusy

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

**Low-frequency optical conductivity of graphene.** — We investigate optical transitions of non-interacting electron systems consisting of two symmetric energy bands touching each other at the Fermi energy (e.g., graphene at half-filling). Optical conductivity is obtained using Kubo formula at zero temperature. We show that for particles whose pseudospin direction is determined solely by the direction of their momentum, the optical conductivity has power-law frequency dependence with the exponent  $(d-2)/z$  where  $d$  is the dimension of the system and  $z$  is the dynamical exponent. According to our result two-dimensional systems with the above pseudospin characteristics always exhibit frequency-independent optical conductivity.

**Dynamics of the contact process in inhomogeneous environments.** — According to our renormalization group and Monte Carlo simulation studies, the local asymmetry (dependence of the spreading on the direction) in the one-dimensional, inhomogeneous contact process, which is a basic model of epidemic spreading, is irrelevant provided the model is symmetric in a statistical sense. If the spreading rates are systematically greater in one direction, two distinct phase transitions occur, which are related to the spreading in the favorable and unfavorable directions, respectively. In the latter, the dynamics are ultra-slow (characterized by logarithmic time-dependence), while the former one is different and characterized by multi-scaling. On small-world networks containing long links with algebraically decaying probabilities, the critical dynamics of the above model are ultra-slow again and the corresponding critical exponents depend on the topology of the network.

**Non-equilibrium quench dynamics in quantum quasicrystals.** — We have studied the non-equilibrium dynamics of a quasiperiodic quantum Ising chain after a sudden change in the strength of the transverse field at zero temperature. In particular, we have considered the dynamics of the entanglement entropy and the relaxation of the magnetization. The entanglement entropy is found to increase with time as a power law, and the magnetization to exhibit stretched exponential relaxation. These behaviors are explained in terms of anomalously diffusing quasiparticles, which are studied in a wave packet approach. The nonequilibrium magnetization is shown to have a dynamical phase transition.

**Boundary critical phenomena of the random transverse Ising model.** — Using the strong disorder renormalization group method, we have studied numerically the critical behavior of the random transverse Ising model at a free surface, at a corner, and at an edge in two-, three-, and four-dimensional lattices. We have determined the corresponding local critical exponents with high numerical precision, the value of which are independent of the form of the disorder. We have also studied critical magnetization profiles in slab, pyramid, and wedge geometries with fixed-free boundary conditions and analyzed their scaling behavior.

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<sup>A</sup> Associate fellow

**Condensation of quasiparticles and density modulation beyond the superfluid critical density.** — We extended our earlier study of the ground state of a bosonic quasiparticle Hamiltonian by investigating the effect of a constant external velocity field. Our main finding is the macroscopic condensation of quasiparticles at a nonzero velocity dependent wave vector  $k$ , and a simultaneous condensation of physical particles at  $\pm k$ . An implication of the latter is a density modulation of wave vectors  $k$  and  $2k$ .

**Galilean invariance in confined quantum systems.** — We investigated Galilean invariance in confined quantum systems, and found some interesting implications of it on the spectrum and the eigenstates of the energy operator. The established properties have deep physical consequences concerning superfluidity and periodic ordering at zero temperature.

## Grant

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

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## S-C. Long range order in condensed systems

**Balázs Ujfalussy**, Gábor Csire, Kamasa Pawel, Krisztina Kádas, Annamária Kiss, Miklós Lajkó, Karlo Penc, István Tüttő, Lajos Károly Varga<sup>A</sup>, Levente Vitos

**Strongly correlated systems.** — We have studied the charge Kondo effect in the spinless interacting resonant level model (IRLM) by means of the continuous-time quantum Monte Carlo method. We derived exact dynamics and thermodynamics of the IRLM numerically for a wide range of parameters such as the Coulomb interaction and hybridization. We have found a quantum critical point in excellent agreement with a simple scaling formula in the negative Coulomb interacting range, where the quasiparticle mass is highly enhanced. Thus, the charge Kondo effect might be relevant to certain Samarium compounds with peculiar, magnetic field independent heavy-fermion behavior.

The low energy physics of Mott insulating states of cold atoms on optical lattices and in materials with spin and orbital degrees of freedom is captured by  $SU(N)$  symmetric Heisenberg models, where  $N$  is the number of localized degrees of freedom. We studied these models on a honeycomb lattice using variational Monte Carlo calculations. For the  $SU(3)$  model we have shown that a plaquette valence bond is realized. For the  $SU(4)$  model our calculations indicate the instability of the algebraic spin-orbital liquid against tetramerization if second neighbor exchange is turned on.

**High Entropy Alloys.** — High-entropy alloys were investigated using first-principles alloy theory. We predicted that at room temperature the paramagnetic  $NiCoFeCrAl_x$  alloys adopt the fcc structure for  $x < 0.60$  and the bcc structure for  $x > 1.23$ , with an fcc-bcc duplex region in between the two phases. The calculated elastic parameters exhibit strong composition and structure dependence. Alloys around the equimolar composition have superior mechanical performance as compared to the single-phase regions. We also studied the surface energy and the surface stress of the homogeneous disordered bcc Fe/Cr system in the concentration interval up to 20 at.% Cr. We found that Cr addition to Fe generally increases the surface energy and surface stress. As a result, the (100) surface of Fe–Cr becomes more stable against reconstruction with increasing Cr concentration. The observed trends have magnetic origin.

The strong softening of the tetragonal shear elastic constant  $C'$  is the main reason for the second magnetostriction peak observed in  $Fe_{(100-x)}Ga_{(x)}$  alloys. We demonstrated that  $C'$  strongly depends on the degree of order of Ga atoms in Fe. The B2 type ordering proves to have an important role on the elastic softening for  $x < 19\%$ , whereas the extreme shear lattice softening and the anomalous temperature dependence of  $C'$  are found to be due to the strong magnetochemical coupling in the  $DO_3$  phase. Ab initio alloy theory was used to determine the elastic properties of Ni-Fe alloys with Fe:Ni ratio 1:3. The interplay between magnetic and chemical effects was investigated and it was found that the influence of long-range chemical order on the bulk properties strongly depends on the magnetic state. It was concluded that magnetic ordering has a substantially larger impact on the bulk parameters of  $Ni_3Fe$  than the chemical ordering.

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<sup>A</sup> Associate fellow



**Beyond rear earth magnets (BREM).** — Permanent magnets of high flux-density are expected to be in high demand in the future due to need of energetics. Currently, most of these magnets are based on the rare-earth elements (RE). The high cost of RE and upcoming supply issues motivate search for RE-free magnets, on which we conduct research in several threads.

One of the promising candidates for BREM materials is the alnico alloy. We performed first-principles calculations to investigate the site preference of ternary alloying addition in  $DO_3$  phase of  $Fe_3Al$ ,  $Co_3Al$  and  $Ni_3Al$  alloys. In  $Fe_3Al$  the discussed ternary elements are found to occupy the Fe sublattice. For both Fe-rich and Al-rich compounds the ternary elements with less 3d electrons than in Fe (Ti in our case) prefer to occupy  $\alpha$ -sites of the Fe sublattice, while elements with a larger number of 3d electrons the  $\gamma$ -sites. In the Fe-rich region, the small enthalpy difference of Ti occupying the  $\alpha$ -sites of Fe and Al sublattices, the site distribution of Ti vary with concentration and temperature. A similar dependency was obtained for Ni distribution between Co and Al sublattice in  $Co_3Al$ . However the concentration dependence is weaker compared to the Ti distribution in Fe-rich  $Fe_3Al$  due to weak concentration dependence of chemical potential from concentration in  $Co_3Al$ . Similar to  $Fe_3Al$  alloy the ternary element prefer to occupy the Co sublattice with a change of preferred sites from  $\alpha$  for Ti and Fe to  $\gamma$  for Ni. In the Ni-rich  $Ni_3Al$  the ternary elements prefer to occupy the Al sublattice, while, in the Al-rich alloy the ternary elements prefer to occupy the Ni sublattice with similar trend - metals with lower number of 3d electrons than in Ni goes to  $\alpha$ -sites. The exception should be made for Co which equally distributed between  $\alpha$ - and  $\gamma$ -sites. The magnetic moments of the transition metal in  $Fe_3Al$  and  $Co_3Al$  are ordered ferromagnetically, whereas the  $Ni_3Al$  was found stay nonmagnetic unless the Fe or Co are added as a ternary element.

We performed a detailed first principles study on the magnetic structure of an Fe monolayer on various surfaces of 5d transition metals. We used the spin-cluster expansion technique to obtain parameters of a spin model, and predict the possible magnetic ground state of the studied systems by employing the mean field approach and in certain cases by spin dynamics calculations. In the case of a Ta substrate we demonstrated that the out-of-plane relaxation of the Fe monolayer causes a transition from ferromagnetic to antiferromagnetic ground state. We examined the relative magnitude of nearest neighbour Dzyaloshinskii-Moriya (D) and isotropic (J) exchange interactions in order to get insight into the nature of magnetic pattern formations. For the Fe/Os(0001) system we calculated a very large D/J ratio, correspondingly, a spin spiral ground state. We found that, mainly through the leading isotropic exchange and the Dzyaloshinskii-Moriya interaction, the inward layer relaxation substantially influences the magnetic ordering of the Fe monolayer.

Large value of exchange biased field (HEB  $\sim 2.52$  kOe) were achieved with Si substitution in the off-stoichiometric rapidly quenched from the melt NiMnAl alloys ( $Ni_{55}Mn_{19}Al_{24}Si_2$ ), which is the highest value reported so far in any Heusler alloy system. A metamagnetic shape memory ribbon obtained by rapid solidification was developed in the Ni(Co)–Mn–Al system by cobalt addition. In the  $Ni_{45}Co_5Mn_{32}Al_{18}$  ribbon, the martensitic transformation temperature is decreased upon application of external magnetic field. An Arrott plot was used to identify the Neel temperature and a cluster model was adopted to explain the presence of ferromagnetic and antiferromagnetic domains in the sample. The permanent magnet properties of Mn-Al-C were optimized by melt spinning technique and subsequent

heat treatments. The optimal structure is a nanostructured tau - phase with interstitially dissolved C atoms obtained by a homogeneous single-phase precursors (epsilon-phase).

## Grants and international cooperation

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

OTKA 109570: Fundamentals of complex, multi-component metallic alloys (L. Vitos, 2013-2017)

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

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

OTKA K106047: Correlated states and excitations in d- and f-electron systems and ultracold Fermi gases (K. Penc, 2013-2017)

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

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

MTA Mobility program: Infrared, ESR, and NMR spectroscopy of functional insulators in high magnetic fields, SNK-64/2013,

Oak Ridge National Laboratory, Beyond Rare Earth magnets, (B. Újfalussy, 2012-2013)

Transzvil Zrt – contract type: KMR 12, 2013,

Watt 22 Kft. – contract type: KMR 12, 2013

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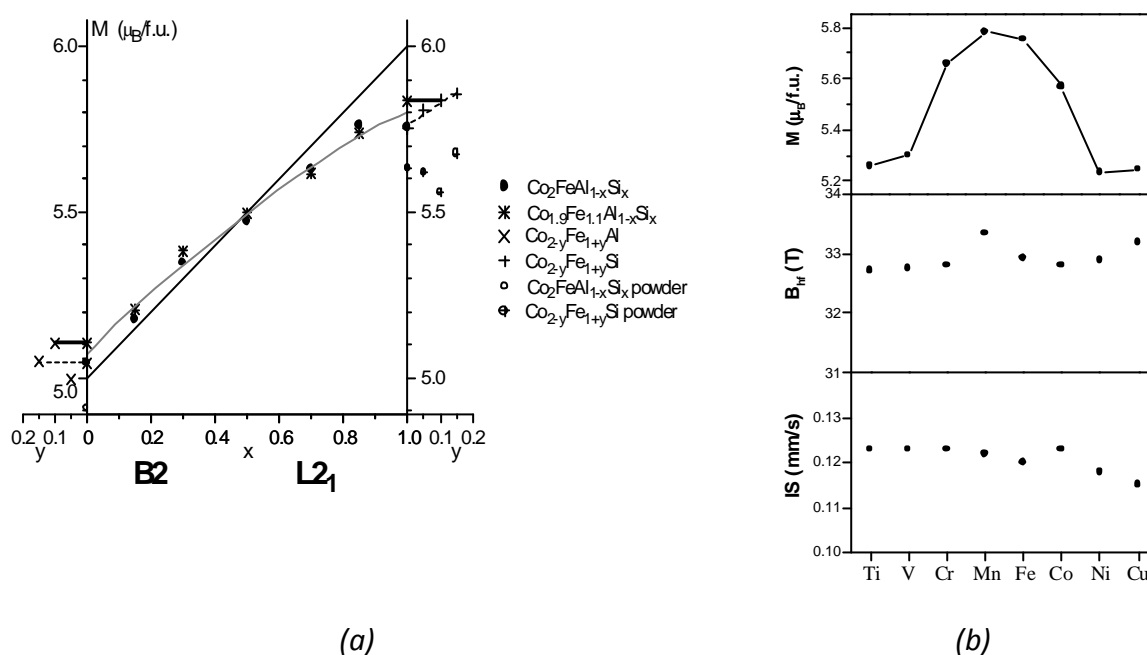
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## S-E. Non-equilibrium alloys

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

**Half metallic ferromagnetic alloys** are indispensable for spintronic applications. There is a controversy between experiment and theory about the half-metallic nature of the  $\text{Co}_2\text{FeSi}$  Heusler alloy deduced from theoretical calculations. Usually a generalized Slater-Pauling type (i.e. valency-controlled) behavior of the average magnetization (theoretically =  $6 \mu_B/\text{f.u.}$ ) is considered as a conclusive proof. In the present study SQUID magnetic and  $^{57}\text{Fe}$  Mössbauer measurements were performed to clarify the situation. Bulk  $\text{Co}_2\text{FeAl}_{1-x}\text{Si}_x$ ,  $\text{Co}_{1.9}\text{Fe}_{1.1}\text{Al}_{1-x}\text{Si}_x$ ,  $\text{Co}_2\text{Fe}_{0.9}\text{TM}_{0.1}\text{Si}$  (TM = Ti, V, Cr, Mn, Co, Ni, Cu),  $\text{Co}_{2-y}\text{Fe}_{1+y}\text{Al}$  and in Si off-stoichiometric  $\text{Co}_2\text{FeSi}$  samples ( $\text{Co}_2\text{Fe}_{1\pm y}\text{Si}_{1\mp y}$ ) were prepared by induction melting. The  $\text{Co}_2\text{FeAl}_{1-x}\text{Si}_x$  shows the  $L2_1$  crystal structure only for  $x \geq 0.4$ , between  $x=0$  and  $0.3$  it has the  $A2$  structure (Fe – Al, Si disorder). The average magnetization of these alloys does not follow the expected Slater-Pauling trend (on the Si side saturation is observed around  $5.75 \mu_B/\text{f.u.}$ ) and similar deviation is observed for the replacement of Fe by transition metal (TM) atom. The effect of the antisite disorder (Fe-Si) on the magnetization and Fe hyperfine parameters was determined and significant decrease in the Co magnetic moment for excess Si neighbourhood is extrapolated. The formerly reported large  $\approx 6 \mu_B/\text{f.u.}$  magnetization for  $\text{Co}_2\text{FeSi}$  was observed only in samples having Fe excess and Si deficiency.



**Figure 1. a:** Average magnetization of the  $\text{Co}_2\text{Fe}(\text{Al},\text{Si})$  and related alloys. The linear composition dependence corresponds to the expected Slater-Pauling behavior; **b:** Average magnetization, Fe hyperfine fields and isomer shifts in the  $\text{Co}_2\text{Fe}_{0.9}\text{TM}_{0.1}\text{Si}$  alloys.

A method was developed to reduce the systematic errors of a superconducting quantum interference device (SQUID) magnetometer which results in a significant increase in the accuracy of the measured magnetic moments.

For **spintronic research** the properties of the interface between Fe and MgO is an important issue for the goal to achieve large tunneling magnetoresistance, as well as, for the

investigations of the magnetoelectric phenomena. With the analysis of low temperature Mössbauer spectroscopy measurements we gave a proof of the property that the interface is chemically sharp; neither  $\text{Fe}_{1-x}\text{O}_x$  nor (Fe, Mg)O oxide phase is formed.

