Contents

Chapter 1

Scientific Work and its Organization at the Institute – an Overview

1.1 History and Development of the Institute

1992-1994 • The Senate of the Max Planck Society decided to set up the Max Planck Institute for the Physics of Complex Systems in November 1992, with *Prof. Fulde* as the Founding Director. The concept for the institute includes three scientific divisions and a large-scale visitors program. The incorporation of a seminar and workshop program within the visitors program was expected to become a significant part of the institute's activities. The program aims at promoting new developments in the field of the physics of complex systems. One important aspect is to provide a high-level platform for young scientists from universities to become acquainted with recent research developments much earlier than was traditionally the case. At the same time, important new research areas in the field of theoretical physics are promoted efficiently. Dresden was chosen as the location for the institute due to its favorable scientific environment and good travel connections. Scientific activities started on July 1st, 1993, in Stuttgart, as proper office space in Dresden was lacking. This was supplied by January 1994 thanks to the support of the TU Dresden, short of office space, but generously offering a temporary accomodation for the institute in a barrack in the Bayreuther Straße, close to the university campus. These were exciting times in Dresden, the early post unification years full of change, (re)construction and new initiatives. The institute was officially inaugurated by Prof. H. Zacher, President of the Max Planck Society, on May 2nd, 1994. Both the State of Saxony and the City of Dresden have contributed significantly to a smooth setting up of the activities of the institute, e.g., by the City of Dresden providing additional temporary office space in a villa with unsettled property claims, free of charge. The institute also had to rent several additional offices close to the barrack. An administration was installed, headed by Mrs. *I. Auguszt*. First guests were invited, and the first workshop took place in March 1994. An independent junior research group on *Nonlinear Time Series Analysis* was founded in 1995 and headed by *Dr. H. Kantz*. Strongly supported by President Zacher, the institute decided to broaden its research spectrum considerably by installing temporary junior research groups. *Dr. M. Bär* started his activities as head of the junior research group *Pattern Formation in Reaction-Diffusion-Systems* in 1995. *Dr. K. Richter* became head of the junior research group *Quantum Chaos and Mesoscopic Systems* in January 1996, and *Dr. M. Dolg* of the group *Quantum Chemistry* shortly afterwards.

1995-1998 • At the same time, plans for the new institute building were beginning to materialize. The architecture firm Brenner und Partner (Stuttgart) with J. Wittfoth won the competitive bidding, and constructions started in September 1995. After less than two years the institute moved into the newly constructed main building, together with the three guest houses. The inauguration of the buildings was held alongside a simultaneous symposium on *Complexity in Physics*, September 23-24, 1997. In the meantime the Seminar- and Guest-Program were gaining momentum, with hundreds of scientists already having visited the institute.

1999-2001 • The next important step was the appointment of *Dr. J. M. Rost* (Freiburg) as head of the second division of the institute in December 1998. *Dr. Rost* started the activities on May 1st, 1999 by setting up the division *Finite Systems*. He appointed *Dr. A. Buchleitner* as head of a research group *Nonlinear Dynamics in Quantum Systems*. After *Dr. Dolg* accepted an offer for a professorship at the University of Bonn in 2000, *Dr. U. Birkenheuer* was appointed as his successor in March 2000. *Dr. K. Richter* soon afterwards also accepted the offer of a chair for Theoretical Physics at the University of Regensburg. This concluded the Junior Research Group *Quantum Chaos and Mesoscopic Systems*. To continue the successful work in this research field with modified premises, *Dr. H. Schomerus* (Leiden) was appointed as head of a new Junior Research Group *Waves in Complex Media and Mesoscopic Phenomena* in November 2000.

2001-2002 • To account for the increasing demand for building bridges between physics and biology, *Dr. F. Jülicher* (Paris) was appointed as head of the third division *Biological Physics* in 2001. Shortly afterwards, two research groups on *Physics of Biological and Soft Matter* headed by *Dr. R. Everaers* (Mainz), and *Biological Physics of Olfaction: From Genes to Networks* headed by *Dr. M. Zapotocky* (New York) started their activities within the third division in 2002. The division *Finite Systems* also continued to broaden its research spectrum by appointing *Dr. A. Becker* (Bielefeld) as head of the new research group *Nonlinear Processes in Strong Fields* in 2002.

2003-2004 • In 2003 *Dr. S. Kümmel* (New Orleans) started the activities of an Emmy Noether-Group *Electronic Structure of Finite Systems*. It was followed in 2004 by setting up a Junior Research Group *Physics of Cell Division* headed by *Dr. K. Kruse* (Dresden). His group was the first of three research groups within a joint research program *Physics of Biological Systems* initiated together with the Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. A second Junior Research Group *Mechanics of Cell Division* of this joint research program was started at the end of 2004 by *I.M. Tolić-Nørrelykke* (Firenze) who works experimentally at the MPI-CBG. The construction of an extension to the institute building was started in the year 2004. *Dr. M. Bär* took up a position as a department head at the Physikalisch-Technische Bundesanstalt in Berlin in the fall of 2004.

2005-2006 • In 2005 *Dr. S. Kümmel* accepted a professorship at University of Bayreuth, and *Dr. H. Schomerus* accepted a faculty position at Lancaster University. *Dr. M. Hentschel* (Regensburg) started the activities of an Emmy Noether group *Many Body Effects in Mesoscopic Systems*. *Dr. S. Grill* (Berkeley) completed the joint research program of the mpi**pks** and the MPI-CBG by starting the Junior Research Group *Motor Systems*. His group is affiliated with both institutes and does both theoretical and experimental work. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* started operation in 2005. It attracts PhD students from many countries and is operating jointly with the Technical University Dresden, the Max Planck Institute for Chemical Physics of Solids, the Leibniz Institute for Solid State and Materials Research Dresden, the Forschungszentrum Rossendorf, the Institute for Low Temperature and Structure Research at the Polish Academy of Sciences Wroclaw, the Institute of Organic Chemistry and Biochemistry Prague, and the Institute of Chemical Technology Prague. The new wing of the institute was completed at the end of 2005. It provides new office space and a new seminar room. In 2006, *Dr. K. Kruse* and *Dr. R. Everaers* accepted professorships at the University of Saarbrücken and the École normale Supérieure in Lyon.

2007-2008 • During this period *Prof. P. Fulde* retired from his position as a director of mpi**pks** and as the head of the department *Electronic Correlations*. *Prof. R. Moessner* was appointed as a new director, and started to set up his department *Condensed Matter* in the beginning of 2008. *Dr. A. Becker* accepted the offer of a JILA fellow together with a faculty position at the University of Colorado, *Dr. A. Buchleitner* took the chair for quantum optics and statistics at the University of Freiburg, and *Dr. M. Zapotocky* moved to a permanent position at the Institute of Physiology of the Czech Academy of Sciences. In return, several new groups were installed. In 2007 *Dr. T. Gross* joined mpi**pks** to head the junior research group *Dynamics of Biological Networks*, and *Dr. B. Lindner* set up the activities of the research group *Stochastic Processes in Biophysics*. In the same year, *Dr. S. Skupin* started his junior research group *Computational Nonlinear and Relativistic Optics*, with close links to the Forschungszentrum Rossendorf. In 2008 the research group *Complex Dynamics in Cold Gases* was founded and headed by *Dr. T. Pohl*, and the research group *New States of Quantum Matter* was founded and headed by *Dr. A. Läuchli*. In the end of 2008 *Dr. S. Kirchner* came to mpi**pks** to head the junior research group *Collective Phenomena in Solid State and Materials Physics* which is operating jointly with the neighboring Max Planck Institute for the Chemical Physics of Solids.

2009-2010 • In 2009 *Dr. K. Hornberger* arrived at mpi**pks** to head the research group *Molecular Quantum Optics*. In the following year 2010 *Prof. R. Ketzmerick* (TU Dresden) was appointed by the Max Planck Society as a *Max Planck Fellow* and started activities of the Max Planck Fellow group *Chaos and Quantum Chaos* at mpi**pks**. Recently *Dr. E. Altmann* arrived to set up the Otto-Hahn group *Dynamical Systems and Social Dynamics*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* was successfully renewed for a second six year period.