**Pressure dependence of magnetic properties in Fe-Mn-B amorphous alloys** – The pressure dependence of the saturation magnetization and Curie temperature was studied in melt-spun  $\text{Fe}_{60}\text{Mn}_{20}\text{B}_{20}$ ,  $\text{Fe}_{56}\text{Mn}_{24}\text{B}_{20}$  and  $\text{Fe}_{75}\text{B}_{25}$  amorphous alloys up to 0.9 GPa corresponding to volume changes up to 0.45%. In addition, in-situ high-pressure (up to 40 GPa) X-ray diffraction was performed to determine the compressibility of the latter two alloys. Both the Curie temperature  $T_C$  (at atmospheric pressure  $T_C = 201 \pm 3$  and  $159 \pm 3$  K) and the low-temperature saturation magnetization  $M_{5K, 5T}$  decrease remarkably with increasing pressure:  $dT_C/dp = -31 \pm 0.5$  and  $-32 \pm 5$  K/GPa and  $d \ln M_{5K, 5T}/dp = -0.15 \pm 0.02$  and  $-0.13 \pm 0.03$   $\text{GPa}^{-1}$  for  $x_{\text{Mn}} = 20$  and 24 at%, respectively. Compared to  $d \ln M_{5K, 5T}/dp = -0.016 \pm 0.003$   $\text{GPa}^{-1}$  measured for  $\text{Fe}_{75}\text{B}_{25}$ , the pressure dependence of  $M_{5K, 5T}$  is one order of magnitude larger in the ternary alloys. The bulk modulus for the  $\text{Fe}_{56}\text{Mn}_{24}\text{B}_{20}$  and  $\text{Fe}_{75}\text{B}_{25}$  glasses were measured to be 152 GPa and 173 GPa, respectively. These data are also compared with the pressure dependence of the hyperfine-field and theoretical calculations of the saturation moment for Fe-B alloys reported in the literature. The results were interpreted within an inhomogeneous itinerant-electron model of ferromagnetism.

## Grants

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

TÉT 10-1-2011-0579 Magnetic interactions in multilayer heterostructures (J. Balogh, 2012.10.01-2014.09.30)

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See also: R-L.3, R-L.5

## S-F. Laboratory for advanced structural studies

**Gyula Faigel**, Gábor Bortel, László Gránásy, Zoltán Jurek, Katalin Kamarás, Gyöngyi Klupp, Éva Kováts, Katalin Németh<sup>#</sup>, Gábor Oszlányi, Áron Pekker<sup>#</sup>, Tamás Pusztai, László Rátkai<sup>#</sup>, Attila Szállás, Zoltán Szekrényes<sup>#</sup>, Gyula Tóth, György Tegze, Miklós Tegze

**Crystalline derivatives of fullerenes.** — Fullerenes are closed shell carbon molecules. The most abundant among them is C<sub>60</sub>. The conjugated bond system makes C<sub>60</sub> ideal precursor of ionic and covalent derivatives. In condensed state the rotation and the supramolecular interactions of the high-symmetry molecules enlarge the possibility of further structures. As a result of the above properties, fullerenes have unusually large number of solid state derivatives, like alkali metal salts, polymers and cocrystals with a series of inorganic and organic molecules.

Lately we worked on fullerene based cocrystals. The study of these systems was extended to endohedral fullerenes. Several new, high-symmetry M<sub>3</sub>N@C<sub>80</sub> compound was prepared, their structure was determined from powder and single crystal diffraction experiments and modeled in the framework of cohesion energy calculations. The solvent-free Sc<sub>3</sub>N@C<sub>80</sub> crystal was prepared in 2 steps via thermal decomposition of its toluene solvate. This simple method may be applied to other hard-to-crystallize fullerenes. The new special double rotor-stator structure of the high stability Sc<sub>3</sub>N@C<sub>80</sub>-cubane was found to be face centered cubic in accordance to previous model calculations. More flexible rotor-stator system, of less stability is the cubic Sc<sub>3</sub>N@C<sub>80</sub>-mesitylene. These results were applied in preparation of analogous cocrystal structures of the potential MRI contrast agent, Gd<sub>3</sub>N@C<sub>80</sub>.

**Infrared spectroscopy.** — In previous years we mostly studied carbon based system, like carbon nanotubes, graphene, and hybrid materials based on these with other organic molecules. This year we concentrated on other type of materials.

We determined the chemical bonding and physical structure of adsorbed hydrogen on silicon and germanium surfaces. In some layers we detected the formation of blisters, a result important for possible hydrogen storage. We also characterized the surface of silicon carbide quantum dots by infrared spectroscopy and near-field infrared measurements on the nanoscale, and proved their potential for application in bioimaging.

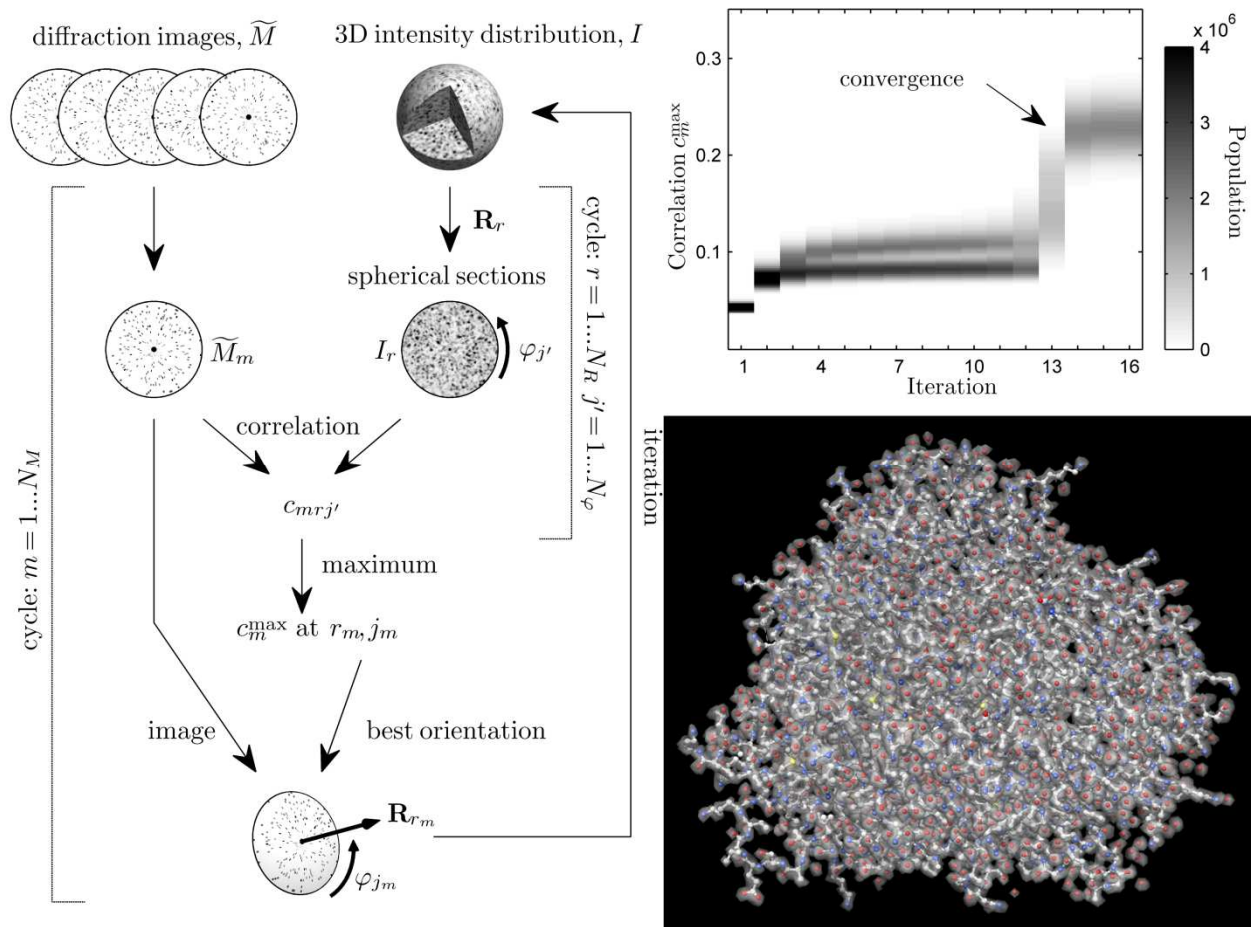
**Single molecule imaging.** — Using the very short (10-100fs) and intense x-ray pulse of an X-ray Free Electron Laser, scattering on a single particle can give useful information on its structure before the sample would eventually be destroyed. Single particles are injected into the x-ray beam and scattering patterns of single particles are collected by 2D detectors and stored individually. One of the most challenging problems of single molecule imaging is how to assemble these noisy patterns of unknown orientations into a consistent single set of diffraction data. We have developed an efficient method to find the orientations of the noisy diffraction patterns. We have also shown that our method is able to select identical particles from a mixture and find their orientations simultaneously. Further, based on our molecular dynamics tool we showed that the orientation of molecules can also be determined from the measurement of fragment distribution. Our method allows

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<sup>#</sup> Ph.D student



measurements of much smaller molecules than previously expected and also relaxes the requirements on the probe beam.



**Figure1.** Selection of different particles and determination of orientation of diffraction patterns. **Left** panel shows the block diagram of the algorithm. The **upper right** panel illustrates the convergence of the iteration. On the **lower right** panel the electron density of the NapAB protein molecule calculated from 100,000 simulated noisy diffraction patterns of the randomly oriented molecule overlaid on its ball-and-stick model. The model is shifted and rotated to the best fitting position.

**Theory of phase transformations.** — A simple dynamical density functional theory is used to investigate freezing of an undercooled liquid in the presence of a crystalline substrate.

We have reviewed the basic concepts and applications of the phase-field-crystal (PFC) method, which is one of the latest simulation methodologies in materials science for problems, where atomic- and microscales are tightly coupled. The PFC method operates on atomic length and diffusive time scales, and thus constitutes a computationally efficient alternative to molecular simulation methods

We have used the PFC theory to model the formation of eutectic dendrites in ternary systems; a spectacular growth form discovered in 2010. We have shown that the two-phase and single phase dendrites have similar shapes. It has been found that the eutectic pattern, appearing on surface of the two-phase dendrites, may include concentric rings, and single- to multiarm

spirals, motifs of which thermal fluctuations choose. The number of spiral arms correlates with the tip radius and the kinetic anisotropy.

## Grants and international cooperation

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

ESA PECS Contract No. 4000104330/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2011–2013).

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

ESA PECS Contract No. 4000104330/11/NL/KML: GRADECET – Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2011–2013).

OTKA K-81348. Ultrafast diffraction imaging of single particles (M. Tegze, 2010- 2014)

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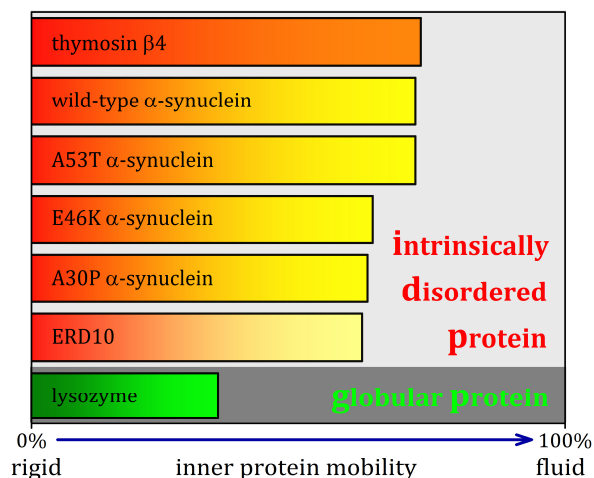
**See also: S-D1, S-D2, S-G2**

## S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Bernadette Sas<sup>A</sup>, Kálmán Tompa, Tamás Verebélyi, Francis Ian Bickford Williams<sup>A</sup>

### Inner protein mobility determined from <sup>1</sup>H-NMR spectra.

—The identification and the proportion of mobile parts (residues) in the protein molecules, the physical characteristics of their motion and the effect of mobility on their reactivity and function are all essential knowledge in molecular biology. Wide-line NMR spectrometry uses the hydrogen atomic nuclei residing in the protein molecules as elementary probes to provide global, non-selective information. We introduced a novel model-free order parameter, the hydrogen mobility (*HM*), which is applicable in describing function-related features of flexibility of proteins. *HM* reflects the motional states of the hydrogen atoms in the studied molecules. Those molecular motions, the correlation times of which fall within the NMR time-scale, reduce the second moment of the spectrum relative to that of the rigid or static system. The difference between the rigid-state and the motionally reduced second moment divided by the rigid-state second moment yields the factor *HM*. The so defined hydrogen mobility depends on the molecular structure, temperature, and also on the chemical environment in the case of solutions. The usefulness of *HM* was tested and demonstrated on small organic molecules. The link of *HM* with structural and functional characteristics was outlined on a range of proteins: *HM* provides a model-free parameter that can clearly distinguish between globular and intrinsically disordered proteins (Fig.1), and can also provide insight into the behavior of disease-related mutants (see  $\alpha$ -synuclein variants in Fig. 1).



**Figure 1.** The hydrogen mobility parameter, *HM* quantifies the inner mobility of a protein. *HM* was calculated from experimental wide-line <sup>1</sup>H-NMR spectra. Intrinsically disordered proteins are more dynamic than the globular proteins as a general rule.

## Grants and international cooperation

SPEC – Saclay: Collaboration agreement with Service de Physique de L'Etat Condensé (SPEC, CEA-Saclay, France) on electron crystals and nano-electronics (2005-2013); principal investigator: F.I.B. Williams.

Joint Project supported by the Korean Research Council of Fundamental Science & Technology (KRCF) and MTA (Hungarian project leader: P. Tompa, Institute of Enzymology, BRC, MTA; participating Wigner scientists: K. Tompa, M. Bokor, 2013-2014)

<sup>A</sup> Associate fellow

## Publications

### Articles

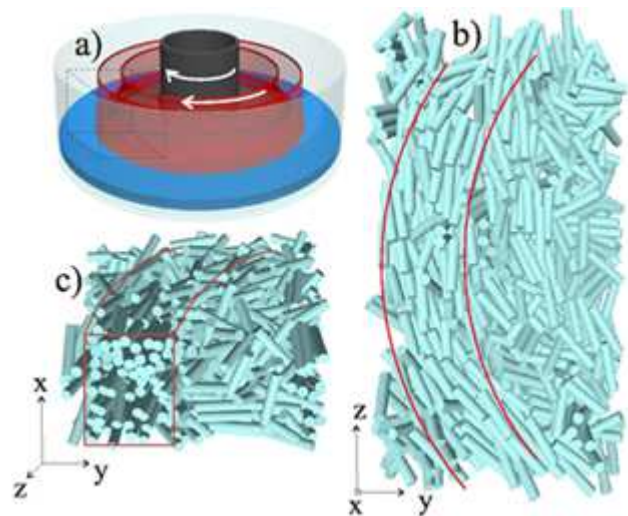
1. Petković I, Williams FIB, Bennaceur K, Portier F, Roche P, Glattli DC: Carrier drift velocity and edge magnetoplasmons in grapheme. **PHYS. REV. LETT.** 110:(1) Paper 016801. 5 p. (2013)
2. Tantos A, Szrnka K, Szabo B, Bokor M, Kamasa P, Matus P, Bekesi A, Tompa K, Han K-H, Tompa P: Structural disorder and local order of hNopp140. **BBA-PROTEINS PROTEOM.** 1834:(1) pp. 342-350. (2013)
3. Tompa K, Bokor M, Han K-H, Tompa P: Hydrogen skeleton, mobility, and protein architecture. **INTRINSIC. DISORDERED PROT.** 1:(1) pp. 77-86. (2013)

## S-H. Partially ordered systems

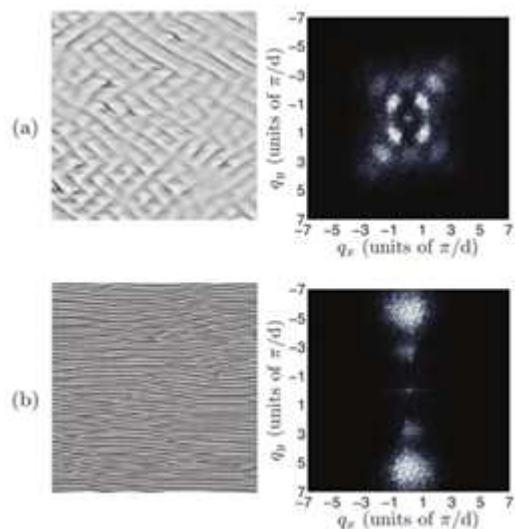
Tamás Börzsönyi, Ágnes Buka, Nándor Éber, Katalin Fodor-Csorba<sup>A</sup>, Antal Jákli, Isván Jánossy, Péter Salamon, Ellák Somfai, Balázs Szabó, Tibor Tóth-Katona, Anikó Vajda<sup>A</sup>

**Granular flows.** — The motion and rotation of individual particles as well as the average flow properties of granular samples under shear was determined using X-ray tomography and optical methods. We have shown, that particles in a sheared dry granular material consisting of elongated grains rotate with fluctuating rotational velocity. The ensemble average of the grain orientation forms a small angle with the streamlines. The average rotational velocity of many particles is angle dependent, it is the smallest when the particle is aligned in the preferred direction and largest perpendicular to the preferred alignment, similarly to the rotation of a single prolate ellipsoid placed in a sheared viscous liquid. A review article was published, summarizing the properties of granular materials composed of shape-anisotropic grains, focusing on packing, dense flows, shaken systems and granular gases.