The institute hosts approximately 100-150 long-term guest scientists at any given time, together with 1200-1500 short-term guests who annually participate in the workshop and seminar program. The new wing of the institute has quickly turned into a new and vibrant focal point of meetings, poster sessions, discussions and collaborations.

The Board of Trustees has supported the work of the institute since 1995, thus providing important connections to the State, the City and the Academia. The research activities of the institute have been accompanied by a Scientific Advisory Board since June 1996.

1.2 Research Areas and Structure of the Institute

The research of the institute in the field of the physics of complex systems ranges from classical to quantum physics and focuses on three main areas, which correspond to the activities in the three divisions:

- With the help of semiclassical methods, the division *Finite Systems* headed by *Prof. Rost* focuses on the nonlinear dynamics of atoms, molecules and clusters.
- The division *Biological Physics* headed by *Prof. Jülicher* studies biological systems with tools of statistical physics and nonlinear dynamics.
- The division *Condensed Matter* headed by *Prof. Moessner* studies the classical and quantum statistical mechanics of condensed matter.

Furthermore, four research groups broaden and strengthen the work of the corresponding divisions. Additional groups interpolate with their research between and add to the above listed research topics, and establish research links with other institutions:

- The Emmy Noether Group *Many Particle Physics in Mesoscopic Systems* is headed by *Dr. Martina Hentschel*. It bridges work between the divisions *Electronic Correlations* and *Finite Systems*.
- The Junior Research Group *Computational Nonlinear and Relativistic Optics* is headed by *Dr. Stefan Skupin* and links the work of mpi**pks** with the Forschungszentrum Rossendorf.
- The Junior Research Group *Collective Phenomena in Solid State and Material Physics* is headed by *Dr. Stefan Kirchner* and bridges the research work between mpi**pks** and the Max Planck Institute for Chemical Physics of Solids.
- The Max Planck Fellow group *Chaos and Quantum Chaos* is headed by *Prof. Roland Ketzmerick* (TU Dresden) and links the research work at mpi**pks** with the Technische Universität Dresden.
- The Otto-Hahn group *Dynamical Systems and Social Dynamics* is headed by *Dr. Eduardo Altmann*. It interpolates research between mpi**pks** and the Technische Universität Dresden.
- The only permanent research group, headed by *Prof. Kantz*, is working on *Nonlinear Time Series Analysis*. Here, methods are applied and developed, related to various aspects of classical chaos, which play an important role also for research on semiclassical topics.

Finally, a joint research program *Physics of Biological Systems* of the mpi**pks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) comprises three closely interacting Junior Research Groups. These joint research groups build a close link between both institutes to promote collaborative work on the physics of cells:

- The Junior Research Group *Dynamics of Biological Networks* is headed by *Dr. Thilo Gross* and operates at mpi**pks**.

- The Junior Research Group *Motor Systems* is headed by *Dr. Stephan Grill*. It is affiliated with both institutes and works both theoretically and experimentally.
- A third experimental Group *Interior Design of the Cell* headed by I.M. Tolić-Nørrelykke is located at the MPI-CBG.

1.3 Workshop and Visitors Program

Central to the mission of the institute is to conduct international *Workshops and Seminars* (p. 112), which makes mpi**pks** an almost unique institute within the Max Planck Society, only comparable with the mathematics institute in Bonn. A small but efficient group of staff headed by *Dr. S. Flach* is responsible for the logistics and the preparation of meetings, and gives advice and support to the (usually external) scientific coordinators on the various aspects of planning and conducting the corresponding event.
The *Visitors Program* (p. 101) offers research visits ranging from a few weeks to two years in duration. Guest scientists use various ways of collaboration by joining research groups at the institute, by doing joint research with other guest scientists, or by starting collaborations with workshop and seminar participants. Further possibilities of collaboration include contacts with the TU Dresden or other local research institutions, well documented, e.g., by common publications (see p. 161).
Proposals for workshops and seminars, as well as applications for guest scientist positions, are evaluated by two different committees. Members of each committee include both external scientists and scientists of the institute.
In order to further strengthen and structure the Visitors Program, mpi**pks** started in 2000 annually to award the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist. The awardees *Prof. S. Aubry* (Saclay) 2009 and *Prof. Y. Kevrekidis* (Princeton) 2010 have spent up to one academic year at mpi**pks** (p. 108).
mpi**pks** also offers one *Distinguished PKS Postdoctoral fellowship* annually. It aims at excellent young researchers, shortly before accepting a tenure track position (p. 102).
In 2007 *Advanced Study Groups* were launched at mpi**pks**. These groups consist of 3-5 experienced researchers, who join forces to do cutting-edge research on a topic from the field of the physics of complex systems. In the year 2009 we hosted the group *Quantum Aggregates* under the leadership of *Prof. J. Briggs*. In the following year 2010 we hosted two large groups. *Dr. M. Zhitomirsky* headed the group *Unconventional Magnetism in High Fields*, and *Prof. G. C. Hegerfeldt* coordinated the activities of the group *Quantum Thermodynamics of Finite Systems*.
The success of our workshop program has led to a new joint program of mpi**pks** with the *Institute for Cross-Disciplinary Physics and Complex Systems (IFISC)* in Palma. Initiated for three years (2008-2010) we conducted workshops in Palma and Dresden, which focus on the theme of the joint program *Trends in Complex Systems* (p. 112).

1.4 Teaching and Training

The institute aims at a broad and far reaching education of young scientists in research, teaching and the organization of research.
Teaching • Standard lecture series are conducted by institute members, both at the TU Dresden and at other universities (p. 147). In addition, the public relations sector of our institute offers institute members possibilities to teach and lecture for high school teachers and high school students, both at mpi**pks** as well as at high schools (p. 151).
International Max Planck Research School • Since 2005 our institute has been running the IMPRS *Dynamical Processes in Atoms, Molecules and Solids* together with the Technical University Dresden, the Max Planck Institute for Chemical Physics of Solids, the Leibniz Institute for Solid State and Materials Research Dresden, the Forschungszentrum Rossendorf, the Institute for Low Temperature and Structure Research at the Polish Academy of Sciences Wroclaw, the Institute of Organic Chemistry and Biochemistry and the Institute of Chemical Technology at Prague. It attracts PhD students from many countries and offers a well-structured PhD training with a large program of lecture courses. Finally mpi**pks** participates in the IMPRS *Molecular Cell Biology and Bioengineering* of the MPI for Cell Biology and Genetics.
Research Organization • The large-scale Workshop and Seminar Program at mpi**pks** offers the unique

possibility for young scientists to take part in the organization of meetings. Out of the 44 events during 2009-2010, young scientists of the institute took part in the coordination of 8. This has a positive educational effect for young scientists, and helps the external coordinators through the permanent contact with a local scientific coordinator.

1.5 Equal Opportunities

Over the last years we were able to increase the percentage of female researchers to 10% of all postdocs and 20% of all predocs holding a contract of more than three months. In addition to the standard measures of ensuring equal opportunities, mpi**pks** participates in the scientific activities on the annual *Girl's Day* and invites female students from high schools to informative lectures and discussions about a career in science. In order to meet the needs of researchers with young children we have created in guest house 3 a *mother & child* apartment, of course also available to fathers with their young kids. Together with an offer for daycare, we have been able to attract several young participants, who could join the scientific program of workshops while their children were looked after in the guest house. This apartment, when not booked for workshop participant purposes, is also available and frequently used by members of mpi**pks** when they need to be accompanied by their young children during working hours in case of an emergency (e.g. sickness in the family or the day care).

1.6 Public Relations

The institute considers itself as a platform for the emergence, exchange, development and promotion of creative ideas in research. While mainly focusing on scientists, this also includes potential future scientists, i.e., high school students, teachers, as well as the general public interested in science. Within our school-contact-program we offer lectures at schools in order to spread the fascination of science as it happens.
Since 1999, mpi**pks** has coordinated, together with the TU Dresden and the City of Dresden, the lecture series *Science in the City Hall*, aimed at promoting public interested in science. Well-known scientists are invited to give lectures for the broad public, which are intended to popularize modern research (p. 150). Furthermore, coordinators of workshops are encouraged to offer a public evening lecture at mpi**pks** in the course of the workshop. Since 2006, when Dresden was awarded the title 'Stadt der Wissenschaft 2006', mpi**pks** has participated in numerous activities which are part of the annual program of the scientific community of Dresden.
In 2007 we initiated the program *Dresden Journalist in Residence* in which the two other MPIs in Dresden also participate (p. 151).

1.7 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment, formed by the TU Dresden and the many other research institutes which surround it. An intensive scientific dialogue with the Physics Department of the TU Dresden takes place, e.g., with regular joint seminars (*Quantum Dynamics* with Prof. Schmidt), with the Max Planck Fellow group *Chaos and Quantum Chaos* headed by *Prof. R. Ketzmerick*, and through a collaboration with Prof. Schwille. mpi**pks** has particular close contacts to the Institute of Theoretical Physics and the Institute of Biophysics at the Physics Department. Institute members are involved in various Research Focus Programs (p. 145). The division *Electronic Correlations* was, and the division *Condensed Matter* is cooperating with the IFW (Institut für Festkörper- und Werkstoffforschung) and with the neighboring Max Planck Institute for Chemical Physics of the Solid State. In particular, both institutes jointly run the Junior Research Group *Collective Phenomena in Solid State and Material Physics* headed by *Dr. S. Kirchner*. The division *Biological Physics* has established close contact to the Max Planck Institute of Molecular Cell Biology and Genetics. There are also intense collaborations with the Biotechnological Center and the newly founded Center for Regenerative Therapies. The divisions *Finite Systems* and *Condensed Matter* cooperate closely with the Research Center Rossendorf, in particular through joint research conducted by the Junior Research Group *Computational*

Nonlinear and Relativistic Optics headed by *Dr. S. Skupin*. This group also cooperates closely with the faculty of physics and astronomy at the Friedrich-Schiller University in Jena, where *Dr. S. Skupin* holds a *Carl Zeiss Junior Professorship for Computational Photonics* since 2009.
National and International • The many different national and international collaborations and contacts are listed in the research group reports below. Furthermore, the institute has a small budget for collaborations with experimental groups (p. 110).

1.8 Departments and Research Groups

Division: Finite Systems
(Head: Prof. Dr. J. - M. Rost)

The department *Finite Systems* studies the dynamics of finite microscopic systems in different environments. One class of environment consists of similar systems as the atom or molecule under consideration (e.g., clusters, quantum aggregates, ultracold Rydberg gases). Strong light pulses form another quite universal type of environment.

The fundamental and formal mathematical aspects of finite systems coupled to an environment and specifically the phenomenon of decoherence has been investigated by *Klaus Hornberger* and his research group. The effect of an ultracold environment on atoms, in particular on many-body Rydberg dynamics, is in the focus of *Thomas Pohl's* research with his group on *Complex Dynamics in Ultracold Gases*.

The research group *Finite Systems* within the department concentrates on clusters (project leader *Ulf Saalmann*), quantum aggregates (project leader *Alexander Eisfeld*) and the interaction of finite systems with strong and short light pulses, inspired by rapid technological development towards ultrashort pulses (attosecond science) and short X-ray pulses (X-ray Free Electron Lasers). Fruitful synergy emerges from the relation between exciton dynamics in traditional quantum aggregates and their counterpart in the context of ultracold Rydberg complexes.

Research topics

Basic coupling mechanisms of short XUV pulses to matter We explore non-equilibrium multi-particle dynamics of ions and electrons triggered by intense sub-femtosecond light absorption. Almost simultaneous absorption of many photons by many bound electrons has become feasible with 4th generation light sources and could be possible with attosecond sources given a strong resonant absorption, e.g., in xenon.

Charge migration in finite systems is a universal result of energy absorption in an extended system. Its consequences, apart from collectivity, are rarely explored as coordinated multi-electron dynamics since – far from equilibrium and often happening on a short time scale – it is difficult to access, experimentally and theoretically.

If X-ray pulses irradiate a cluster of atoms, inner shell electrons are removed ("photo-electrons"), and the large space charge created, leads to field ionization of atomic outer-shell electrons. These electrons can screen a fraction of the ions reducing their repulsion and therefore, their motion, which is crucial for single molecule imaging, an important future application of X-FEL radiation. Recently we have investigated an alternative to reduce the effect of the large space charge: Instead of supplying screening electrons, one can think of removing positive charge by transferring electrons from light elements (hydrogen) to heavier elements so that the light bare H^+ leave the complex and reduce thereby the space charge. Prototypical systems are clusters of CH_4.

Time-resolved electron transport Only recently time-resolved studies in quantum dots have become possible. We are interested in the time-dependent response of interacting electrons in single or double dot systems coupled to contacts. In particular pump-probe scenarios – standard tools in atomic and molecular physics – have been hardly considered for quantum transport. Having developed especially efficient propagation schemes, we have followed the coherent time evolution of electrons in double quantum dots induced by fast bias-voltage switches. Such devices have the potential for a controlled

manipulation of charge qubits. Taking Coulomb interactions into account, we have also investigated non-adiabatic charge pumping through single-level quantum dots which may be used to produce quantized currents for metrological purposes.

Ultracold Rydberg dynamics An ultracold environment harmonizes perfectly with Rydberg dynamics with its inherently small energy scale. Consequently, this field has gained enormous momentum recently, holding hopes for information science and offering very flexible possibilities to design and investigate condensed matter like systems of very different character. In most applications the focus is on electron dynamics with the atomic motion as an annoying but unavoidable fact. In contrast we concentrate on the interplay of electronic and atomic motion akin to chemical dynamics.

We have found that this interplay produces surprising dynamical features such as internal quantum reflection in Rydberg dimers (bound systems formed with a ground state and a Rydberg atom), or abundant conical intersections in an ultracold Rydberg gas. With Rydberg dressing only a small admixture of Rydberg character is added to the electronic ground state wavefunction, producing very stable poly-atomic systems with well defined geometries in a trap. This allows one to study archetypical molecular situations, e.g., a conical intersection not influenced by other channels as in a standard molecule. Ultracold trapped Rydberg atoms may also be prepared together with ground state atoms such that they form a system with properties of quantum aggregates. While in traditional aggregates, the position of the atoms is hardly controllable, this can be achieved in the ultracold realization by entangling atomic motion and electronic excitation. Thereby, we have found an efficient way to transport electronic entanglement and coherence along an atomic chain, akin to Newton's cradle in the classical case.

Quantum aggregates Self-organized aggregates of dye molecules are versatile quantum systems with applications in photography, opto-electronics, solar cells, photo-biology and as supra-molecular fibers. In addition, new types of quantum aggregate have emerged: e.g. assemblies of ultra-cold Rydberg atoms, as discussed above, "molecules" and "crystals" composed of quantum dots or arrays of nano-size metallic particles.

For aggregates embedded in a glassy host we have found that static disorder strongly influences the optical and transfer properties (Anderson localization). A broadening of the absorption spectrum upon aggregation occurs for stable Levy disorder. This is in contrast to a strong narrowing which follows from the commonly assumed Gaussian disorder.

For a Helium-nanodroplet as an environment it has turned out that a proper inclusion of internal vibrational modes is essential to explain measured aggregate spectra of the organic semiconductor PTCDA.

Perspectives for the future

With additional FEL sources coming on line and more users getting interested, the general emphasis in theoretical research shifts towards simulation of specific situations and experiments. In contrast to this trend we will continue to concentrate on general principles of interaction and their simple formulation for light-matter interaction in the attosecond- and XUV- as well as X-ray-short pulse parameter regime, including the development of simplified models for a better understanding, such as the concept of Coulomb complexes.

Our approach to describe large molecules or clusters under short pulses has been so far based on the classical motion of all charged particles where the activation of these particles through photons is modeled by rates since due to the wavelength, the light does not resolve bound orbital structure for IR down to VUV radiation. This changes for XUV to X-ray radiation where we plan a more detailed formulation with the help of the coherent state approach. It offers formally a quantum framework but still based on classical trajectories.