**Liquid crystal composite materials.** — We have demonstrated that in ferronematics (liquid crystals doped with magnetic nanoparticles), both the threshold of the magnetic Fréedericksz transition and the dielectric response to low magnetic fields (far below the Fréedericksz transition) depend not only on the volume concentration of the magnetic particles, but also on the size. According to the results, the larger is the particle, the bigger are the effects (a larger decrease of the threshold of the Fréedericksz transition and a more pronounced linear response to low magnetic fields). Furthermore, we have shown that the type and the shape anisotropy of the particles also make impact on these processes and, we have also pointed out the possible importance of the initial pretilt.



**Figure 1.** Shear induced ordering of elongated particles. Image (a) shows the experimental split bottom shear cell, while images (b) and (c) show the reconstructed particle positions and orientations from the tomographic images.

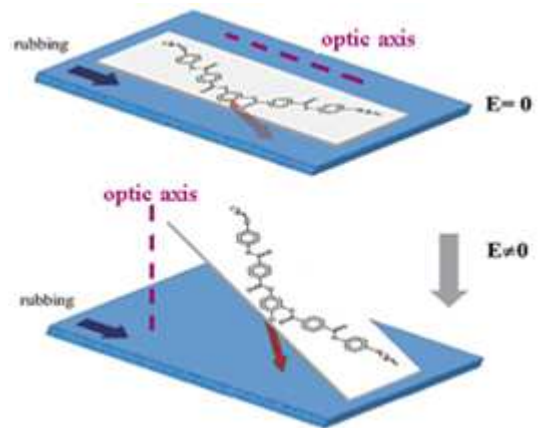


**Figure 2.** Snapshots and their 2d Fourier transforms for (a) oblique EC rolls and (b) flexodomains.

<sup>A</sup> Associate fellow

**Electric field driven pattern formation.** — Characteristics of electric field induced patterns, including their temporal variations within the driving period, have been explored in the nematic 1008 in the  $10 \text{ mHz} < f < 100 \text{ Hz}$  frequency range. The neighbouring figure shows typical snapshots and the corresponding 2d Fourier transforms for the two basic mechanisms: (a) oblique rolls of electroconvection (EC) patterns and (b) parallel stripes of flexodomains (FDs), and demonstrates their morphological differences. Unlike FDs, EC patterns at low frequencies do not have a sharp threshold, indicating an imperfect bifurcation with increasing imperfection toward lower  $f$ . By measuring the threshold voltages and critical wave numbers of FDs the temperature dependence of the flexoelectric parameter  $|e_1 - e_3|$  could be determined.

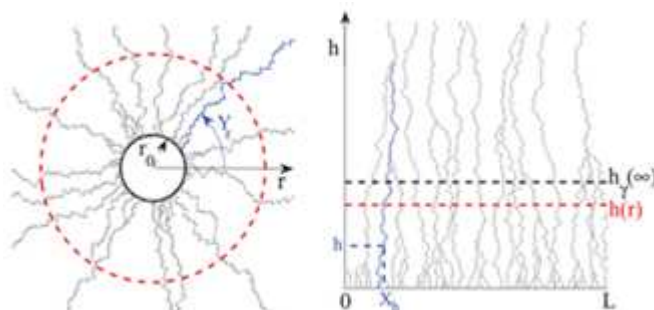
**Properties of bent-core mesogens.** — Banana shaped (bent-core) molecules form a special novel class of liquid crystals. Electric field induced optically isotropic state has been detected in planar samples of a bent-core mesogen synthesized in our laboratory. The phenomenon indicates a  $90^\circ$  rotation of the optical axis as shown in the figure which can be regarded as a clear proof for the field-induced biaxiality the 'banana' nematic phase of this compound. The effect is present in mixtures of bent-core and rod like nematics too.



**Figure 3.** Alignment of the bent-core molecule, its permanent dipole moment and the optic axis without (above) and with (below) an applied electric field.

**Scale-invariant dynamics in expanding space.**

— We established an exact relation between the statistical properties of scale invariant space-time trajectories of interacting particles in uniformly expanding and in fixed geometries. This relation generalizes standard conformal transformations as the natural symmetry of self-affine growth processes. The mapping corresponds to a nonlinear time transformation which converges to a finite value for a large class of trajectories. This enables an exact analysis of asymptotic properties in expanding domains, which are often nontrivial and random due to amplification of initial fluctuations.



**Figure 4.** Expanding radial growth structure and the same structure on a fixed domain with periodic boundary conditions, illustrated for the case of coalescing random walks. The distribution of the rescaled radial structure at radius  $r$  is identical to the distribution of the fixed domain structure at height  $h(r)$ .

## Grants and international cooperation

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

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

OTKA K      Electro and photomechanical effects in organic soft materials (I. Jánossy, 2010-2014)

MTA Infrastructure Devel.      Modern experimental tools, rheomicroscope      (Á. Buka, T. Börzsönyi)

MÖB-DAAD (Hungarian-German bilateral)      From anisotropic liquids to anisotropic granular materials (T. Börzsönyi, 2012-2013)

NFÜ-TÉT\_CN (Hungarian-Chinese bilateral)      Nonlinear structures in mesogens (Á. Buka, 2013-2015)

MTA-SAS (Hungarian-Slovak bilateral)      Nanoparticles in anisotropic soft matter (T. Tóth-Katona, 2013-2015)

MTA-ASCR (Hungarian-Czech bilateral)      Photosensitive mesogenic monomers (T. Tóth-Katona, 2013-2015)

MTA-INSA (Hungarian-Indian bilateral)      Dynamics of soft condensed matter (N. Éber, 2013-2015)

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- biaxiality. *J. PHYS. D* 46:(45) Paper 455101. 7 p. (2013)
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15. Stannarius R, Wegner S, Szabó B, Börzsönyi T: Shear alignment and orientational order of macroscopic rodlike grains. *AIP CONF. PROC.* 1542: pp. 74-77. (2013)

## S-I. Electrodeposited nanostructures

László Péter, Imre Bakonyi, Kata Berkesi, Katalin Neuróhr, Lajos Pogány, Bence Tóth, Bence Lázár

**Electrodeposited magnetic/non-magnetic multilayers.** —  $\text{Ni}_{50}\text{Co}_{50}/\text{Cu}$  multilayers with 1 to 8 nm layer thicknesses have been successfully prepared with electrochemical deposition. The total sample thickness ranged up to 700 nm. The  $\text{Ni}_{50}\text{Co}_{50}$  composition shows high magnetoresistance among the Ni-Co alloys, and this composition could be kept constant with the electrodeposition method by optimizing all deposition conditions. The value of the giant magnetoresistance (GMR) was obtained for samples with 5 to 6 nm Cu layer thickness, independently of the thickness of the Ni-Co layer. It has been shown that the magnitude of the GMR is strongly related to the surface roughness of the multilayers, which, on the other hand, is influenced by the deposition conditions.

**Electrodeposition from non-aqueous solvents.** — Electrodeposition of nickel and iron was elaborated by using pure methanol as a solvent and metal chlorides as the solute. While the iron deposited was spontaneously oxidized in air, the nickel samples proved to be stable. The chemical analysis showed that no impurity originating from the methanolic media could be detected in the electrodeposited Ni metal samples. Scanning electron microscopy showed the formation of a nanocrystalline nickel coating. The X-ray diffraction study of the nickel samples showed that the lattice parameters of the deposit are in good agreement with the properties of pure nickel. All samples were of polycrystalline nature without any texture.

On the surface of electrodes immersed in non-aqueous media (typically, on the negative electrodes of lithium ion batteries), a surface layer with mixed electrical and ionic conductivity can form. For modelling the alternating current behaviour of such layers, we have developed an equivalent circuit that treats the electrical and ionic conductivities as independent current channels. The proposed equivalent circuit can be considered as an advanced model as opposed to the earlier ones because of the following reasons: a) all equivalent circuit elements are directly related to some measurable quantity; b) it can simulate the actual number of time constants of the system without adding any artificial circuit element; c) the temporal change of the high-frequency resistivity is coupled with the relevant physical quantity.

**Radiotracer method in electrochemistry.** — Concerning the radioelectrochemical study of anion adsorption on porous electrodes, it was shown that the apparent difference between the adsorption and desorption rates originates from the mass transport coupled in serial with the adsorption step. During the anion adsorption on porous electrodes, the transport of the anion to the adsorption site is the rate-determining step. During the desorption, however, the concentration gradient of the same anion (which is the driving force of the anion release) is higher by about 4 orders of magnitude than during the adsorption. Therefore, the exit of the anions from the porous surface layer takes place essentially instantaneously.

**Various applied research projects.** – Electrodeposition of compact and fairly thick ( $d > 100 \mu\text{m}$ ) amorphous Ni-P alloys without crystalline inclusions and having a small final surface roughness has been developed for application in neutron physical devices. The surface

roughness of the samples after polishing was between 1 and 2 nm, which makes the samples suitable to prepare neutron mirrors after further surface treatments.

We have been taking part in a risk analysis project related to the service lifetime extension of the Nuclear Power Plant of Paks. In the framework of this project, the electrochemical and corrosion properties of stainless steel samples were studied. The aim of this work is the determination of pitting corrosion resistance of the samples and the identification of the parts of higher-than-average risk potential.

## Grants and international cooperation

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

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

## Long-term visitor

N. Rajasekaran, Ph.D. student, Central Electrochemical Research Institute, Karaikudi, India, Oct. 2012 – April 2013 (hosts: L. Péter and I. Bakonyi)

## Publications

### Articles

1. Berkesi K, Horváth D, Varga K, Németh Z, Pintér T, Péter L: Development and application of the in situ radiotracer thin gap method for the investigation of corrosion processes II. Validation of the thin gap method adapted for the application of porous surfaces. **ELECTROCHIM. ACTA** 109: pp. 790-797. (2013)
2. Horváth D, Berkesi K, Varga K, Péter L, Kovács T, Buják R, Pintér T: Development and application of the in situ radiotracer thin gap method for the investigation of corrosion processes. I. Adaptation of the thin gap method for the application of porous surfaces. **ELECTROCHIM. ACTA** 109: pp. 468-474. (2013)
3. Neuróhr K, Csik A, Vad K, Molnár G, Bakonyi I, Péter L: Near-substrate composition depth profile of direct current-plated and pulse-plated Fe-Ni alloys. **ELECTROCHIM. ACTA** 103: pp. 179-187. (2013)
4. Péter L: A systematic approach to the impedance of surface layers with mixed conductivity forming on electrodes. **J. SOLID STATE ELECTR.** 17: pp. 3075-3081. (2013)
5. Tóth BG, Péter L, Dégi J, Révész Á, Osztzky D, Molnár G, Bakonyi I: Influence of Cu deposition potential on the giant magnetoresistance and surface roughness of electrodeposited Ni-Co/Cu multilayers. **ELECTROCHIM. ACTA** 91: pp. 122-129. (2013)

6. Tóth BG, Péter L, Dégi J, Bakonyi I: Magnetoresistance and surface roughness study of electrodeposited Ni<sub>50</sub>Co<sub>50</sub>/Cu multilayers. *J. ELECTROCHEM. SOC.* 160:(8) pp. D307-D314. (2013)

#### **Conference proceeding**

7. Berkesi K, Horváth D, Varga K, Németh Z, Pintér T, Péter L: Development and application of the in situ radiotracer thin gap method for the investigation of corrosion processes II. Validation of the thin gap method adapted for the application of porous surfaces. *ELECTROCHIM. ACTA* 109: pp. 790-797. (2013)

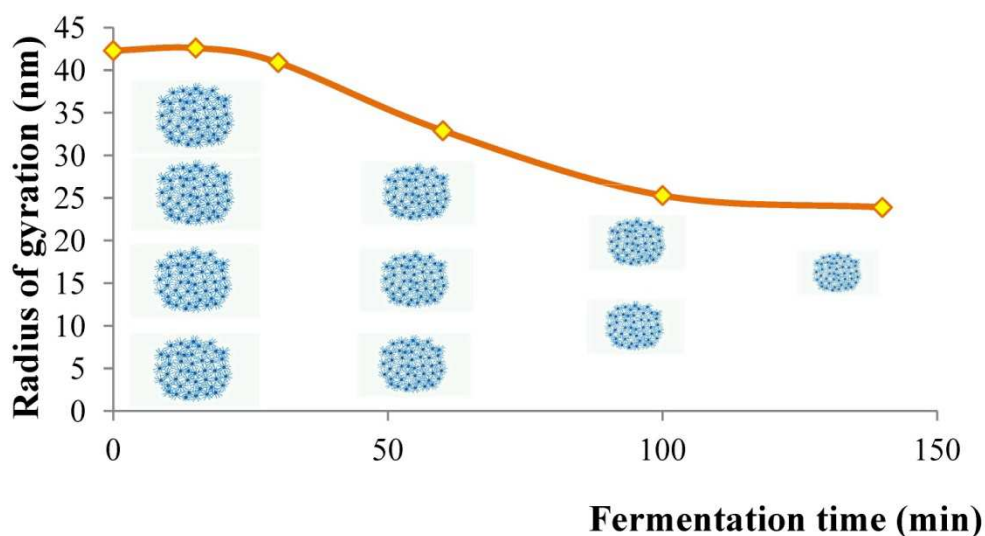
## S-L. Nanostructure research by neutron scattering

László Almásy, Gergely Eszenyi, Margit Fábrián, György Káli, Adél Len, Márton Markó, Gergely Nagy, László Rosta, Alex Szakál, Noémi Kinga Székely, Gyula Török, Renáta Ünneper, Tamás Veres

**Hydrogen bonding in aqueous solutions.** — Aqueous solutions of cyclic and aromatic amines exhibit anomalous behavior of their physico-chemical properties in the function of composition. This behavior is due to the specific intermolecular interactions, amongst which the hydrogen bonding is the most complicated factor due to its directionality. Small-angle neutron scattering and ultrasound measurements revealed that the mixtures are strongly inhomogeneous even at temperatures much below the liquid-liquid phase separation region. The transient structures that form the basis unit of the two phases are shown to be the water-amine complexes, which can further aggregate through hydrogen bonds involving the hydration water molecules. Ultrasound relaxation shows that the aggregates are dynamic structures with nanoseconds-order relaxation times. This mechanism of phase separation is suggested to be generally valid for aromatic amine aqueous solutions.

**Milk protein structure.** — Casein is one of the main substrate of microbial transglutaminase, mTG, also known as meat-glue in gastronomy. This enzyme is industrially produced by submerged fermentation of *Streptomyces mobaraensis*. It is widely used for dairy and meat products because of its protein cross-linking action, resulting in a polymerized protein molecule made up of  $\epsilon$ -( $\gamma$ -glutamyl)-lysine bonds.

The process of fermentation and the effect of mTG enzyme on dairy products fermentation have been studied by small angle neutron scattering (SANS). The role of the casein is to increase the stability of the formed micelle-network. During the fermentation process the micelles and the formed nanogel structure undergo structural changes on the nanometer scales. Following the nanostructure development of model yogurt solutions and low-fat set-

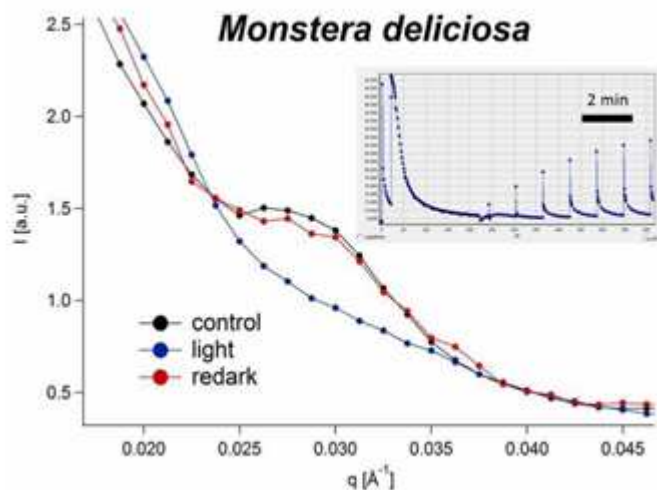


**Figure 1.** Changes in the size of the casein micelles radii of gyration in function of the fermentation time.

type yogurt products during their production, the decrease of size of the casein micelles was seen during the first hours of fermentation. The effect of the mTG on the studied model and real yogurt solution was also verified (Fig. 1); in the presence of mTG a faster fermentation and a larger syneresis degree was observed resulting in better product stability. The ability to follow the structure changes in situ during fermentation allows studying the contribution of the different factors in these complex and technologically important systems.