We are only beginning to understand the phenomena of exciton dynamics coupled to atomic motion in the context of ultracold Rydberg aggregates. The great flexibility of ultracold Rydberg systems and the possibility for experimental realization offer a wide potential which can be developed in various directions, several of which we follow in the department with *Thomas Pohl* and his research group as well as parts of the *Finite Systems* research group. In the latter we will concentrate on developing an understanding how transport of coherence and entanglement can proceed over many sites in large ultracold Rydberg networks. Due to the universal character of dipole-dipole forces, such an understanding will give us a

handle to address the same question in large molecular networks which has recently become of great interest, e.g., for light harvesting complexes.

Cooperations

With experimental groups
We have active collaborations with

- Prof. Stienkemeier (Freiburg) regarding molecular aggregates in helium nano-droplets,
- with Profs. Berrah (Kalamazou, USA) regarding photo ionization of fullerenes and fulllerene negative ions,
- with Thomas Möller (Berlin) related to cluster experiments at the two FELs in Hamburg and Stanford.
- A close interaction via the *Max Planck Advanced Study group at the Center for Free Electron Laser Studies* has been established with Prof. Ullrich (Heidelberg).

With theoretical groups (some examples):

- on STM image maps of metallic carbon nanotubes with M. Garcia (Kassel, Germany)
- on noise in quantum systems with K. Singh (Mohali, India)
- on semiclassical theory with A. Ozorio de Almeida (Rio, Brazil)
- on photo processes in endohedrals with H. Chakraborty (Maryville, USA) and S. Manson (Atlanta, USA)
- on quantum aggregates with V. Malyshev (Groningen, Netherlands).

Local cooperations
The interaction with Prof. Schmidt's group from the TU Dresden has intensified with a well defined research program concerning quantum-classical mixed description in all degrees of freedom of small systems (atoms and molecules) in strong laser fields. With Dr. Großmann from the TU Dresden we enjoy a productive collaboration on *semiclassical propagation techniques* which will be expanded to include coherent state methods in quantum formulations. Also, a collaboration on quantum aggregates exists with Prof. Strunz, TU Dresden.

Research Group: Molecular Quantum Optics
(Head: Dr. Klaus Hornberger (since 11/09))

The group was established in November 2009; it currently hosts two PhD students (T. Fischer, F. Platzer), two postdocs (C. Gneiting, A. Jacob), an associated guest scientist (S. Tesfa), and an associated postdoc (K. Härkönen).

A main goal of our research is to investigate systems and phenomena that lie in the transient region between classical physics and the quantum regime. Based on the theory of open quantum systems we are studying to what extend one can understand the emergence of classical physical properties and the laws of classical physics if one views quantum theory as universally valid. These questions arise naturally if one deals with the dynamics of ever larger molecules as they interact with their natural environment. The increasing complexity of such quantum objects makes it impossible to use a complete microscopic description, forcing us to identify the general principles and mechanisms behind the quantum-to-classical transition. In parallel to this, we are developing experimentally realizable proposals to probe the boundary region between quantum behavior and classical physics, and to verify quantum phenomena at scales that have not been reached so far. This includes demonstrating the wave nature of ultra-massive particles, such as large metal clusters, by means of a near-field interference effect, as well as establishing entanglement with respect to macroscopically distinct properties of quantum systems.

Matter wave interference with complex molecules In collaboration with the experimental group around M. Arndt at the Univeristy of Vienna, we have been devising novel near-field interference schemes. They are targeted to work with particles of extremely high mass, corresponding to de Brogle wave lengths in the sub-picometer range. The latest development, the Kapitza-Dirac-Talbot-Lau interferometer, features a standing light wave as a central optical element in a near-field diffraction setup. It already established the wave nature of objects with masses exceeding 1600 proton masses and sizes exceeding 30Å. Our studies suggest that it should be possible to demonstrate interference with metal clusters of masses on the order of 10^6 atomic mass units. Since the coupling of the center of mass motion to rotational and internal degrees of freedom may start to play a role at these scales, we are currently studying what consequences such interactions will have on the visibility of interference fringes.

The paradox of molecular chirality It is not obvious, due to the parity invariance of the molecular hamiltonian, how to understand from first principles why large molecules often show up as enantiomers, i.e. in a chiral configuration which cannot be brought into congruence with its mirror image. We showed that this phenomenon, which is often viewed as a paradigm for the emergence of classical properties from the underlying quantum theory, can be explained as the result of specific environmental interaction processes. We also proposed an experiment for testing our quantitative predictions. It relies on earlier ideas of using lasers to split a racemic molecular beam into jets of left- and right-handed molecules. Since these proposals do not account for the potentially detrimental effect of molecular rotation, we are currently investigating its consequences by incorporating the orientation dynamics.

In another research project related to the rotation dynamics of extended bodies we study whether environmental interactions can explain how the classical non-linear Euler equations of motion for the orientation state come about. As a first step towards this, we constructed a Wigner-Weyl phase space representation of the rotation states of an asymmetric top molecule.

Incoherent control by measurements Coherent techniques of quantum control prove to be increasingly difficult when applied to large quantum systems such as poly-atomic molecules. As a way around this we are investigating how the incoherent dynamics induced by continuous monitoring can provide a more robust means of steering quantum dynamics towards desired target states. Our first results demonstrate the potential use of non-selective measurements of position or, more generally of configurational molecular degrees of freedom, for the optimization of transition probabilities.

Spatial entanglement of material particles Experimental demonstrations of entanglement between non-interacting material objects so far only involve internal degrees of freedom. We have developed methods and worked out experimental scenarios for establishing non-local quantum correlations in the state of motion of far separated free particles. A specific experimental proposal is based on the judicious Feshbach dissociation of a molecular Bose-Einstein condensate of fermionic lithium atoms. This admits a Bell test to establish that the entangled properties, the positions of each particle, are macroscopically distinct.

Cooperations

- M. Arndt (Universität Wien, Austria) and his experimental group on interference phenomena with large molecules and metal clusters
- H.-P. Breuer (Universität Freiburg) on quantum Monte Carlo methods for solving Markovian quantum dynamics
- J. Madroñero (Technische Universität München) on a complex scaling application to open quantum systems
- S. Nimmrichter (Universität Wien, Austria), a co-supervised PhD student, on the theory of molecular near-field interference
- H. Ulbricht (University of Southampton, UK) on molecular interference experiments, in particular the influence of grating wall dispersion forces
- B. Vacchini (Università di Milano and INFN Sezione di Milano, Italy) on the derivation and the properties of the quantum linear Boltzmann equation

Research Group: Complex Dynamics in Cold Gases
(Head: Dr. T. Pohl)

The group was established in September 2008, and currently hosts three PhD students (Georg Bannasch, Nils Henkel, Rick Mukherjee) and two postdoctoral guest scientists (Sevilay Sevinçli, Rejish Nath). Our research is centered around the behavior of cold and ultracold atomic gases. In particular, we are interested in their response to laser radiation, which may cause correlated, many-body dynamics to emerge directly as atoms are ionized or excited to high lying states. As outlined below, the understanding of this process and the back-and-forth interaction between light and correlated matter raises rather diverse questions, and opens up promising avenues for applications in optical and information science.

Ultracold plasmas, formed by photoionization of laser-cooled atoms, occupy an exotic parameter regime of plasma physics in which the potential energy greatly exceeds the thermal energy of the charges. Such plasmas are created far from equilibrium, and, thus, provide an ideal platform to study non-equilibrium phenomena in strongly correlated Coulomb systems. We have developed efficient microscopic approaches to study atomic reactions, relaxation processes and collective phenomena under such strong coupling conditions. Further we are exploring the utility of laser light to probe and even control the plasma dynamics. Parts of this work is being done in a joint theoretical-experimental effort with the group of Prof. T.C. Killian at Rice University, USA.

Bose Einstein condensates of long-range interacting particles are another focus of our research activities. Recently, we considered off-resonant laser coupling to high-lying Rydberg states as a means of overcoming the lifetime-limitation set by excited state decay. At the same time, such a "Rydberg-dressing" produces a peculiar effective interaction, featuring long-range tails and a soft core at small distances, which prevents condensate collapse, as otherwise occurring dipolar condensates. We have shown that this approach provides a promising physical setting to realize a continuous supersolid state in ultracold atoms and allows to create entirely self-trapped structures, i.e. three-dimensional bright solitons, for the first time in Bose Einstein condensates. While these results are largely based on a mean-field description, we recently started to explore effects of thermal and quantum fluctuations, within a collaboration with the group of Prof. Peter Zoller (Innsbruck University). Future work, will address collective interactions, arising from higher-order correlations between dressed excitations, and rotating systems, which suggest an interesting competition between supersolid ordering and the emerging Abrikhosov-lattice of vortices due to the rotation.

Optical lattices, filled with ultracold atoms, have become a remarkably versatile toolbox to address fundamental condensed matter physics problems. A paradigm example are Hubbard-type models, where atoms tunnel between adjacent lattice sites and feature local onsite interactions. In an effort to extend such settings to long-range interacting systems, we have worked out a scheme for strong magic-wavelength trapping of ground- and Rydberg-states, that exploits the availability of two valence electrons in alkaline-earth atoms. This combination of tight lattice confinement and strong state-dependent interactions, for example, provides an essential pre-requisite for implementations of digital quantum simulators and scalable quantum computers. Among next steps, we currently study a novel approach for controlled Rydberg-state-enabled charge transport in such an alkaline-earth lattice and explore suitable, robust protocols for the generation of non-classical many-body states in Strontium Rydberg-atom lattices, which may provide an entanglement-resource for applications in high-precision frequency metrology.

Nonlinear optics is commonly based on higher order light-matter interactions, such that the resulting nonlinearities are often of perturbative nature. In this respect, the combination of slow-light techniques and strongly interacting Rydberg states in an ultracold gas promises new perspectives for the field, which, only recently, have attracted increased experimental and theoretical interest. In the past few years, we have developed complementary numerical methods as well as analytical approaches that allow to study this problem. Our calculations provide an excellent description of recent experiments and reveal a universal scaling relation that illuminates the origin of the optical nonlinearities, emerging from the highly correlated light-driven gas dynamics. We predict giant nonlinear susceptibilities that are many orders of magnitude larger than realized in other optical media, which could make several applications, such as few-photon optical switches, possible. Having established a theory for the optical response of an ultracold

interacting gas, future work will address the propagation of light in such a medium, which suggests a rich nonlinear dynamics driven by strong and highly nonlocal Rydberg-state-induced interactions.

Quantum optics. The above results, i.e. the tremendous enhancement of optical nonlinearities in cold Rydberg gases, also holds great promise for applications in quantum optics. In a recent collaboration with the groups of Prof. Mikhail D. Lukin (Harvard University) and Prof. Michael Fleischhauer (University of Kaiserslautern) we approach this question by considering the dynamics of two-photon pulses under conditions of electro-magnetically induced transparency (EIT). Here, we could show that the strong atomic interactions map onto effective photon interactions of unprecedented strength, which, in turn, permits to entangle single photons with atoms, to perform two-photon phase gates and to realize deterministic single-photon sources, with current experimental capabilities. Generally, the propagation of multi-photon fields in interacting EIT media, including the quantum nature and spatial propagation of light, poses a challenging many-body problem, for which an appropriate theoretical framework is yet to be developed. In this respect, our results for the two-excitation dynamics provide important intuition for understanding the full quantum many-body problem, which will be tackled in future work.

Cooperations

In the past few years we have initiated and continued fruitful collaborations with the experimental groups of

- Prof. Thomas C. Killian (Rice University, USA) on relaxtion processes in ultracold plasmas
- Prof. Matthias Weidemüller (University of Heidelberg, Germany) on coherent population trapping
- Prof. Charles S. Adams (Durham University, UK) on nonlinear light absorption in cold Rydberg gases
- Dr. Matthew Jones (Durham University, UK) on ultracold Strontium gases

and have established theory collaborations with the groups of

- Prof. Peter Zoller (University of Innsbruck) on lattice formation in rotating Bose-Einstein condensates
- Prof. Mikhail D. Lukin (Harvard University, USA) and
  Prof. Michael Fleischhauer (University of Kaiserslautern, Germany) on photonic phase-gates
- Prof. Mark Saffman (University of Wisconsin, USA) and
  Prof. Wieslaw Królikowski (Australian National University) on selftrapping of matter-waves

Division: Biological Physics
(Head: Prof. Dr. F. Jülicher)

The department Biological Physics studies active dynamic phenomena in cells and tissues. From the point of view of physics, biological systems represent a highly organized and inherently dynamic form of condensed matter. This living matter is active and can exhibit spontaneous movements and flows, oscillations, as well as unusual material properties. On a large range of length and time scales self-organized processes take place.

Patterns in space and time emerge from the collective behaviors of many subunits on smaller scales (e.g. molecules and molecular aggregates in cells and cells in tissues). These subunits are coordinated by mechanical coupling but also by molecular signaling systems in the cell. Methods and concepts from statistical physics, non-equilibrium physics as well as nonlinear dynamics are the basis of our theoretical approaches to understand the dynamics of living matter.

In addition to the study of physical principles which play a key role in cells and tissues, current problems of cell and developmental biology are studied theoretically in close cooperation with biologists. These

projects aim at a theoretical and quantitative description of biological processes (e.g. cell locomotion, cell division, pattern formation in cells and tissues). The goal is to develop novel methods and concepts to unravel the function and organization of living systems.

The department Biological Physics started its activities in 2002. The research of our department is characterized by many close interdisciplinary cooperations with experimental groups. Most important is a close cooperation with the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. This cooperation is organized around a joint research program on "Physics of Biological Systems" which consists of three research groups that are affiliated with both institutes. A rich variety of collaborative projects exist in the context of this research program. Our group is also linked to the International Max-Planck Research School on Cell Biology, Bioengineering, and Biophysics, managed by the MPI-CBG. In addition, our group has intense collaborations with the Institut Curie in Paris and the AMOLF in Amsterdam in the context of a European Associate Laboratory.

Current research topics include:

Physics of active fluids and gels. Cellular dynamics is an important example of the behaviors of active matter. In collaboration with the Institut Curie in Paris, we develop hydrodynamic theories of active fluids and gels. Spatial anisotropies in incompressible active gels lead to rich physics. Active gels represent a paradigm for the dynamics of the cell cytoskeleton. In this case, the multicomponent character of the system becomes important. Furthermore, active chiral processes give rise to interesting dynamics with broken symmetries that are relevant for biology. The concept of active gels also plays a role for the study of tissue dynamics on large scales.

Physics of cells. Cells are highly dynamic systems as exemplified by cell locomotion or cell division. Cell division is a spatiotemporal process by which a cell is physically divided in two daughter cells. An important situation is the case where cell division is asymmetric and leads to two different daughter cells. Our work focusses on the dynamics and spatial organization of the mitotic spindle and the centrosome and on flows and transport processes that occur during cell division. Recently, we have shown that liquid-liquid phase separation leads to the formation of highly dynamic fluid drop-like objects in the cytoplasm. This is a novel physical principle by which the cell cytoplasm is spatially organized.

Dynamic organization and patterning of tissues. A paradigm for the formation of patterns and morphologies in tissues is the problem of vertebrate segmentation. This process, which forms the precursors of the segmented vertebrate structure, is based on cellular genetic oscillations which interact via molecular signaling systems. As a result, a collective spatio-temporal pattern of gene activity emerges that subsequently gives to the segments. Our work has shown that time delays in the oscillator coupling are key to understand the collective behaviors of oscillating cells. Key predictions of our theory could be observed in recent experimental studies.

An important model system for the patterning of tissues during the development of organisms are epithelia, which are two dimensional tissues. In recent years we have intensely studied the development of the fly wing which is an important model system for the patterning of two-dimensional tissues. A key result was the finding that large scale polar order in the plane of the wing is organized by cell flow patterns. These cell flows couple to polarity via their shear and rotational components.

Cell locomotion and swimming. Many cells can move on solid surfaces or swim in fluids. These movements are generated in the cell cytoskeleton, in particular by the activity of molecular motors. We study fundamental aspects of self-propulsion of cells but also of artificial systems, as well as the question of how swimmers can steer towards a target. A simple artificial swimmer is a colloidal particle which locally catalyzes a chemical reaction on its surface. The generic physics that allows such a chemical motor to swim provides a beautiful example of active interfacial processes that generate fluid flows. Similar surface flows are ubiquitous in biology.