**Photosynthesis mechanisms in plants.** — In the past years we developed a method to measure plant leaves by SANS, which opened the possibility to investigate the correlation between thylakoid membrane ultrastructural changes in high light and the non-photochemical quenching (NPQ) of the singlet excited state of chlorophyll-a, an important photoprotective mechanism observed only in intact leaves and whole cells. SANS curves of *Monstera deliciosa* (a shade plant) leaves exhibited strong change on a timescale of 1-2 minutes, parallel with the formation of the NPQ of the chlorophyll fluorescence (Fig. 1). These changes are almost fully reversible but can be inhibited with certain reagents. Interestingly, the structural reorganizations in leaves of other higher plants which are not shade plants (spinach, *Arabidopsis thaliana*) under similar conditions were considerably less pronounced.

We also used several mutants and strains of the green alga *Chlamydomonas reinhardtii* and the diatom alga *Phaeodactylum tricornutum* in order to understand the relationship between NPQ and the ultrastructural changes in the thylakoid membrane system. We found that the structural reorganizations do not strictly correlate with the ability for NPQ. Pilot experiments performed on wild type *Arabidopsis* leaves, as well as on leaves from kinase and phosphatase mutants showed the way to study state transition related structural changes. Similar studies have been performed earlier on green algae. Measurements of different mutants of *Arabidopsis thaliana* in which different peripheral antennae are missing, reveal that the



**Figure 2.** Excess-light-induced reversible changes in the thylakoid membrane ultrastructure and the magnitude of NPQ, reflected by variations in the SANS profile and the chlorophyll-a fluorescence transient of the intact leaves of *Monstera deliciosa*.

protein-composition of membranes has strong influence on the interthylakoidal distances.

The Hofmeister series is a classification of ions based on their ability to salt-out (precipitate) or salt-in proteins and other physical properties of soluble proteins, with a mechanism not fully understood. In order to elucidate the action of Hofmeister salts on membrane proteins and multilamellar membrane system, we performed SANS experiments on isolated plant thylakoid membranes; these experiments revealed very fast structural rearrangements with chaotropic salts, while kosmotropic salts exerted no effect.

## Grants and international cooperation

EU-FP7 – CHARISMA – Cultural Heritage Advanced Research Infrastructures: Synergy for a multidisciplinary approach to conservation/restoration (L. Rosta, 2009-2013)

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

OTKA-A08-3 OMFB-00590/2010 Structure and dynamics of self-organized lamella molecular systems (Mezei F. 2010-2012)

International Atomic Energy Agency: Project No. CRP1575, Development, Characterization and Testing of Materials of Relevance to Nuclear Energy Sector Using Neutron Beams (Gy. Török 2012-2013)

NFÜ-MAG ZRt. TÉT-0018 South-Africa, Structural Analysis of Treated Textile Fibres (Gy. Török 2011-2013)

cooperations without specified grants: JINR, Dubna, Russia, PNNPI, Gatchina, Russia, Institute of Physics, Kosice, Slovakia, Pharmaceutical Faculty, Comenius University, Bratislava, Slovakia, PSI, Villigen, Switzerland, ILL, Grenoble, France, IFE, Kjeller, Norway, INPC, Mianyang, China.

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22. Baranyai R, Makai M, Pálffy H, Rosta L (szerk.): Progress Report on the activities at the Budapest Research Reactor. Budapest Neutron Centre 2010-2012. Budapest, KFKI, 2013.
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See also: R-M.1, S-M.5

## S-M. Neutron optics

János Füzi, László Cser, Zoltán-Imre Dudás, Zoltán László<sup>#</sup>, Márton Markó, Ferenc Mezei, János Orbán<sup>#</sup>

**Neutron instrumentation development.** – Serving the quest of neutron spectroscopy research for understanding the structure and dynamics of solid state matter on nano- and picometric scale, the main task of the Neutron Optics Research Group is the ongoing improvement of the neutron delivery system and spectrometer suite deployed around the 10-MW Budapest Research Reactor (BRR), central element of the Budapest Neutron Centre (BNC). One of the key and largest research facilities in Hungary, it is the base for a significant domestic and international user community to serve for exploratory and applied research in many fields of science and technology as well as for methodological developments in neutron beam techniques. Relevant examples are investigations of hydrogen storage materials, high temperature and radiation resistant structural materials, welding technology development, understanding the mechanism of photosynthesis.

The deployment of the new focusing small angle neutron scattering spectrometer has reached the commissioning phase. We successfully tested the chopper system, focusing optics and event based data acquisition system. The instrument extends the available range of the existing BNC YS spectrometer by one order of magnitude towards lower scattering vector values and allows detection correlation to sample excitations.

A significant achievement in the field of knowledge transfer towards innovation-intensive industry has been realized in the frame of a bilateral contract: researchers of the Neutron Spectroscopy Department participated in the design, commissioning and on-site acceptance testing of three instruments manufactured, delivered and installed by Mirrotron Ltd for the Mianyang Research Reactor in China: a polarized time of flight neutron reflectometer, a small angle scattering spectrometer and a triple axis diffractometer.

**Neutron detectors.** – In the frame of the NMI3 Detectors JRA we participate in the search for new types of neutron detectors: boron fluoride, respectively thin solid boron converter solutions, to replace the expensive <sup>3</sup>He isotope. We have also engineered a novel signal processing technique for particle counters with delay line encoding, that allows conservation of a wealth of useful information on the signal itself.

As a member of the consortium lead by Mirrotron Ltd in the frame of the NFÜ-MAG ZRt. KMR\_12-1-2012-0226 project, our goal is to improve the count rate capability, position resolution and homogeneity of neutron detectors with delay-line readout. The position resolution of multiwire proportional counters is limited by the wire spacing and stopping power of the filling gas mixture. In-house developed wiring technology allows wire spacing as low as 0.8 mm. With neighbouring wires connected in pairs to increase the total charge of the induced signals, the theoretically achievable resolution is 1.6 mm. The interpolation of the delayed signals lead to an experimentally measured resolution of 1.3 mm.

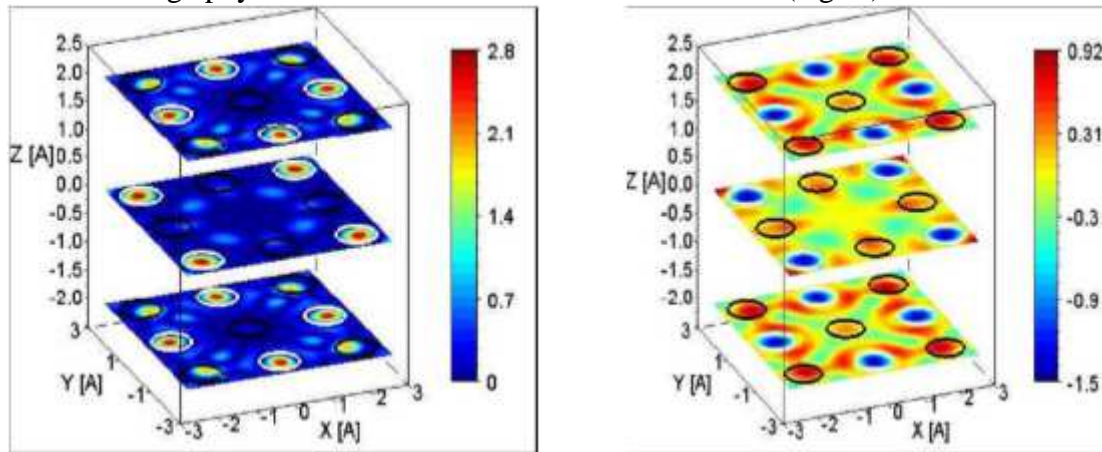
**Atomic resolution neutron holography.** – In order to extend the applicability of neutron holography to polycrystalline samples, we have worked out a novel mathematical procedure

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<sup>#</sup> Ph.D student

for inter-nuclear distance determination from wavelength-dependent holographic signal. We carried out the proof of principle experiment at the ISIS facility. The method opens the way towards direct imaging of local distortions in the vicinity of impurity atoms in a large set of materials with industrial relevance.

A novel holographic data processing method, called double reconstruction (DR) makes use of both internal source (ISR) and internal detector (IDR) reconstruction. It efficiently suppresses the spurious spots observed on applying exclusively either ISR or IDR. The signs of the positive and negative amplitudes are well pronounced, allowing one to distinguish nuclei with positive and negative scattering lengths. The successful use of 2D multietectors for neutron holography has been demonstrated for the first time (Fig. 1).



**Figure 1. Left:** The intensities of holographic images of the system PdH<sub>0.51</sub> reconstructed by the internal detector reconstruction. **Right:** The amplitudes of the holographic image reconstructed by the double reconstruction method (right). The layers of the reconstructed images are parallel to the (001) lattice planes at  $z = -2, 0$  and  $2 \text{ \AA}$ , respectively. The positions of the 6 first and 8 second neighbour Pd atoms (marked by black circles) and the 12 first neighbour H atoms (marked by white circles) arranged around the hydrogen atom at the centre of the coordinate system (not shown) are indicated.

## Grants and international cooperation

NFÜ-MAG ZRt. KMR\_12-1-2012-0226 Development of components for new generation neutron research instrumentation (L.Rosta, 2012-2015)

OTKA-A08-3 OMFB-00590/2010 Structure and dynamics of self-organized lamellar molecular systems (Mezei F. 2010-2013)

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

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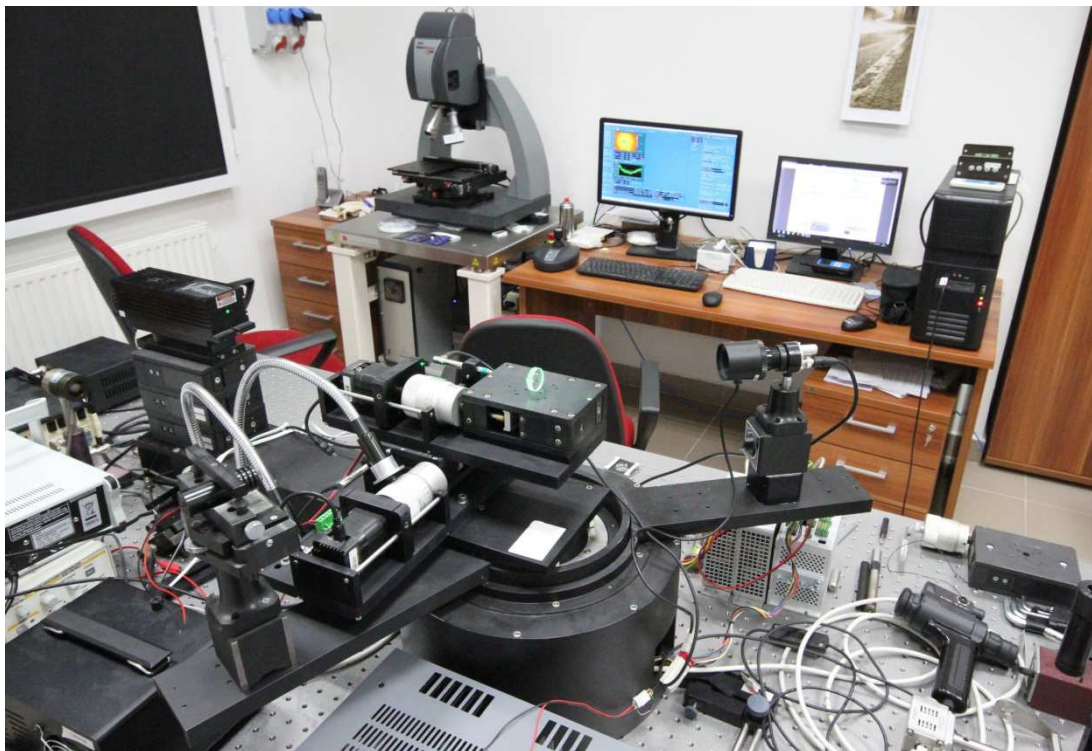
**See also: R-L.1, S-L.27**

## S-N. Laser applications and optical measurement technics

**Aladár Czitrovsky**, Kárpát Ferencz, Péter Jani<sup>A</sup>, Attila Kerekes, Attila Tibor Nagy, Dániel Oszetzky, Lénárd Vámos

**Helios project.** — In the scope of the project, which was successfully accomplished last year, a new laboratory was built, including clean room environment, where 4 new laser facilities were developed. Using these facilities we can generate attosecond pulse train by high harmonic generation; determine the damage threshold of optical substrates and layers by different laser pulses, having wide pulse duration range; study the 3 photon pre-ionization of Rb plasma for AWAKE experiment in case of the Resonance Enhanced Multi-Photon Ionization (REMPI) scheme, proposed by us earlier (CERN-co-operation), and investigate the statistical properties of plasmon processes with high temporal resolution.

**New optical laboratory.** — Another new optical diagnostic laboratory was built for 3D optical profiling and mapping of the surfaces with sub-nanometre vertical resolution. The ZYGO 7100 interferometric system is capable of studying the quality of optical elements, layers and substrates. This system is also available for measurement of mechanical vibrations having submicron amplitude. A two arm goniometric light scattering system was developed for studying the optical homogeneity of bulk optical materials. The angular distribution of scattered intensity can be automatically measured over high dynamic range.



*Laboratory for metrology of optical materials*

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<sup>A</sup> Associate fellow



*Laser mirrors and optical coatings*

**Optical coatings.** — The optical coating technology group produced high quality 4" Ti:Sapphire laser mirrors, which were successfully applied in a long-resonator laser system having 80 m length.

**Drug delivery in human airways.** — We have developed a research infrastructure for theoretical and "in-vitro" experimental study of toxic aerosol and aerosol drug deposition in realistic hollow human lung models (KTIA\_AIK\_12 project). CFD simulations of the air flow velocity and direction in idealistic airway geometry was validated by experimental measurements performed by the non-contact laser Doppler velocimetric

system developed by us previously. We started to build the further parts of the above system to determine physical and chemical parameters of different aerosol drugs deposited in realistic airway geometries – the topology of the deposition, concentration, size distribution, composition, etc. The realistic hollow airway models were constructed on the base of CT images of human lungs together with pulmonologists.

## **Grants and international cooperation**

ELI-09-1-2010-0010 NFÜ Establishing of Budapest Research Centre for ELI laser technology - hElios project (A. Czitrovsky, 2010-2013)

MTA Infrastructural developments, IF -011/013 (A. Czitrovsky, 2013)

82013-00 (410) /EAC EAC Conference (A. Czitrovsky, 2011)

KTIA\_AIK\_12-1-2012-0019, Theoretical and experimental Investigation of aerosol deposition in human airways in case of lung diseases, (A. Nagy, 2013-2015)

Austro-Hungarian Bilateral Co-operation – TÉT\_10-1-2011-0725, Study of optical properties of aerosols and their climate relevance with dual wavelength optical particle spectrometer

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4. Fűri P, Balásházy I, Czitrovsky A, Nagy A, Pándics T, Dura Gy, Kerényi T, Farkas Á, Jókay Á, Madas B, Nikovits T: A vörösiszap por fizikai tulajdonságainak, légúti depozícióeloszlásának és az egészségre gyakorolt hatásának elemzése (Analysis of physical properties, deposition distribution and its impact on health of red mud dust, in Hungarian). In: Kertész Zs, Szikszai Z, Angyal A, Furu E, Szoboszlai Z, Török Zs (eds.): XI. Hungarian Aerosol Conference. 95 p. (Debrecen, Magyarország, 2013.10.18-2013.10.20.) Debrecen: ATOMKI, 2013. pp. 42-43. (ISBN:978-963-8321-50-3)
5. Kerekes A, Veres M, Nagy A, Himics L, Oszetzky D, Kugler Sz, Czitrovsky A: Inhalációs készítmények légúti depozíciójának lokális meghatározása in vitro módszerrel (Determination of local deposition of inhalational pharmaceuticals in human airways, in Hungarian). In: Kertész Zs, Szikszai Z, Angyal A, Furu E, Szoboszlai Z, Török Zs (eds.): XI. Hungarian Aerosol Conference. 95 p. (Debrecen, Magyarország, 2013.10.18-2013.10.20.) Debrecen: ATOMKI, 2013. pp. 40-41. (ISBN:978-963-8321-50-3)
6. Nagy A, Czitrovsky A, Kerekes A, Szymanski WW: Terepi optikai mérések aeroszolok forrásazonosításának céljából (Source apportionment of aerosols by field measurements using optical methods, in Hungarian). In: Kertész Zs, Szikszai Z, Angyal A, Furu E, Szoboszlai Z, Török Zs (eds.): XI. Hungarian Aerosol Conference. 95 p. (Debrecen, Magyarország, 2013.10.18-2013.10.20.) Debrecen: ATOMKI, 2013. pp. 86-87. (ISBN:978-963-8321-50-3)