Physics of hearing. Hair cells are highly sensitive mechanosensors which in our ears transduce sound vibrations to electrical signals. Our ear is able to operate over a vast dynamic range of 12 orders of magnitude and to detect extraordinarily weak stimuli. This is achieved by active processes which perform nonlinear frequency-selective amplification. This cochlear amplifier is based on the generic properties of dynamic oscillators. However, the exact identity of the amplifier is still under debate. In the mammalian cochlea, both spontaneous hair bundle movements and hair cell electromotiliy are likely important elements of the amplifier. We are studying the interplay of active processes in the cochlea on

scales ranging from individual hair cells to the ensemble of hair cells lined up along the basilar membrane to investigate the nature of the cochlear amplifier.

Perspectives. The close collaboration between the mpi**pks** and the MPI-CBG has in recent years stimulated many new research projects between physics and biology. The goal of this research is to develop quantitative and theoretical approaches to understand dynamic processes in cells and tissues. In order to expand and further develop these activities, the Max Planck Society is currently planning to create a *Center for Systems Biology of Cells and Tissues* in Dresden that is jointly operated by the two institutes. It is planned to hire additional research group leaders as well as a new director at MPI-CBG. The new center will integrate theoretical activities with experimentalists. A novel research activity that will be attracted to the new center is image informatics which complements the existing activities between theoretical physics and biology. By combining experimental biology with theoretical physics and computer science, the activities in Dresden will be significantly strengthened. This will also allow us to move towards new challenges such as the study of the dynamics of cells and tissues in three dimensions.

Cooperations

- Max Planck Institute for Molecular Cell Biology and Genetics, Dresden
  - Collaboration with the groups of Jonathon Howard, Anthony Hyman and Stephan Grill on cell division, cellular pattern formation and dynamics.
  - Collaboration with Suzanne Eaton and Christian Dahmann on the dynamic organization of epithelia.
  - Collaboration with Andy Oates on the segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns.
  - Collaborations with Ewa Paluch on active cell mechanics and cell adhesion.
  - Collaboration with Marino Zerial on the dynamics of endosomal transport and signaling networks in cells.
  - Collaboration with Stefan Diez on the collective behaviors of molecular motors.
- Institut Curie, Paris
  - Collaboration with Jean-Francois Joanny and Jacques Prost on the physics of active gels, the dynamics of the cytoskeleton and cell locomotion.
  - Collaboration with Pascal Martin on the physics of mechanosensory hair cells.
- AMOLF, Amsterdam
  - Collaboration with Marileen Dogterom on cytoskeletal dynamics.
- University of Geneva
  - Collaboration with Marcos González-Gaitán on the dynamics of morphogens in growing tissues and their role in growth control.
- Stanford University, USA
  - Collaboration with Julie Theriot on oscillations in cell locomotion.

Research Group: Stochastic Processes in Biophysics
(Head: Dr. Benjamin Lindner)

In many biophysical systems we face a fascinating mixture of nonlinear dynamics, different kinds of fluctuations, complex signals, and adaptation processes involving multiple time scales. In our group we study selected problems from neurobiology and cell biophysics in the framework of stochastic nonlinear dynamics. Besides intense computer simulations of simplified biophysical models, we develop novel analytical approaches for the respective statistics of interest to gain deeper insights into the underlying processes. We have tight collaborations with experimental colleagues and seek for applications of our analytical results to help designing new experimental paradigms. Specifically, we work on:
Stochastic Neural Activity. The generation of action potentials by neurons (nerve cells) is inherently

noisy. Many sources of fluctuations like, for instance, synaptic transmission failures, channel noise and, most importantly, quasi random input from other neurons contribute to the statistics of the subthreshold membrane voltage and the variable timing of neural spikes (action potentials). Using simplified linear and nonlinear integrate-and-fire neuron models, we have calculated the spontaneous firing and interspike-interval statistics of neurons that are subject to (i) stochastic adaptation; (ii) short-term synaptic plasticity (synaptic facilitation and depression); or (iii) stochastic oscillations. In specific cases, these statistics allow conclusions about otherwise inaccessible parameters like, for instance, the number of adaptation channels in sensory neurons. Another central problem of interest is to understand how neurons encode time-dependent signals into spike trains and how their coding properties are influenced by features like short-term plasticity, noise, and adaptation. Using linear response theory, we study the coding problem in different variants that allow to isolate the effects of a certain feature on signal transmission.

Stochastic Dynamics of Hair cells. One well-studied example of the transduction of sensory stimuli is hearing. In the mechano-sensory hair cell of the inner ear organs air pressure variations (sound) are transduced into electrical currents that can be transmitted and processed by the neurons of the brain. Outer hair cells of the cochlea, however, serve also another task, namely, the active amplification of the basilar membrane vibration in response to sound stimuli. Although it is commonly accepted that hair cells are an essential part of the active cochlear amplifier, details of this amplification are still poorly understood and different hypothesis are hotly debated. The hair cell possesses a small organelle, the hair bundle, which is a key element in the transduction and amplification process. Single hair bundles in vitro show all signatures of an active amplification that are, however, diminished by a large amount of intrinsic noise. In models of different complexity as well as in experiments, we explore how by means of mechanical hair bundle coupling this intrinsic noise can be reduced and thus amplification properties of the bundle can be enhanced.

Diffusion and transport in cells. Transport and diffusion processes are essential for the functioning of biological cells. Vesicles are transported along filaments by means of molecular motors but may also suffer subdiffusive motion in the cytoplasm when detached from filaments. In experiments, the behavior of vesicles is often explored by local mean-square-displacement analysis. We study the properties of this algorithm in terms of simple Langevin models. Another topic in this project is the dynamics of assemblies of molecular motors, which are essential for the active transport in the cell. We investigate how biophysical models of motor assemblies can be approximated by much simpler phenomenological models like the active Brownian particle.

Ongoing collaborations

Experimental groups:

- Pascal Martin, Institut Curie Paris, France
- Jan Benda, LMU and BCCN München, Germany
- Doris Heinrich, LMU München, Germany
- Iva Tolić-Nørrelykke, MPI-CBG Dresden, Germany
- David Russell and Alexander Neiman, Ohio University, Athens, USA

Theoreticians:

- Alexander Neiman, Ohio University, Athens, USA
- Nenad Pavin, mpi**pks** Dresden, Germany
- Frank Jülicher, mpi**pks** Dresden, Germany
- Lutz Schimansky-Geier, HU Berlin, Germany

We have a number of collaborations with experimental groups studying the stochastic activity of and providing us with data from neurons (Benda and Neiman/Russell) and sensory hair cells (Martin). Related theoretical work is carried out together with researchers from Dresden (Jülicher and Pavin) and Athens,

Ohio (Neiman). Problems from cell biophysics are explored in collaboration with experimental groups from Munich and Dresden. Specifically, we work on intracellular diffusion and transport (Heinrich) and on the problem of capturing of kinetochores (Tolić-Nørrelykke). Active motility models are studied in a joint project with a research group in Berlin (Schimansky-Geier).

Division: Condensed Matter
(Head: Prof. Dr. R. Moessner)

In condensed matter physics, complex behaviour arises due to the interactions between a large number of microscopic degrees of freedom; these fundamental degrees of freedom can themselves be very simple. The resulting behaviour is fascinating in its richness: many different phases exist as distinct 'vacua', each with its own characteristic properties such as ground-state correlations, excitations, and dynamics in and out of equilibrium. The *Condensed Matter* division studies such collective behaviour. Most fundamentally, the aim is to connect the macroscopic behaviour of matter with the microscopic properties of its constituent particles. This work is not only aimed at identifying and understanding novel behaviour, but also at identifying the principles according to which we can understand how the physical world is organised.

To achieve this, we utilise the methods of many-body physics, both of analytical (e.g. field theories, exact solutions), and numerical (e.g. Monte Carlo, exact diagonalisation) nature. To guide and test theory, a broad range of results from experimental investigations are available, which themselves profit from the combinatorial richness supplied by the periodic table of elements, and from the possibility to custom-tailor degrees of freedom and their interactions. Progress often nucleates around experimental breakthroughs, such as the possibility to investigate real-time quantum dynamics and well-controlled time-dependent Hamiltonians in systems of cold atoms, or very clean electronic systems provided by semiconductor heterostructures and graphene.