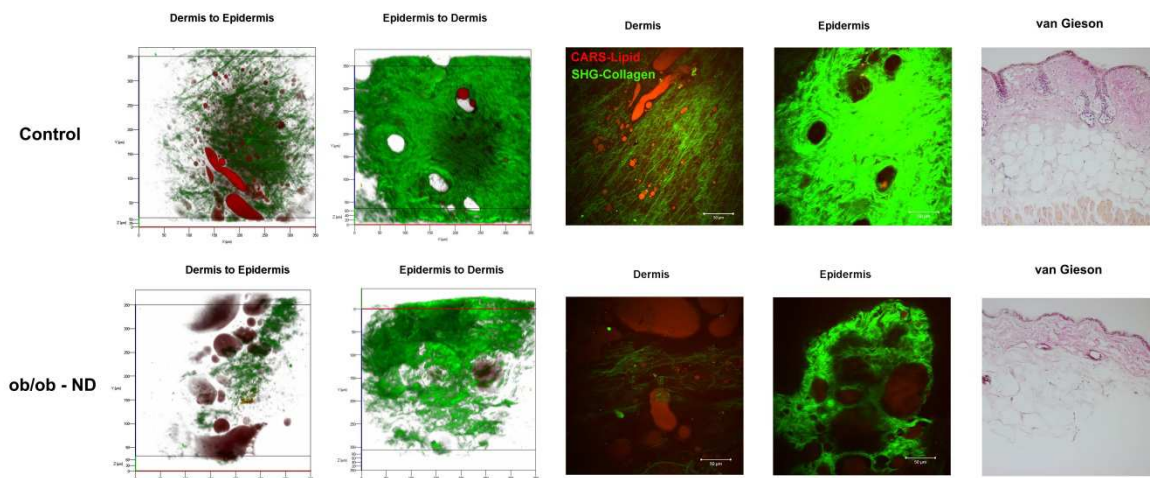
**See also: S-I.5**



## S-O. Femtosecond lasers

Róbert Szipőcs, Attila Csákányi, Dóra Haluszka<sup>#</sup>, Attila Kolonics, Zoltán Várallyay

**Nonlinear 3D microscopy.** — We performed a high number of experiments related to *in vivo* optical disease diagnosis, such as basalioma detection, characterization of obesity or *in vivo* drug monitoring, in collaboration with our scientific partners Semmelweis University, Department of Dermatology and a pharmaceutical company, Genetic Immunity, respectively. For these measurements, we upgraded our standard scanning two-photon absorption fluorescence microscope (*Axio Examiner LSM 7 MP*, product of Carl Zeiss) by a second harmonic generation (SHG) and a coherent anti-Stokes Raman scattering (CARS) detection unit, which could be efficiently used for label-free detection of the collagen network (by SHG) and adipocytes (by CARS) in the skin and for instance. As an example, we show a set of microscope images recorded for characterization of obesity in murine skin *in vivo* by CARS and SHG microscopy using our cost efficient, Yb-fiber laser based wavelength extension CARS unit. In Fig. 1, correlation between skin collagen content and the size of adipocytes is shown. Dermal collagen content and morphology alterations were measured from the skin surface to deeper layers of the dermis (0-60  $\mu\text{m}$ ) by SHG microscopy using a Ti:sapphire laser operating at 796 nm. We examined the interaction between adipocytes and fibroblast at normal (control) and obese (ob-ob) circumstances revealed by SHG, CARS and van Gieson staining also. 3D composite images verify the distribution of collagen at epidermal-dermal border and the location of adipocytes mainly at the dermis. Magenta staining at histochemistry images revealed also the lack of the collagen mass in obesity.



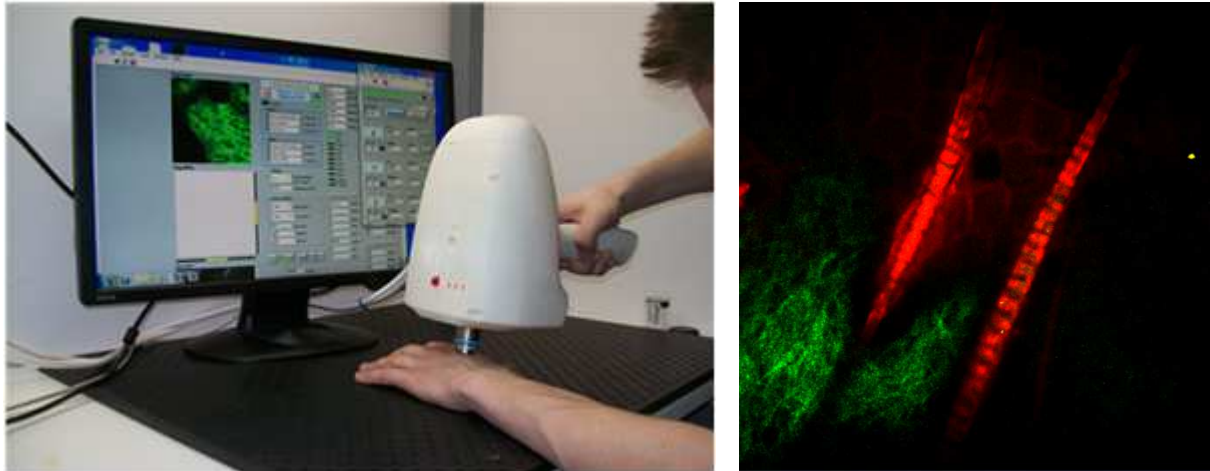
**Figure 1.** Correlation between skin collagen content and the size of adipocytes in murine skin.

For biomedical diagnostic applications, we have developed a small size, cost efficient, hand-held version of a similar 3D nonlinear microscope system (FiberScope), which uses our picosecond pulse Yb-fiber laser system as light source for nonlinear processes (2P, SHG) in the investigated tissue. Among others, it can be used for basal cell carcinoma (skin cancer) detection, which is the most common cancer. In Fig. 2 (right), we show a test image having

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<sup>#</sup> Ph.D student

been recorded at the proper fiber laser wavelength for a murine skin sample. On the left, the photo of the FiberScope system is shown.



**Figure 2. Left:** Photo of our handheld nonlinear microscope system (FiberScope) developed for basal cell carcinoma detection. **Right:** Corresponding test image recorded for a murine skin sample at the properly set fiber laser wavelength (SHG and 2P)

## Grants and international cooperation

- OTKA 76404 Design and application of photonic crystal fibers for femtosecond pulse optical fiber lasers, laser amplifiers and optical parametric oscillators (Coordinator: R. Szipócs, 2009-2013)
- 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 (Coordinator: R. Szipócs, 2009-2014)

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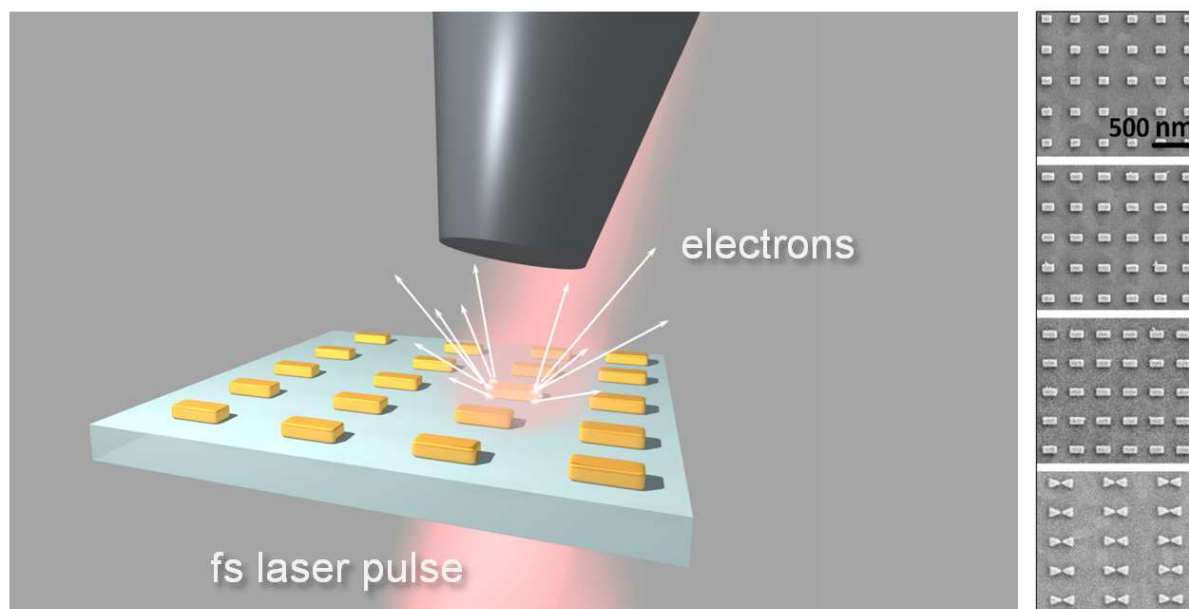
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## S-P. Ultrafast, high intensity light-matter interactions

Péter Dombi, Norbert Kroó, Győző Farkas, Sándor Varró, István Márton, Péter Rácz

We carried out experimental investigations on ultrafast strong-field photoemission processes from tailored metallic nanostructures. We could define structures where the femtosecond photoemission process and electron acceleration was significantly enhanced thanks to hot spots on the nanoparticles. We established for the first time that the electron acceleration process in these nanoparticle fields is ponderomotive in its nature and we could find clear correlation between the nanolocalized field enhancement and the electron spectrum measured with a retarding field analyzer. Results of these experiments carried out in the Budapest laboratory were published in a high-impact paper in Nano Letters and it was also also featured in several popular science reports in Hungary. Theory and nanoparticle fabrication support for these experiments were provided by a leading plasmonics group at the University of Graz in a close collaboration.

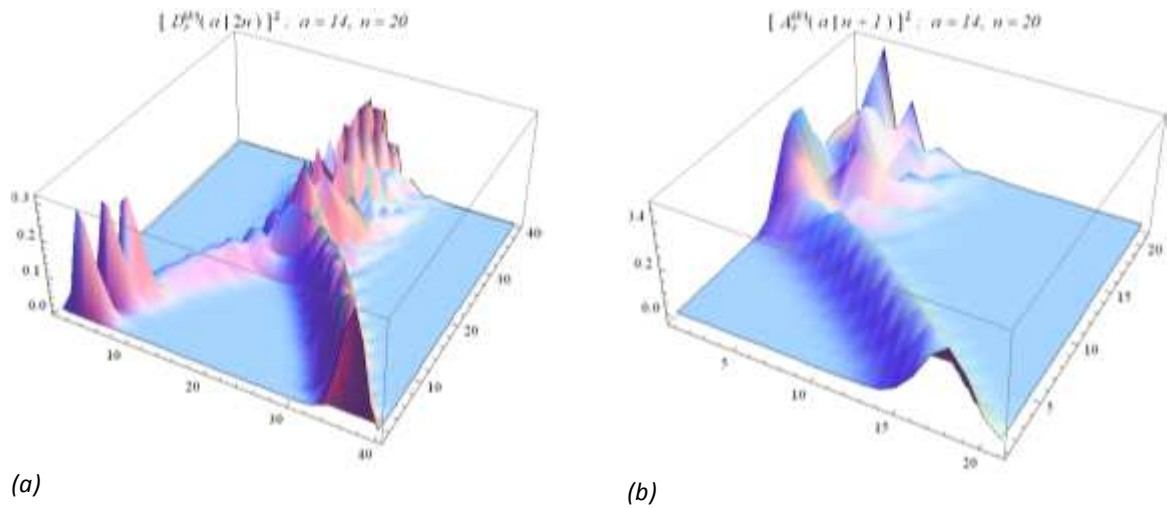


**Figure 1.** Experimental scheme on photoemission from metallic nanoparticles, including nanorods on a glass substrate. The illuminating femtosecond laser beam comes from below and the spectrometer tube collecting the electrons is also depicted. The different nanoparticles investigated are shown on the right-hand-side.

In addition, with the help of the infrastructure development grant of the Hungarian Academy of Sciences, we set up a multifunctional femtosecond light source, covering the 300 nm – 15  $\mu\text{m}$  wavelength range which will be suitable for the investigation of ultrafast process in various media including plasmonic nanoparticles, functional molecules etc. Research at these workstations on various subjects are under way and further developments and upgrades are also planned.

We also performed femtosecond fiber optics experiments related to femtosecond pulse compression in various optical fibers. These yielded some fundamental new discoveries in the field of nonlinear fiber optics that we published in 2013. Follow-up experiments on chirp conversion in large-mode-area fibers is being made public in Optics Letters in 2014.

Here we highlight one of our theoretical results; exact analytic solutions have been determined of the Dirac and Klein-Gordon equations of a charged particle propagating in a classical monochromatic electromagnetic plane wave in a medium of index of refraction smaller than unity. Besides Gordon's (1927) and Volkov's (1935) exact solutions *in vacuum*, our new solutions are the by now only closed-form analytic solutions for the same interaction with a plane radiation field *in a medium*. In the Dirac case the solutions are expressed in terms of new complex polynomials, and in the Klein-Gordon case the found solutions are expressed in terms of Ince polynomials. In each case they form a doubly infinite set, labelled by two integer quantum numbers. These integer numbers represent quantized momentum components of the charged particle along the polarization vector and along the propagation direction of the electromagnetic radiation. Since this radiation may represent a plasmon wave of arbitrary high amplitude, propagating in an underdense plasma, the solutions obtained may have relevance in describing possible quantum features of novel acceleration mechanisms. In Fig. 2. we show the distribution of the high-harmonics in the Dirac and in the Klein-Gordon wave functions for a particular transverse electron momentum eigenvalue  $p_x = 20 \times \hbar \omega_p / c$ , and for different longitudinal quantum numbers.



**Figure 2.** An overview of the high-harmonic spectra on a three-dimensional list plot for a Dirac (a), and for a Klein-Gordon (b) particle.

In Fig. 2 the fundamental parameter  $a$ , which determines the strength of the interaction, has the value  $a=14$  and the transverse momentum quantum number has been taken  $n=20$ . The parameter  $a = 4eF_0\lambda_p / \hbar\omega_0$  equals the work done on the charged particle by the electric force of the laser field along the plasma wavelength  $\lambda_p$  divided by the photon energy, where  $F_0$  is the electric field strength of the laser field. The different longitudinal eigenvalues, whose indices  $k=1, 2, \dots, 40$  and  $k=1, 2, \dots, 20$  are displayed on the right axis, correspond to different harmonic spectra. The discrete points are connected by a smoothed surface in order to guide the eye. In this numerical illustration a Ti:Sa laser field of photon energy  $\hbar\omega_0 = 1.56eV$  and of  $I_0 = 100MW/cm^2$  peak intensity has been considered, and the plasmon energy was  $\hbar\omega_p = 1eV$ .

## Grants and international cooperations

OTKA K 109257: Time-resolved investigation of functional molecules and metal nanoparticles (P. Dombi, 2013-2017)

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

MAX PLANCK INSTITUTE of Quantum Optics (Garching, Germany), Ultrafast photoemission from metallic nanotips (P. Dombi)

UNIVERSITY OF ALBERTA, Edmonton, Canada, Field-enhanced electron acceleration with few-cycle laser pulses (P. Dombi)

INSTITUTE FOR PHOTONIC SCIENCES, Barcelona, Ultrafast electron acceleration experiments with mid-infrared lasers (P. Dombi, P. Rácz)

KARL-FRANZENS-UNIVERSITÄT, Graz, Austria, Investigation of femtosecond photoemission from nanostructures (P. Dombi)

INSTITUTE FOR QUANTUM PHYSICS, University of Ulm (Ulm, Germany), Wigner functions (S. Varró)

INSTITUTE FOR QUANTUM OPTICS, University of Ulm (Ulm, Germany), Radiation properties of nitrogen-vacancy centers in diamond. (S. Varró); Surface plasmon research. (S. Varró and N. Kroó).

INSTITUTE FOR APPLIED PHYSICS, Theoretical Quantum Physics, Technical University of Darmstadt (Darmstadt, Germany), Quantum optics. (S. Varró).

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## S-Q. Crystal physics

László Kovács, István Bányász, László Bencs, Gábor Corradi, Gabriella Dravec, István Földvári, Ivett Hajdara, Nikoletta Laczai<sup>#</sup>, Krisztián Lengyel, Gábor Mandula, Ágnes Péter, Katalin Polgár, Zsuzsanna Szaller, Éva Tichy-Rács<sup>#</sup>

**Crystal growth.** — Maintaining the near planar solid-liquid interface during high temperature top seeded solution growth, optically defect free stoichiometric LiNbO<sub>3</sub>:Mg single crystals of 30 mm diameter were grown. For the growth of large, defect free paratellurite a high gradient Czochralski method has been improved. Li<sub>6</sub>Y(BO<sub>3</sub>)<sub>3</sub> single crystals of 25 mm have been Czochralski grown in a Pt crucible alloyed to withstand the highly corrosive materials.

**Phase transition and dielectric behaviour of pure and doped potassium lithium niobate (KLN) crystals.** — The temperature dependence of the dielectric constant  $\epsilon_z$  of pure and doped KLN was measured to study the composition dependent phase transition. For a Nb content above 52 mol% the phase transition was found to be of relaxor type occurring in a broad temperature range and with a frequency dependent  $\epsilon_z$ , which indicates the existence of two polarisation mechanisms. Alkali additives (Na, Rb or Cs) do not modify the dielectric behaviour of KLN, but Ta or Ti substituting for Nb increase  $\epsilon_z$ .

**Photorefractive damage resistance of LiNbO<sub>3</sub>:Zr crystals.** — Several tetravalent dopants increase the photorefractive damage resistance (PDR) of LiNbO<sub>3</sub> crystals. Optical methods including ultraviolet absorption, infrared absorption of hydroxyl ions, Raman spectroscopy, and the Z-scan method have been used to determine the PDR threshold in Zr-containing flux-grown stoichiometric LiNbO<sub>3</sub> (sLN). All methods used to characterize the sLN:Zr crystals indicate that samples containing more than  $\approx 0.085$  mol% Zr are above the PDR threshold.

**Calculation of OH<sup>-</sup> vibrational frequencies in congruent LiNbO<sub>3</sub> crystal.** — The atomic positions in a LiNbO<sub>3</sub> supercell consisting of 3x3x3 hexagonal unit cells and containing a NbLi antisite ion compensated by 4 nearby Li vacancies and an added proton were optimised using the SIESTA software. Adiabatic potential energy surfaces for the proton were created by varying the proton coordinates. Frequencies of the vibrational stretching, bending and combination modes of OH<sup>-</sup> were determined by a newly developed quantum chemical method including the influence of effective mass. Measurements of the infrared absorption spectrum of a long (22 mm) LiNbO<sub>3</sub> crystal confirmed the calculated band positions within 100 cm<sup>-1</sup>.

**Coherent radiative processes in rare earth doped LiNbO<sub>3</sub>.** — A simple, pulsed or CW pump-probe measurement scheme developed to measure the homogeneous linewidth of an atomic transition in an inhomogeneously broadened spectral line of a dopant ion in a single crystal was applied to the <sup>2</sup>F<sub>7/2</sub> – <sup>2</sup>F<sub>5/2</sub> optical transition of Yb in LiNbO<sub>3</sub>:Yb<sup>3+</sup>, and the <sup>4</sup>I<sub>11/2</sub> – <sup>4</sup>I<sub>15/2</sub> Er transition in LiNbO<sub>3</sub>:Er<sup>3+</sup> crystals. A fast dynamic real-time calibration process was developed by using a 500 mm long Fabry-Pérot interferometer to determine the precise temporal dependence of the piezo-modulated laser frequency. In the case of the Yb<sup>3+</sup> dopant, in addition to the main spectral hole, a narrower spectral hole component was also observed with a strongly temperature dependent dipole relaxation time of  $\sim 130$  ns at 9 K.

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<sup>#</sup> Ph.D student

**Model of  $O^-$  hole polarons in  $LiNbO_3$ .** – Models have been constructed to describe the partly resolved hyperfine structure of the low temperature ESR spectra of  $O^-$  hole polarons in  $LiNbO_3$ , the latter playing a basic role in many applications. Assuming that the hyperfine structure arises due to maximally 2  $^{93}Nb$  and 2  $^7Li$  nuclei adjacent to the hole localised on a single oxygen, the simulated spectra show excellent agreement with experiment. This demonstrates that delocalised models suggested earlier in the literature can be disregarded.

**Waveguides.** – Planar optical waveguides were designed and fabricated in Er-doped tungsten-tellurite and aluminosilicate glasses using high-dose irradiation with 200 keV electrons. Micro-Raman measurements indicated irradiation-induced structural changes in layers of 20 – 30  $\mu m$  thickness. Channel optical waveguides were produced in Er-doped tungsten-tellurite glass and both types of bismuth germanate crystals using wide beams of 3.5 MeV  $N^+$  ions with a silicon mask or a 5 MeV  $N^+$  microbeam. Transmission optical gratings were fabricated in Pyrex and Schott IOG glasses using microbeams of MeV energy carbon and oxygen ions. Atomic force microscopy of the gratings revealed a sinusoidal surface relief.

**$Li_2B_4O_7$ -based dosimeters and detectors.** – To optimise the luminescent yield in  $Li_2B_4O_7$ -based tissue-equivalent materials for thermoluminescent dosimeters and neutron detectors, ceramic and single crystal samples with various activator dopants have been produced and irradiated. For  $Li_2B_4O_7:Mn$  ceramics irradiated at room temperatures the thermoluminescence peak observed at 500 K is optimal for dosimetric purposes while samples with single crystal structure are inferior due to vanishing concentrations of the built-in Mn.

**Scintillators.** – The melt-assisted method has been applied for the synthesis of polycrystalline yttrium oxysilicate ( $Y_2SiO_5$ ). As a flux, several alkaline metal compounds ( $NaCl$ ,  $NaF$ ,  $LiF$ , 46.3 mol %  $Li_2O$  – 53.7 mol %  $B_2O_3$  eutectic,  $Li_2B_4O_7$ ) having lower melting point than the required  $X_2$ -phase of  $Y_2SiO_5$  have been used. From  $Y_{1.99}Ce_{0.01}SiO_5$  and the fluxes at varying ionic ratios, pastilles have been prepared and annealed at 1400 °C in vacuum. For verifying the phase purity, XRD and Raman spectrometry, while for optical properties, luminescence spectrometry has been applied. The samples prepared with  $LiF$  ( $Y_{3+}/Li_{10+}=10$ ) gave the  $X_2$ -phase as the main reaction product, and the strongest luminescence yield.

**Analytical methods for environmental purposes.** – The determination of ethyl carbamate in wine by HPLC was optimised. Atmospheric  $SO_2$ ,  $NO_2$ ,  $O_3$  and acidic aerosols were analysed in samples from Tanzania and Cuba, and the exhaust plumes of seagoing ships were monitored in the port of Rotterdam. Principal component analysis identified sea spray, local combustion, vehicular traffic, biomass burning, re-suspended road dust, soil/crustal and long-range transport as major pollution sources. A simultaneous, multi-element graphite furnace AAS method was developed for the determination of the toxic elements As, Cd, Cr, Cu, Pb, and Se in water samples of various sources.

## **Grants and international cooperation**

OTKA CK 80896: Scintillator materials for medical imaging purposes (L. Kovács, 2010-2013)

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



OTKA K 101225: Fabrication of integrated optical elements via ion beam implantation and irradiation for telecommunication applications (I. Bányász, 2012-2014)

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

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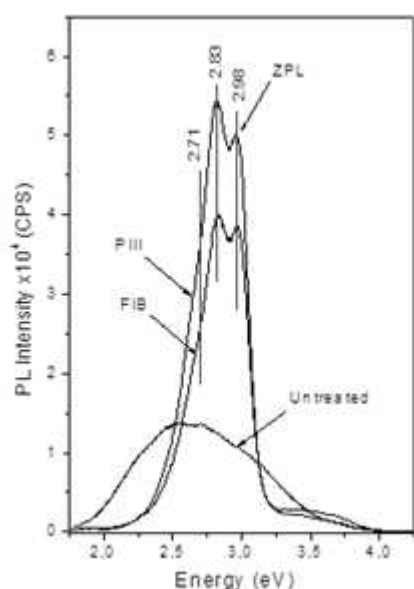
### Others

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16. Kovács L: Eredmények a magyar kristályfizika utóbbi éveiből. *FIZIKAI SZEMLE* 63:(1) pp. 7-11. (2013)

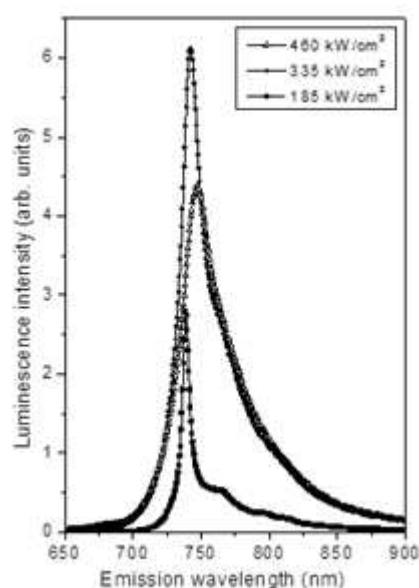
## S-R. Nanostructures and applied spectroscopy

Miklós Veres, László Himics, Margit Koós<sup>A</sup>, Sára Tóth

Due to their unique properties preparation and characterization of nanodiamond structures with specific light-emitting defect centers are among the most intensely studied areas of diamond research. A novel method has been developed for the creation of nitrogen-related N<sub>3</sub> defect centers in diamond nanoparticles by employing low-energy implantation (using plasma immersion ion implantation (PIII) or fast ion bombardment (FIB) methods) of He<sup>+</sup> and N<sub>2</sub><sup>+</sup> ions followed by two-stage heat treatment. This color center has an intense photoluminescence band around 415 nm (2.98 eV) and could have a great potential in magneto-optics, quantum computing and coherent light sources in the deep-blue wavelength range.



**Figure 1.** Room temperature photoluminescence spectra excited by  $E_{ex}=4.597$  eV photon energy of untreated and implanted (using PIII and FIB techniques) diamond nanocrystals after heat treatments at 750°C (in vacuum) and 450°C (in air).



**Figure 2.** Effect of the excitation power on the photoluminescence from diamond in the region of SiV-related emission band.

Extensive characterization of the silicon-related SiV color center was performed in different diamond structures, important for biomedical applications. The light emission of the center was found to be stable up to 1350°C, however red shift and considerable broadening of the zero phonon line occurred at higher excitation intensities. This phenomenon was explained by the contribution of the neutral vacancy-related GR1 center to the emission of the SiV defect's zero phonon line.

A novel method has been developed to determine the distribution of inhaled drugs in human airways based on Raman spectroscopy. Different aerosol medications were inhaled

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<sup>A</sup> Associate fellow

into artificial lung models prepared by reproduction of computer tomographic data of human airways with 3D printing. The amount of the deposited drug was determined from the intensity distribution of characteristic Raman peaks in mapping Raman spectra recorded in different points of the artificial lung.

## Grant

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

## Publications

### Articles

1. Karmenyan A V, Perevedentseva E, Veres M, Cheng C–L: Simultaneous Photo-luminescence and SERS Observation of Nanodiamond at Laser Deposition on Noble Metals. *PLASMONICS* 8:(2) pp. 325-333. (2013)
2. Kozyukhin S, Veres M, Nguyen HP, Ingram A, Kudoyarova V: Structural Changes in Doped  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  Thin Films Studied by Raman Spectroscopy. *PHYSICS PROCEEDIA* 44: pp. 82-90. (2013)
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See also: S-N.2, S-N.3

## Supplementary data

## Education

### Graduate and post-graduate courses

#### ***Eötvös Loránd University, Budapest***

- Advanced Experimental Particle Physics (G. Vesztergombi)
- Algebraic Bethe Ansatz and its applications (F. Woynarovich)
- Cavity Quantum Electrodynamics (P. Domokos, J. Asbóth)
- Cognitive Neuroscience (L. Négyessy)
- Computational Neuroscience (Z. Somogyvári)
- Electrons in solids (I. Tüttő)
- Electrons in solids (J. Sólyom)
- Inner structure of compact stars (G.G. Barnaföldi and M. Vasúth)
- Introduction to Experimental Particle Physics (G. Vesztergombi)
- Introduction to general relativity, (M. Vasúth)
- Introduction to gravitational theory and high energy physics (G.G. Barnaföldi and M. Vasúth)
- Jet physics (P. Lévai)
- Macromolecules I. (S. Pekker)
- Many-body physics I. (G. Szirmai)
- Many-body physics II. (G. Szirmai)
- Mathematical modelling in neuroscience (G. Orbán, M. Bányai, Z. Somogyvári)
- Metastable Metallic Materials (T. Kemény)
- Neural Modelling (Z. Somogyvári, M. Bányai, D. Cserpán)
- Nuclear Solid State Physics I (D.L. Nagy)
- Nuclear Solid State Physics II (D.L. Nagy)
- Open Quantum System Theory (L. Diósi)
- Phase structure of strongly interacting matters (P. Lévai)
- Plasma physics of the Solar System (K. Szegő)
- Relativistic heavy ion collisions (P. Lévai)
- Renormalization methods for strongly correlated systems (Ö. Legeza)
- Statistical learning in the nervous system (G. Orbán, M. Bányai, Z. Somogyvári)
- Superconductivity (I. Tüttő)
- Topological insulators (J. Asbóth)

#### ***Budapest University of Technology and Economics***

- Advanced thermodynamics (P. Ván)
- Chapters from High-temperature Plasma Physics (G. Kocsis)
- Coherent control of quantum systems (Z. Kis)
- Group theory in solid state research (G. Kriza)
- Infrared and Raman spectroscopy (K. Kamarás)
- Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (L. Kovács)
- Interacting spin systems (K. Penc)
- Introduction to theoretical plasma physics (A. Bencze)

- Ion beam analysis, part of the course Experimental methods in materials science (E. Szilágyi)
- Low temperature plasma physics (Z. Donkó)
- MHD in low-dimensional systems (A. Bencze)
- Neutron scattering I, part of the course Experimental methods in material science (B. Nagy, L. Bottyán)
- Nuclear Solid State Physics I (D.L. Nagy)
- Nuclear Solid State Physics II (D.L. Nagy)
- Spectroscopy and structure of matter (K. Kamarás)
- Superconductivity (G. Kriza)

### ***Semmelweis University, Budapest***

- Neuroinformatics (L. Négyessy, F. Bazsó, Z. Somogyvári, L. Zalányi, M. Bányai) Szent István University, Gödöllő
- Biophysics (Z. Szókefalvi-Nagy, SZIE AOTK)
- Computer Aided Engineering (L. Zoltan)
- Machine elements I. (L. Zoltan)
- Machine elements II. (L. Zoltan)

### ***University of Szeged***

- Analytical mechanics (L. Fehér)
- Application of statistical physics (F. Iglói)
- Experimental methods of nuclear physics (T. Csörgő)
- Fundamental processes in nonlinear laser-matter interactions (S. Varró)
- Introduction to theoretical physics I. (L. Fehér)
- Nuclear and Particle Physics I (T. Csörgő)
- Quantum field theory (L. Fehér)
- Selected topics in mathematical physics (L. Fehér)
- Statistical physics (F. Iglói)

### ***University of Pécs***

- Calculus I. (K. Szlachányi)
- Calculus II. (K. Szlachányi)
- Control theory (J. Füzi)
- Digital Control (J. Füzi)
- Electronics (J. Füzi)
- Mathematical methods in physics IV. (P. Ádám)
- Numerical methods (P. Ádám)
- Operating systems (B. Kollár)
- Probability theory (P. Ádám)
- Quantum mechanics I. (J. Janszky)
- Quantum mechanics II. (J. Janszky)
- Quantum mechanics II. (P. Ádám)
- Statistical physics (K. Szlachányi)

— Theoretical physics III. (P. Ádám)

#### ***University of Debrecen***

— Particle Physics, MSc Course (D. Horváth)

— Quantum Field Theory (T.S. Biró)

— Structure and Experimental Test of the Standard Model, PhD Course (D. Horváth)

#### ***University of Miskolc***

— Description of weak gravitational waves in General Relativity (I. Rácz)

#### ***Óbuda University, Budapest***

— Chemistry and Physics of Polymers (S. Pekker)

#### ***Rolls-Royce University Technology Centre, Cambridge University, UK***

— Phase field modelling and solidification (L. Gránásy, T. Pusztai, G. I. Tóth, G. Tegze)

#### ***National University of Public Service, Budapest***

— Mathematical analysis – theory and practice (B. Tóth)

### **Laboratory practices and seminars**

#### ***Eötvös Loránd University, Budapest***

— Experiments on liquid crystals (Á. Buka, N. Éber, T. Tóth-Katona)

— Laboratory practice (T. Pusztai)

— Laboratory practice in solid state physics and materials science (K. Tompa and M. Bokor)

— Laboratory practice - MHD (Z. Németh)

— Physical chemistry laboratory practice (K. Neuróhr)

— RBS and ERDA analysis, extended practice for physics student (E. Kótai).