Finally, the concepts and methods of statistical mechanics have a much wider range of applicability beyond materials-based many-body physics. For instance, they permit us to take a broader view of subjects such as quantum complexity theory, where they can be used to attack questions about typical rather than worst case complexity in computational ensembles.

Research Topics

The search for emergent magnetic monopoles: In 2008, we predicted that the class of magnetic materials which goes under the name of spin ice should exhibit elementary excitations in the form of magnetic monopoles. Subsequently, a multi-faceted experimental effort got underway with the aim of testing this prediction, as this would in particular confirm spin ice to be the first three-dimensional magnetic material in which fractionalisation occurs, in a phase described by a weakly fluctuating emergent gauge field. We collaborated with Santiago Grigera and Alan Tennant who conducted a set of thermodynamics and neutron scattering experiments. In providing a parameter-free, quantitative Debye-Hueckel theory for the measured heat capacity, we were able to establish that the interacting magnetic monopoles could be described as a weakly interacting magnetic Coulomb liquid. In addition, we analysed the spin correlations due to the 'Dirac' strings of flipped spins which run between different monopoles. In a separate line of work, we investigated the phase ordering kinetics upon approaching the Coulomb phase, with particular view of generating a large out-of-equilibrium population of monopoles at low temperature. Also, we provided a theoretic framework to explain the irrational charge of the magnetic monopoles which also accounts for previously known instances of irrational charge in one dimension.

Disorder in spin liquids: The interplay of disorder and interactions presents one of the most fascinating and challenging aspects of condensed matter physics. In the context of spin systems with quenched disorder, the physics of spin glasses and infinite randomness phases are just two instances of conceptually new physics which have arisen in the past. It is natural to ask more generally what happens when quenched disorder is introduced in a magnetic system exhibiting a novel correlated ground state. Indeed, besides a search for new types of disorder-induced phases, the properties of many quantum systems can be probed sensitively through the controlled introduction of impurities. We have started to address this set of questions in the context of Kitaev's honeycomb model, one of the few analytically tractable instances of a gapless quantum spin liquid. We have found that impurities nucleate a magnetic moment

which is almost free. Also, vacancies bind a flux of an emergent gauge field, a feature which strongly influences the interactions between a pair of them.

Real-time quantum dynamics and quantum quenches: When passing through a quantum critical point by changing the control parameter at a finite rate in time, time evolution is necessarily non-adiabatic – a system initialised at $T = 0$ leaves its ground state. The concomitant production of defects (e.g. excited states, vortices) is described by Kibble-Zurek theory. We have applied these ideas to mono- and bilayer graphene in the presence of strong in-plane or perpendicular electric fields, respectively. We predict that the non-linear electric conductivity of graphene grows with $\sqrt{E}$ (E being the electric field), in line with subsequent experimental observations. A time dependent gate voltage in bilayer graphene results in population inversion around the Dirac cone, which can in principle provide a coherent source of infra-red radiation with tunable spectral properties.

Quantum information and quantum complexity theory: There is an extensive research effort under way aimed at constructing a quantum computer capable of manipulating wavefunctions rather than operating on states of classical bits. The potential advent of such a new tool raises the question: which classes of computational problems will quantum computers find easier, in a complexity-theoretic sense, than their classical counterparts. And, given the existence of such classes, what algorithms will be needed for actually leveraging the power of quantum computers. As the first step in that direction, we have studied the quantum version, k-QSAT, of the classical k-SAT optimisation problem, which has itself been investigated using the powerful methods of the (classical) statistical mechanisms of disordered systems. We pursue an analogous programme of utilising insights and tools from quantum many-body theory for k-QSAT. For $k > 3$, k-QSAT is in the quantum complexity class QMA_1, the analogue of the classical NP-complete complexity class.

Exotic phase transitions: The competition between different types of complex (magnetic and non-magnetic) order and disorder is one of the central themes of quantum magnetism. Motivated by experiments on $Na_4Ir_3O_8$, we derived an effective low-energy Hamiltonian in a strong coupling expansion. Our analysis uncovered a phenomenology which transparently combined a number of generic phenomena such as a sequence of phase transitions leading to an ultimately very complex order which go along with the generation of low energy scales at which excitations on geometries of effectively reduced dimensionality emerge. On the classical side, we continued our studies of phase transitions out of topological phases – these generically lie outside the standard Landau-Ginzburg–Wilson framework as they involve a phase not described by a standard local order parameter; we found an 'infinite order' phase transition which can be realised in spin ice under pressure. We have also investigated two-dimensional arrays of submicron monodomain magnetic islands, which can be constructed liphografically (and probed locally) with exquisite control over their local geometry.

Multiband superconductivity: Motivated by the concrete example of superconductivity in the pnictides, we have pursued a systematic study of the fundamental modelling of this class of systems. Special emphasis is placed on experimental diagnostics of novel behaviour and on identifying an appropriate 'minimal theory' for the pnictides. We have in particular demonstrated that a simple model of itinerant electrons in several bands can already at weak to moderate coupling account for much of the structure seen in inelastic neutron scattering experiments. We have also analysed quasiparticle interference phenomena as probed using scanning tunnelling microscopy. This has provided information about the nature of the order underpinning superconductivity.

Perspectives

The condensed matter division at **mpipks** was constituted in late 2007 with the arrival of Roderich Moessner as director. The first group leader to join, in the course of the year 2008, was Andreas Läuchli, a computational physicist whose particular expertise lies in the study of novel phases in quantum lattice systems. Frank Pollmann's arrival at the beginning of this year to head a group working on "Topology and correlations in condensed matter" has complemented the line-up. His interests lie in the study of strongly correlated phases in low dimension, in particular in the development of new algorithms for their investigation. Next, Andreas Läuchli will in turn leave the division to take up a professorship at the University of Innsbruck in Austria later of this year.

In the future, our work will pursue a number of detailed studies of the physics of strong interactions, when it is combined with other ingredients. For example, the recently initiated line of research on the

role of disorder in exotic strongly correlated phases is going to be continued. Particular emphasis will be placed on questions relating to the interactions between disorder-induced local perturbations of the correlated state on one hand, and suitable connections to experiment, with either neutrons or alternative local probes (e.g. nuclear magnetic resonance), on the other.

Another new and promising direction we plan to pursue is the combination of itinerant degrees of freedom and geometric frustration. Following some preliminary work (e.g. on supersolidity in bosonic systems), we plan to consider also fermionic degrees of freedom, in part motivated by recent experiments on itinerant magnetic compounds such as $Pr_2Ir_2O_4$.

Given the immense progress in constructing models realising new quantum disordered states and the continuing stream of candidate systems proposed as their realisations, we plan to reinforce the study of the question how to diagnose these, either in experiment or in numerical simulations. This is conceptually of fundamental importance as it reverses the original motivation for the study of gauge theories proposed by Wegner.

Cooperations

- Joint group with Max Planck Institute for the Chemical Physics of Solids:

  At the beginning of 2009, a joint research group in the field of quantum condensed matter was set up between **mpipks** and the Max-Planck-Institut für Chemische Physik fester Stoffe. This group on "Collective phenomena in solid state and materials physics" has a research activity centred on the field of quantum phase transitions, which substantively complements the research undertaken in the condensed matter division. It is headed by Stefan Kirchner.