— Solar-terrestrial relation for astrophysics students (M. Tátrallyay)

— Solid-state physics seminar (I. Tüttő)

#### ***Budapest University of Technology and Economics***

— Infrared and Raman spectroscopy (K. Kamarás)

— Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (K. Lengyel)

— Laboratory practice on investigation methods in materials science (M. Bokor and K. Tompa)

— Medical biology measurements (B. Sódor)

— Practice course in electrodynamics for energy-engineers (A. Szakál)

— Practice course in mathematics (A. Szakál)

— Problem solving courses in thermodynamics (T. Fülöp)

— Problem solving course in heat exchange (P. Ván)



- Raman spectroscopy, part of the Biophysics laboratory practice (M. Veres)
- Seminar to the Physics 2 course for bachelor students in electrical and software engineering (B. Nagy)

### ***University of Pécs***

- Control theory seminar (J. Füzi)
- Electronics laboratory practice (J. Füzi)
- Operating systems (B. Kollár)

## **Diploma works**

### ***Eötvös Loránd University, Budapest***

L. Ábrók, Supervisor: Zs. Kis)

G. Bíró, Flow phenomena in anisometric granular materials (BSc, Supervisor: T. Börzsönyi)

A. Budavári, (Supervisor: Zs. Kis)

### ***Budapest University of Technology and Economics***

A. Incze, Supporting real-time ultra fast video diagnostics development for plasma physics experiments, (Supervisor: T. Szepesi)

A. Karsa, Protein-ion interaction on molecular level (MSc, supervisor M. Bokor)

B. Nagy, Femtosecond Laser Induced Damage Threshold Measurements with Compressed Laser Pulses (MSc, supervisor: P. Dombi)

M. Timár, Investigation of strongly correlated systems by renormalization methods (BSc, supervisor: Ö. Legeza)

### ***University of Pécs***

E. Molnár, Az Urizar-Tóth fotonszám-fázis határozatlansági összefüggés intelligens állapotai (Supervisor: P. Ádám)

## **Ph.D students**

### ***Eötvös Loránd University, Budapest***

- Á. Agócs, Database management for large particle physics experiments at CERN LHC (Supervisors A. Benczur and G. Vesztergombi)
- A.G. Agócs, Interaction between high-pT hadrons and quark-gluon plasma in CERN LHC ALICE experiment (Supervisor P. Lévai)

- G. Barcza, Development and application of the non-local density matrix renormalization group (non-local DMRG) method to low-dimensional spin and fermionic models (Supervisors Ö. Legeza and F. Gebhard<sup>\*</sup>)
- Gy. Bencédi, Identification of high-pT particles in CERN LHC ALICE experiment (Supervisor P. Lévai)
- D. Berényi, Particle production in time-dependent strong fields in the ELI and the CERN LHC experiments (Supervisor P. Lévai)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor G. Kocsis)
- G. Csire, Quasiparticle spectra of the metal-superconducting heterostructure.
- Z. Darázs, Quantum control with measurements (Supervisors T. Kiss and A. Csordás)
- M. Dolgos, Metastable structures in stratified systems (Supervisor L. Bottyán)
- A. Dombi, Quantum dynamics of atomic motion in multimode optical resonator fields (Supervisor P. Domokos)
- E. Gáspár Merse, Characterization of spontaneous activity in the visual cortex (Supervisor: G. Orbán)
- I. Hagymási, Heavy-fermion behavior in the periodic Anderson model (Supervisor J. Sólyom)
- G. Kónya, Many-body physics in cavity QED (Supervisor P. Domokos)
- N. Laczai, Fabrication of nano-scintillator materials for medical imaging purposes (Supervisor L. Bencs)
- K. Lukács, Investigation of the evolution of the interplanetary magnetic field (Supervisor G. Erdős)
- K. Márton, Ultrarelativistic hadron-nucleus collisions at CERN SPS energies (Supervisors A. László and D. Varga<sup>\*</sup>)
- F. Máté Nagy, Numerical study of gravitational wave generation.
- K. Németh, Chemical functionalization of carbon nanotubes (Supervisor K. Kamarás)
- K. Neuróhr, Electrochemical preparation of multilayers with giant magnetoresistance (Supervisor L. Péter)
- L. Oláh, Analysis of identified particles by ALICE HMPID (Supervisor G.G. Barnaföldi)
- M. Pápai, Modelling the electronic, structure of transition metal compounds (Supervisor G. Vankó)
- T.N. Papp, Open quantum systems (Supervisor L. Diósi)
- S. Pochybova, High energy quark and gluon jets in proton-proton and heavy ion collisions (Supervisor P. Lévai)
- L. Rátkai, Phase-field modelling of columnar to equiaxed transition with fluid flow (Supervisor T. Pusztai)
- P. Salamon, Flexoelectricity in liquid crystals (Supervisor N. Éber)
- B. Szabó, Experimental investigations of granular flows (Supervisor T. Börzsönyi)
- É. Tichy-Rács, Synthesis, crystallization and spectroscopy of rare-earth-alkaline orthoborates (Supervisor K. Polgár)
- B. Tóth, Giant magnetoresistance (GMR) in multilayers (Supervisors I. Bakonyi and L. Péter)
- R. Ünnepe, Study of self-assembly functional nano particles by neutron scattering (Supervisor F. Mezei)

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<sup>\*</sup> Not a member of the Wigner RCP

- K. Ürmössy, Advanced statistical methods in high energy physics (Supervisor T.S. Biró)
- T. Verebélyi, NMR and DSC study of protein solutions (Supervisor K. Tompa)
- A.J. Zsigmond, Study of high density QCD matter in Pb+Pb and p+Pb collisions in the CMS experiment at the LHC (Supervisors F. Siklér and G.I. Veres\*)

#### ***Budapest University of Technology and Economics***

- M. Bányai, Neural sampling in a hierarchical model of the visual cortex (Supervisor G. Orbán)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor: G. Kocsis)
- D. Cserpán, Doctoral School of Informatics (Supervisor Z. Somogyvári)
- M. Lajkó, Theoretical studies of strongly frustrated spin and charge systems (Supervisor K. Penc)
- M. Lampert, Study of plasma turbulence and zonal flows on various tokamak devices (Supervisor S. Zoletnik)
- J. Orbán, Investigation and development of signal processing electronics for position sensitive particle counters (Supervisors L. Rosta and Cs. Sükösd\*)
- A. Szakál, Investigation of the structure and dynamics of metal-hydrogen systems with neutron scattering (Supervisor L. Cser)
- Sz. Szalay, Quantum entanglement in finite-dimensional Hilbert spaces (Supervisor: Ö. Legeza)
- T. Szarvas, Modeling of wave propagation and quantum optical processes in structured dielectrics (Supervisor: Zs. Kis)
- Zs. Szekrényes, Infrared spectroscopy of self-assembled structures on surfaces (Supervisor K. Kamarás)
- B. Tál, Measurements of fast transients in a tokamak plasma (Supervisor G. Veres)

#### ***Semmelweis University, Budapest***

- M. Ashaber, Wiring functional tactile cortical representations, combined optical imaging, light- and electron microscopic track tracing studies in the primate somatosensory cortex (Supervisor L. Négyessy)
- E. Pálfi, The role of somatosensory cortical inhibition in tactile functions (Supervisor L. Négyessy)

#### ***Pázmány Péter Catholic University, Budapest***

- B. Jákli, Control of biomechatronic robotic arm (Supervisor L. Négyessy)

#### ***University of Szeged***

- A. Barna, Stability and contrast improvement of ultrashort KrF laser pulses for laser-plasma experiments (Supervisor I. Földes)
- L. Himics, Nanocrystalline diamonds for advanced applications (Supervisor M. Koós)
- H-M. Tóháti, Optical spectroscopy of confined luminescent materials (Supervisor K. Kamarás)

#### ***University of Pécs***

- M. Aladi, Generation of high-harmonics from gases, clusters and solids (Supervisor I. Földes)
- B. Bódi, High harmonic generation with shaped ultrashort laser pulses (Supervisor: P. Dombi)
- L. Kecskés, Complex chaos in the dynamics of qubits (Supervisor T. Kiss)
- A. Kerekes, Development of optical instrumentation for environmental measurements (Supervisor A. Nagy)
- A. Zs. Kovács, Collective dynamics in strongly coupled many-particle systems (Supervisors: Z. Donkó, P. Hartmann)
- B. Kollár, Quantum information in quantum-optical networks (Supervisor T. Kiss)
- Z. László, Magnetic bearings for neutron beam phase space tailoring (Supervisors J. Nagy, J. Füzi)
- I. Márton, Ultrafast photoemission from plasmonic structures (Supervisor: P. Dombi)
- E. Molnár, Conditional realization of nonclassical quantum states of light by linear optical processes (Supervisor: P. Ádám)
- N. Sándor, Optical information writing and coherent processing using metastable quantum states (Supervisor G. Dzsotjan)
- P. Sinkovicz, Spin liquid phases (Supervisor G. Szirmai)
- Sz. Terdik, Realization of unphysical processes for qubit systems (Supervisor: P. Ádám)
- Á. Varga, Quantum state discrimination (Supervisor P. Ádám)

***University of Pannonia, Veszprém***

- K. Berkesi, Investigation of radioactive contamination on smooth and increased surfaces of noble metal electrodes (Supervisor L. Péter)

***Szent István University Gödöllő***

- Z. László, Magnetic bearings for neutron beam phase space tailoring equipment (Supervisors J. Nagy, J. Füzi)

## **Dissertations**

### **Ph.D**

M. Lajkó: Fluctuating moments in one and two dimensional Mott insulators, 114p. 2013

Sz. Szalay: Quantum entanglement in finite-dimensional Hilbert spaces, 162 p. 2013.

K. Neuróhr: Fémek nanoszerkezetek elektrokémiai leválasztása és vizsgálata (Electrochemical deposition and study of metallic nanostructures), 113 p. 2013.

B. Tóth: Elektrolitikus nanoszerkezetek mágneses ellenállásának vizsgálata (Study of the magnetic resistance of electrochemical nanostructures), 116 p. 2013.

I. Hajdara: A kálium-lítium-niobát kristály tulajdonságai és hibaszerkezete (Properties and defect structure of potassium lithium niobate crystals), 112p. 2012

### **D.Sc**

K. Kecskeméty, Nagyenergiájú ionpopulációk a Helioszférában (Energetic ion populations in the Heliosphere)

J. Balogh, Interfaces and impurities in nanostructured materials

L. Péter: Elektrokémiai úton leválasztott fémek nanoszerkezetek (Electrodeposited metallic nanostructures), 128 p. 2013.

## Memberships

- P. Ádám — Member of the Laser Physics Committee of MTA.
- 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)
- J. Balogh — Int. Board on the Application of the Mössbauer Effect (IBAME), 2012-2017
- G.G. Barnaföldi — Hungarian Representative in EU ESF CompStar 2008-2013.  
— 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
- F. Bazsó — Programme Committee Member, International Conference on Artificial Neural Networks ICANN 2012 Sept. 11-14, Lausanne
- L. Bencs — Editorial Board member of Environmental Monitoring and Management  
— Editorial Board member of ISRN Analytical Chemistry
- T.S. Biró — Member of the Scientific Advisory Committee of the European Physical Journal (representing MTA and ELFT, until August 31, 2012)  
— Co-Editor of the European Physical Journal A: Hadrons and Nuclei;  
— Chairman of Wigner FK RMI TT (Scientific Advisory Board)  
— Member of International Advisory Board for Strangeness in Quark Matter conferences; (Birmingham UK 2013)  
— Member of Physics PhD School Advisory Board at TU Budapest (BME)  
— Member of Physics PhD School, Eötvös Loránd University, Budapest  
— Editor of The European Physics Journal A (Hadrons and Nuclei) Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
- T. Börzsönyi — National Scientific Research Fund (OTKA), Physics Panel Member
- Á. Buka — Electronic-Liquid Crystal Communications, Editorial Board  
— International Liquid Crystal Conference, International Advisory Board  
— National Scientific Research Fund (OTKA), Physics Panel Member  
— Solid State Physics Committee of MTA, Member
- G. Cseh — Member of the Hungarian Nuclear Society
- L. Cser — International Scientific Advisory Council of BNC (Budapest Neutron Centre)

- L. Csernai — Member of the Editorial Board, International Journal of Modern Physics E - Nuclear Physics
- 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
- A. Czitrowszky — Chairman of the Working Group Instrumentation in EAA  
 — Member of the Board of International Aerosol Association  
 — Member of Gesellschaft für Aerosolforschung  
 — President of the Hungarian Aerosol Society  
 — Member of the ELI\_ALPS Scientific Advisory Committee  
 — President of the Hungarian Branch of the European Optical Society  
 — Head of the Optical Chapter of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology (Budapest)  
 — Member of the Editorial Board of "Fizikai Szemle"  
 — Chairman of the Optical Chapter of Roland Eötvös Physical Society  
 — Chairman of the Committee for the Lasers Physics and Spectroscopy in MTA  
 — Founding member of Ph.D. school at the University of Pécs
- L. Diósi — Management Committee, EU COST Action Fundamental Problems in Quantum Physics  
 — Member of Editorial Advisory Board, The Open Nuclear & Particle Physics Journal
- 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 — Conference series "Symposium of the Phenomena in Ionized Gases", Member of International Scientific Committee, from 2006  
 — Conference series "Strongly Coupled Coulomb Systems", Member of International Advisory Board, 2007-  
 — Conference series "Symposium on Application of Plasma Processes,"

Member of International Scientific Committee, from 2008

- P. Dombi — Senior Member of SPIE (Photonics Society), USA
- G. Erdős: — Chairman of the Committee on Astronomy and Space Physics of MTA  
— National Representative of COSPAR
- N. Éber — Member of The Open Crystallography Journal, Editorial Board  
— Member of the Journal of Research in Physics, Editorial Board
- 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
- G. Faigel — XFEL In-kind Review Committee member  
— XFEL SAC member
- K. Fodor-Csorba — Member of the Hungarian Chemical Society
- T. Fülöp — Member of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)
- J. Füzi — Editorial Board Member, Pollack Periodica  
— Editor, IEEE Transactions on Magnetics, SMM21 Budapest issue
- L. Gránásy — Member of the ESA Topical Team “Solidification of Containerless Undercooled Melts”, SOL – EML  
— Member of The Minerals, Metals, and Materials Society, USA  
— Solid State Physics Committee of MTA  
— Mathematics and Science Committee of AKT
- P. Hartmann — Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" Member of International Scientific Committee, 2008-2014
- J. Janszky — Member of the Laser Physics Committee of MTA
- K. Kamarás — Editorial Board Member, European Physical Journal B



- Z. Kis — Member of the Editorial Board of the Physical Review A
- T. Kiss — Member of the Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP)  
— Member of the Management Committee of COST Action MP1006  
— Member of the Laser Physics Committee of ELFT
- G. Kocsis — Member of the Hungarian Nuclear Society  
— Member of the European 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
- 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
- K. Kutasi — Conference series “International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment,” member of International Scientific Committee, from 2006  
— Conference series of “Central European Symposium on Plasma Chemistry” Member of International Scientific Committee, 2013-
- 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)

F. Mezei

- International Scientific Advisory Council of BNC (Budapest Neutron Centre)
- Chairman of the Physical Society Publication Committee
- American Physical Society
- European Neutron Scattering Association (ENSA) Committee
- Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA
- International Council for Scientific and Technical Information, University of California, San Diego
- ESS Lund, Technical Director of Machine

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
- Budapest Neutron Centre (BNC), International Scientific Advisory Committee, 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
- C-ERIC consortium, Working Group, 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

- L. Péter — Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)  
 — Representative for Hungary, International Society of Electrochemistry (2011-2013)  
 — Council Member of Graduate School of Chemistry, ELTE (2009-)  
 — Editor for Electrochemistry (Central European Journal of Chemistry, 2009-)
- 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)
- L. Rosta — International Scientific Advisory Council of BNC (Budapest Neutron Centre)  
 — European Spallation Source, Steering Committee
- F. Siklér — Hungarian delegate to European Committee for Future Accelerators (ECFA)  
 — Member of CMS Publication Committee, Heavy Ions editorial board
- E. Somfai — IOP member  
 — Member of the American Physics Society
- J. Sólyom — Chairman of the Physics Section of the Hungarian Academy of Sciences
- 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
- K. Szegő — Member of Committee on Astronomy and Space Physics of MTA  
 — Member of IAA  
 — Guest Editor of Space Science Reviews
- T. Szepesi — Member of the Hungarian Nuclear Society
- E. Szilágyi — International Committee of the Conference series of Ion Beam Analysis, member
- Z. Szőkefalvi-Nagy — Member of the Editorial Board, International Journal of PIXE  
 — Honorary Member of the International Advisory Board, PIXE  
 — Member of the Committee of International Relations of MTA
- K. Tompa — Member of the Natural Science Committee of the Hungarian Scholarship Board (2011-2013)
- Gy. Török — Member of IAEA JRC-1575

- Member of JRC-NET
- B. Ujfalussy
  - President of the Overseeing Committee of Loránd Eötvös Physical society
  - Secretary of the Materials Science Group of Loránd Eötvös Physical society
- 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)
- P. Ván
  - Member of the Scientific Advisory Board of Joint European Congress in Thermodynamics (Brescia, Italy 2013)
  - Executive chairman of the Organizing Committee of 6th Finno-Ugric International Conference of Mechanics with Special Symposia (Ráckeve, 2013)
  - Editor of The European Physics Journal A: Hadrons and Nuclei Topical Issue on Relativistic Hydro- and Thermodynamics in Nuclear Physics
- G. Veres
  - Member of the Hungarian Microscopy Society
  - Member of the Hungarian Aerosol Society
- I. Vincze
  - Member of the Council of Doctors at 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

## Conferences

### **CETS2013 7<sup>th</sup> Central European Training School on Neutron Scattering**

The school was held in Budapest, Hungary, from 27th May to 31st May 2013 and organized by the Neutron Spectroscopy Department at the Budapest Neutron Centre (BNC) with support of the associate laboratories of our research centre.

The main scope of this course was to provide insight into neutron scattering techniques and their application for studies on structure and dynamics of condensed matter. After attending the lectures the students participated in practical works in groups (powder diffractometer, small-angle neutron scattering instrument, polarized neutron reflectometer, three-axis spectrometer, time-of-flight (TOF) spectrometer, prompt-gamma activation analysis were used). The course consisted of 5 days lectures and experimental works. A lecture by Ferenc Mezei (BNC/ESS) gave an overview on the research with neutrons and future prospects at the European Spallation Source. Further lectures were given by renowned scientist from various European institutions. CETS was also an opportunity to include in the programme a half-day series of poster presentations of the participants, where interesting and useful discussions were made about possible material science investigations using neutrons.

### **Soft Magnetic Material 21-Conference, Budapest 1-4 September 2013**

320 participants from 37 countries, 8 exhibitors.

### **Conference “Artificial Atoms: from Quantum Physics to Applications”, 20-23 May 2013**

The conference was organized as a joint scientific meeting of two consortia of the 7th Framework of the EU, the FP7 ICT DIAMANT (Diamond based atomic nanotechnologies) and the FP7 ITN CCQED (Circuit and Cavity Quantum Electrodynamics). The conference took place in the main building of the Hungarian Academy of Sciences. Besides scientists from the consortia and from EU, guests arrived from the USA, Australia, Japan and Chile. The three-days meeting which was attended by approx. 70 scientists, boosted the cooperation between researchers of materials science and quantum mechanics.

### **International Workshop on Stoichiometric Lithium Niobate, 18-20 September, 2013, Goslar, Germany**

The workshop, co-organized by the Crystal Physics group, was attended by 40 scientists.

## Seminars

Weekly meetings of the Budapest and Debrecen Compact Muon Solenoid (CMS) groups:

<http://www.grid.kfki.hu/twiki/bin/view/CMS/WeeklyBudapestDebrecenMeetings>

Talks for the annual Zimányi School

<http://zimanyischool.kfki.hu/13/agenda>

## RMI Seminars

- 18-01-2013 Kunszt Zoltán (ETH Zürich), Rögös út a Higgs-bozon felfedezéséig (A hard way to the discovery of the Higgs boson)
- 25-01-2013 Diósi Lajos (Wigner RMI), Stochasztikus Schrödinger egyenletek és a kvantumfizika alapjai (Stochastic Schrödinger equations and the principles of quantum physics)
- 22-03-2013 Kunszt Zoltán (ETH Zürich), Az ATLAS és CMS legújabb Higgs-adatai és elméleti interpretálásuk (Latest Higgs data of Atlas and CMS, and their theoretical interpretation)
- 12-04-2013 Noa Mitsui (Wigner RMI), Geophysics, power laws, and mechanism of friction
- 16-04-2013 Andrew Lowe (CERN, ATLAS), Jet substructure and superstructure for new physics searches
- 26-04-2013 Gogohia Vahtang (Wigner RMI), The discovery of the mass gap and confinement of gluons
- 03-05-2013 Christoph Sieg (Humboldt University, Berlin), Perturbative spectra of gauge theories with gravity duals
- 10-05-2013 Minkyoo Kim (Sogang University, Seoul) é Algebraic curves and integrability in string theory
- 17-05-2013 Jakovác Antal (BME), Részecske kép kölcsönható rendszerekben (Particle picture in interacting systems)
- 24-05-2013 Lukács Árpád (RMI), Lehetséges-e a vonósugár, azaz mikor negatív a sugárzási nyomás? (Is the tractor beam possible, or when is the radiation pressure negative)
- 21-06-2013 K. V. Zhukovsky (Lomonosov University, Moscow), Planar Undulator Performance and Harmonic Generation in a Constant Magnetic Field
- 28-08-2013 Kazuhiro Sakai (Ritsumeikan University, Japan), Integrability of BPS equations in ABJM theory
- 30-08-2013 Jeffrey Kelling (Helmholtz Zentrum, Dresden Rossendorf), Performing kinetic lattice Monte-Carlo simulations of far-from-equilibrium processes on GPUs
- 02-09-2013 Szilagyai Bela (Caltech): Stretching the limits of Numerical Relativity
- 06-09-2013 Takihiro Hatano (Earthquake Research Institute, University of Tokyo), Nonequilibrium thermodynamic relations and their generalization to athermal systems
- 11-09-2013 Kertész János (BME), Értékkeremtés kollaboratív internetes környezetben: Wikipédia szerkesztői háborúk (Value creation in a collective internet environment: Wikipedia editorial wars)
- 13-09-2013 Katsushi Ito (Tokyo Institute of Technology), N=4 SYM in Omega background
- 31-10-2013 Dr. Péter Buzás, Hogy fedezték fel újra a színlátást az emlősök és melyek

- ennek a funkcionális következményei? (How the mammals rediscovered color sight, and what are its functional consequences? Biophysics seminar)
- 11-12-2013 Dr. Gábor Juhász, Az idegrendszer kutatás szemléletváltása: a rendszerbiológia, a translációs medicina és a molekuláris medicina együttes hatásai (Change of view in neural research: the collective effects of system biology, translational medicine and molecular medicine, Biophysics seminar)

## SZFI Seminars

- 03-01-2013 András Bartók (Laboratoire de Génie Electrique de Paris France), AMR szenzorok multiscale (többléptékű) modellezése (Multiscale modeling of AMR sensors)
- 04-01-2013 Péter Kómár (Harvard University, USA), Optomechanika több foton módussal (Optomechanics with multiphoton mode)
- 04-01-2013 Gábor Halász (Rudolf Peierls Centre for Theoretical Physics, Oxford, United Kingdom), Mozgékony defektusok Kitaev hatszögrács modelljében (Mobile defects in Kitaev's hexagonal lattice model)
- 08-01-2013 Pál Jóvári (SZFI), Többkomponensű kalkogén üvegek szerkezetvizsgálata (Structural study of multi-component chalcogenide glasses)
- 15-01-2013 Péter Hartmann (SZFI), Fény-mező elvű térbeli részecske detektálás (Particle detection on light-field principle)
- 22-01-2013 Kinga Kutasi (SZFI), Reaktív kisülési plazmák a biomedika és nanotechnológia szolgálatában (Reactive discharge plasmas in the service of biomedics and nanotechnology)
- 29-01-2013 Sándor Varró (SZFI), Alagút-effektus és Wigner-idő (Tunneling effect and Wigner-time)
- 05-02-2013 László Temleitner (SZFI), Rendezetlenség kristályos fázison - diffrakció és szimuláció (Disorder on crystalline phase – diffraction and simulation)
- 12-02-2013 Ihor Korolov (SZFI), Development of an experimental apparatus for charge transfer rate coefficient measurements
- 19-02-2013 Imre Vincze (SZFI), Félfémes  $\text{Co}_2\text{FeZ}$  ( $Z=\text{Al,Ga,Si,Ge}$ ) - hoax? (Semi metallic  $\text{Co}_2\text{Fe}_z$  ( $Z=\text{Al,Ga,Si,Ge}$ ) – a hoax?)
- 26-02-2013 Annamária Kiss (SZFI), Újszerű Kondo-fizika urános és samáriumos nehézfermion rendszerekben (Novel Kondo-physics on uranium and samarium containing heavy-fermion systems)
- 28-02-2013 Igor Jex (Czech Technical University in Prague), Quantum walks with linear optics
- 05-03-2013 András Holl (Library of the H.A.S., Konkoly Observatory), Open Access - arXiv,

SCOAP3, REAL

- 12-03-2013 Imre Hagymási (SZFI), Periodikus Anderson-modell korrelált vezetési elektronokkal (Periodic Anderson model with correlated conduction electrons)
- 19-03-2013 Juhász Róbert (SZFI), Dinamika inhomogén közegben: A diffúziótól a járványterjedésig (Dynamics in inhomogeneous medium. From diffusion to the spread of diseases)
- 19-03-2013 Oliver Mülken (Universitat Freiburg), Exciton Dynamics in Open Quantum Systems - from Quantum to Random Walks
- 26-03-2013 Zoltán Horváth (SZFI), Unortodox lézerek földön s egen (Unorthodox lasers on earth and in the sky)
- 26-03-2013 Árpád Lukács (RMI), Lehetséges-e a vonósugár, azaz mikor negatív a sugárzási nyomás? (Is the tractor beam possible, or when is the radiation pressure negative)
- 02-04-2013 László Péter (SZFI), Hogyan pácoljunk vaslemezt? avagy egy tudományostechnikai innovációs beruházás igaz története a XXI. századi Magyarországról (How to pickle an iron plate? or the true story of a scientific-technological innovational project from XXI. century Hungary)
- 09-04-2013 Prof. Florian Gebhard (Philipps Universitaet Marburg), Excited states in polydiacetylene chains: A Density-matrix-renormalization-group study
- 11-04-2013 Péter Salamon (SZFI), Extraordinary properties of bent-core and rod-like nematic liquid crystals
- 16-04-2013 Aranka Derzsi (SZFI), Elektronfűtési mechanizmusok rádiófrekvenciás gázkisülésekben (Electron-heating mechanisms in radiofrequency gas discharges)
- 16-04-2013 Renáta Ünnep (SZFI), Fotoszintetikus szervezetek tilakoid membrán szerkezetének vizsgálata kisszögű neutron szórásvizsgáló berendezés (SANS) segítségével (Investigation of the structure of thylakoid membranes in photosynthetic structures by small angle neutron scattering (SANS))
- 23-04-2013 Zoltán Jurek (SZFI), Véges méretű rendszerek dinamikája intenzív röntgenimpulzusban (Dynamics of finite size systems in intensive X-ray pulses)
- 30-04-2013 Krisztina György (SZFI), Atomabszorpciós spektrometriai kutatások optikai egykristályok vizsgálatára (Atomic absorption spectroscopy research for studying optical single crystals)
- 06-05-2013 Athanasios Speliotis (Institute of Materials Science, NCSR "Demokritos", Athens), Fe-Pt thin films for perpendicular magnetic recording media
- 07-05-2013 Krisztián Szász (SZFI), Ponthibák azonosítása félvezető szerkezetekben hiperfinom tenzor számításával (Identification of point defects in



semiconductor structures by hyperfine tensor calculations)

- 07-05-2013 Balázs Szabó (SZFI), Nyírási lokalizáció és rendeződés szemcsés anyagokban (Shearing localization and self-organization in granular materials)
- 14-05-2013 Kovács István János (Magyar Földtani és Geofizikai Intézet), Ásványok infravörös fényben (Minerals in infrared light)
- 16-05-2013 Lajkó Miklós (SZFI), Fluktuáló momentumok egy- és kétdimenziós Mott-szigetelőkben (Fluctuating momentums in one and two dimensional Mott-insulators)
- 21-05-2013 Mark W. Meisel (Microkelvin Laboratory, University of Florida), Design and Discovery of New Photocontrolled Magnets: Nanoscaled 'Alchemy'
- 22-05-2013 Judit Zöldföldi (Universität Stuttgart, Materialprüfungsanstalt), A legdrágább féldrágakő: lápisz lazuli - archeometriai vizsgálatok (The most expensive semi-precious stone: lapis lazuli – archeometric studies)
- 23-05-2013 Katalin Neuróhr (SZFI), Fém nanoszerkezetek elektrokémiai leválasztása és vizsgálata (Electrochemical deposition and study of metallic nanostructures)
- 28-05-2013 Alex Szakál (SZFI), Atomi felbontású holográfia polikristályos mintán (Atomic resolution holography on polycrystalline sample)
- 28-05-2013 Lénárd Vámos (SZFI), 1 kHz / 4 mJ-os lézerrendszer installálása és femtoszekundumos roncsolási küszöb mérése (Installation of a 1 kHz / 4 mJ laser system, and measurement of femtosecond damage threshold)
- 04-06-2013 Nikoletta Laczai (SZFI), Polikristályos ittrium-oxi-ortoszilikátok előállítása és vizsgálata (Preparation and study of polycrystalline yttrium oxo-silicates)
- 04-06-2013 Bence Tóth (SZFI), A termomágneses Curie-switch (The thermomagnetic Curie-switch)
- 11-06-2013 Ivett Hajdara (SZFI) A kálium-lítium-niobát kristály fázisátalakulásának vizsgálata (Investigation of the phase transition of potassium-lithium-niobate crystal)
- 11-06-2013 Péter Rácz (SZFI), Ultragyors jelenségek vizsgálata nanolokalizált elektromágneses terekben (Study of ultrafast phenomena in nanolocalised electromagnetic fields)
- 18-06-2013 Zoltán Bodrog (SZFI) Hibaszimmetriák, szimmetriahibák - Kvantumbitek megvalósítása kristálybeli ponthibákkal (Symmetry of defects, defects of symmetry – realization of quantumbits by crystalline point defects)
- 25-06-2013 Dóra Haluszka, Attila Kolonics and Róbert Szipócs (SZFI), In vivo nemlineáris 3D mikroszkópia és néhány alkalmazása az orvosi diagnosztika és a gyógyszeripar területén (In vivo nonlinear 3D microscopy and some applications in the fields of medical diagnostics and pharmacology)

- 27-06-2013 Jonathan Edge (Lorentz Institute, Leiden University), Metallic phase of the quantum Hall effect in four-dimensional space
- 25-07-2013 Géza Tóth (University of the Basque Country UPV/EHU), Efficient algorithm for multi-qudit twirling for ensemble quantum computation
- 13-08-2013 Ronald Dickman (Federal University of Minas Gerais, Brasil), Analysis of an information-theoretic model for communication
- 03-09-2013 Obuse Hideaki (Department of Applied Physics, Hokkaido University, Japan), Network model for 2D and 3D  $Z_2$  topological insulators and its relation to quantum walks
- 24-09-2013 Ellák Somfai (SZFI), Skálainvariáns dinamika táguló térben (Scale invariant dynamics in expanding space)
- 01-10-2013 Urmas Nagel (National Institute of Chemical Physics and Biophysics, Tallinn, Estonia), Terahertz Spectroscopy of Spin Waves in Multiferroic BiFeO<sub>3</sub> in High Magnetic Fields
- 08-10-2013 Brian Tarasinski (Instituut-Lorentz, Leiden), Scattering approach to topological phases in quantum walks
- 15-10-2013 Verebélyi Tamás (SZFI), Kalorimetria a világban és itthon (Calorimetry in the world and here)
- 22-10-2013 Attila Kerekes (SZFI), Inhalációs aeroszolok célzott légúti depozíciójának mérés technikája (Metrology of targeted respiratory deposition of inhalational aerosols)
- 29-10-2013 Varró Sándor (SZFI), Wigner Jenő és a 'kvantum disszidensek' (Eugene Wigner and the 'quantum dissidents')
- 05-11-2013 Katalin Kamarás (SZFI), Töltött szén nanocsövek (Filled carbon nanotubes)
- 07-11-2013 Luca Salasnich (University of Padova), Time-dependent density functional of the Fermi gas in the BCS-BEC crossover
- 12-11-2013 Philippe Claudin (École Supérieure de Physique et Chimie Industrielles), Sand dunes, ripples, chevrons and bars -- formation mechanisms and scaling laws
- 19-11-2013 Farkas Illés (ELTE TTK), Technológiai, társadalmi és biológiai hálózatok átfedő moduljainak azonosítása és értelmezése (<http://CFinder.org>) (Identification and interpretation of overlapping modules of technological, social and biological networks)
- 26-11-2013 Simon Ferenc (BME, Faculty of Physics), A spin-relaxáció új, egyesített elmélete (New, unified theory of spin-relaxation)
- 28-11-2013 Andrzej Sienkiewicz (Ecole Polytechnique Fédérale de Lausanne), Biophysical applications of electron spin resonance (ESR)

- 03-12-2013 Gyöngyi Pergerné Klupp (SZFI), Fém-szigetelő átalakulás követése kémiai nyomás változtatásával fulleridekben (Tracking of metal-insulator transformation by changing the chemical pressure in fullerenes)
- 09-12-2013 Marta Bajko and Juan Carlos Perez (CERN), Superconducting magnets and related technology in LHC and LHC upgrades
- 10-12-2013 Kövér Ákos (MTA Institute for Nuclear Research), Elektronspektrométerek fejlesztése az ATOMKI-ben (Development of electron spectrometers in the ATOMKI)
- 10-12-2013 Ricz Sándor (MTA Institute for Nuclear Research), Aszimmetrikus fotoelektron emisszió foton-atom és foton-H<sub>2</sub> molekula kölcsönhatásban (Asymmetric photoelectron emission in photon-atom and photon-H<sub>2</sub> molecule interactions)
- 17-12-2013 Viktor Ivády (SZFI), Theoretical investigation of the single photon emitter carbon antisite - vacancy pair in 4H-SiC & the role of the screening in the density functional applied on correlated orbitals in an sp<sup>3</sup> electron bath