- Manifold collaborations with theory groups internationally, e.g.:
  - England: Oxford University (John Chalker); University of Cambridge (Gunnar Möller)
  - France: École Normale Supérieure Lyon (Peter Holdsworth), Université Paris VI (Jussieu) and Paris X/Orsay (Benoit Douçot/Mark Goerbig)
  - Hungary: Budapest University of Technology and Economics (Balazs Dora)
  - India: Tata Institute for Fundamental Research (Kedar Damle)
  - Italy: ICTP Trieste (Antonello Scardiccio)
  - Ukraine: National Academy of Sciences (Oleg Derzkho)
  - United States: Princeton University (Shivaji Sondhi); University of Wisconsin at Madison (Andrey Chubukov)

- Collaborations with experimental groups, e.g.:
  - Argentina: UNLP-Conicet La Plata – Santiago Grigera (non-equilibrium behaviour in spin ice)
  - Brazil: Instituto de Fisica de Sao Carlos, USP – Vanderlei Bagnato (Vortex configurations in trapped BECs)
  - Germany:
    - Helmholtz-Zentrum Berlin – Alan Tennant (Magnetic materials with Coulomb phases); Dimitri Argyriou (inelastic neutron scattering in novel superconductors)
    - High magnetic field laboratory, Helmholtz Zentrum Dresden-Rossendorf – Sergei Zherlitsyn, Jochen Wosnitza (ultrasound studies on frustrated magnets)
    - IFW Dresden – Bernd Buechner (NMR spectroscopy in iron-based superconductors)
    - MPI-CPfS – Frank Steglich (non-centroysmmetric superconductors)
    - TU Braunschweig – Peter Lemmens (Raman spectroscopy in iron-based superconductors)
  - Hungary: Budapest University of Technology end Ecomonomics – Ferenc Simon (electron spin resonance, graphene)

Research Group: New States of Quantum Matter
(Head: Dr. A. Läuchli)

The research group "New states of quantum matter" started its activity at the **mpipks** in September 2008. It presently hosts three postdoctoral members (V. Alba, D. Charrier and I. Rousochatzakis) as well as three associated members within the condensed matter department (E. Bergholtz, M. Haque and D. Kovrizhin). We also enjoyed the presence of several visitors for shorter term research activities (K. Agarwal, B. Chakrabarti, B. Hetenyi, D. Schwandt and S. Wenzel).

The goal of our research group is to understand strongly correlated quantum systems based on numerical simulations and to uncover and characterize new quantum states emerging in these systems. We study problems ranging from quantum magnetism and ultracold atomic gases to superconductivity and the fractional quantum hall effect. During the report period we worked particularly on the following topics:

Entanglement Properties of the Fractional Quantum Hall states — We put forward a new approach to obtaining the scaling behavior of the entanglement entropy in fractional quantum Hall states from finite-size wavefunctions. By employing the torus geometry and the fact that the torus aspect ratio can be readily varied, we can extract the entanglement entropy of a spatial block as a continuous function of the block boundary. Other than the topological information, the study of entanglement scaling is also useful as an indicator of the difficulty posed by fractional quantum Hall states for various numerical techniques. We also analyzed the entanglement spectrum of Laughlin states on the torus and showed that it is arranged in towers, each of which is generated by modes of two spatially separated chiral edges. This structure is present for all torus circumferences, which allows for a microscopic identification of the prominent features of the spectrum by perturbing around the thin torus limit. We are currently also investigating the structure of entanglement spectra for other quantum many body systems.

Novel ordered phases and spin liquids in the vicinity of Mott transitions — While the Mott transition and the phases in its vicinity are quite well understood for Hubbard models of two-flavored fermions (e.g. electrons) on hypercubic lattices, the same does not hold true when either increasing the number of flavors to three or more - as could be possible for earth-alkaline atoms in an optical lattice - or when considering more complex lattices such as the triangular or the honeycomb lattice. We made progress along these lines using computational techniques to reveal the nature of the Mott insulating state of three flavored fermions on several realistic lattices, and provide evidence for a spin liquid phase close to the Mott transition of two-flavored fermions on the triangular lattice which is of possible relevance for a class of organic conductors.

Critical properties of orbital-only models — Orbital-only models emerged recently as prototype systems enabling the understanding of relevant aspects of the collective dynamics of orbital degrees of freedom. In a different context, orbital-like models are attracting considerable theoretical interest due to their ability to sustain topologically ordered phases with possibly anyonic excitations, as exemplified by the Kitaev honeycomb model. A variety of properties have already been uncovered for orbital-only models, but most of these are restricted to ground state or low-temperature properties. Much less is known about finite-temperature properties and in particular the nature of thermal phase transitions. We have now performed a comprehensive Monte Carlo investigation of the nature of the finite-temperature phase transitions in two popular orbital-only models on the three-dimensional cubic lattice: the e_g and the t_{2g} models. The e_g model displays a continuous phase transition to an orbitally ordered phase. A detailed analysis of the critical exponents reveals significant deviations from the well known set of exponents of the $O(N)$ familiy. Furthermore at T_c a $U(1)$ symmetry emerges, which persists for $T < T_c$ below a crossover length scaling as $\Lambda \sim \xi^a$, with an unusually small $a \approx 1.3$. For the t_{2g} model we find however a *first order* transition into a low-temperature lattice-nematic phase without orbital order.

Algorithmic developments — We made algorithmic progress on two sides. On the one hand, we put forward a new formulation of the hybridization expansion continuous-time Quantum Monte Carlo algorithm for single impurity problems (relevant e.g. for dynamical mean-field theory (DMFT) applications), which systematically exploits the sparse structure of the impurity hamiltonians to achieve a significant speedup compared to the previously used dense matrix implementation. Using this new formulation it is now possible to perform DMFT simulations based on fully SU(2) invariant interactions such as Hund's terms for 3d transition metal compounds. A second line of algorithmic development is to parallelize our existing exact diagonalization codes for quantum spin systems for massively parallel distributed memory

architectures. Together with developers from the MPG computing center in Garching we are working on this challenging project, with the aim to push the limits of accessible system size from currently 42 spins to possibly 48 or 50 quantum spins in the future.

Cooperations

- Theory groups
  - Lausanne, École Polytechnique Fédérale de Lausanne, collaboration with the group of F. Mila on topics in frustrated quantum magnetism.
  - Palaiseau, École Polytechnique, collaboration with C. Kollath on nonequilibrium properties of strongly correlated systems.
  - Zürich, ETH Zürich, collaboration with P. Werner on algorithmic aspects of DMFT solvers.
  - Toulouse, Laboratoire de Physique Théorique, collaboration with S. Capponi and M. Mambrini on topics in frustrated quantum magnetism.
  - Dortmund, TU Dortmund, collaboration with the group of K.P. Schmidt on magnetic systems close to the Mott transition.
  - Dresden, MPI-CPfS, collaboration with the group of H. Rosner on ab-initio modeling of magnetic insulators.
- Experimental groups
  - Collaborations with neutron scattering group at the University College London (Ch. Rüegg) on the modeling and interpretation of inelastic neutron scattering experiments performed on low-dimensional quantum magnets.
  - Dresden, MPI-CPfS, collaboration with the group of H. Rosner on the experimental characterization of magnetic insulators.

Research Group: Nonlinear Time Series Analysis
(Head: Prof. Dr. H. Kantz)

This group was established in 1995 with a research programme in nonlinear dynamics and time series analysis. Over the years the focus has shifted. Time series analysis is nowadays only part of our activities, with particular emphasis on predictions. The main guideline for us is the aim to understand, model, and predict fluctuations in open, i.e., driven systems. This comprises research in non-equilibrium statistical physics, low- and high-dimensional dynamical systems, nonlinear stochastic processes, and in models of the atmosphere. More precisely, in these settings we aim for an understanding of the magnitude distributions and temporal (and spatial, where applicable) correlations of fluctuations, and of the details of the mechanisms behind. Particular motivation arises from the study of extreme events, which often occur as natural disasters and then have large impact on human civilization. Extreme events in driven systems are very large but rare fluctuations, where first of all dynamical mechanisms (feedback loops) exist which drive the system so far off its normal state, but where secondly the frequency and magnitude of such excursions in phase space are constrained by physical conservation laws.

Non-equilibrium fluctuation theorems. For thermodynamic systems out of equilibrium, a number of strict relations for ratios of probabilities of fluctuations are known as *fluctuation theorems*. One model where we study these is the fluctuating lattice Boltzmann model, a kinematic model for a viscous gas in contact with a heat bath. In the thermodynamic limit, its dynamics is equivalent to the one of the Navier-Stokes equations. For small system size, one can study non-equilibrium fluctuations and verifies the validity of theorems such as Crooks or Jarzynski. Through the theorems one can probe which system parameters correspond to the thermodynamic temperature. Another interesting feature is that non-equilibrium-fluctuations in this model are equivalent to equilibrium fluctuations, i.e., they are thermal fluctuations due to exchange of energy with the heat bath. This is not a general feature, since macroscopic dynamical instabilities would create very different fluctuations. It is therefore an interesting issue to understand under which conditions non-equilibrium fluctuations are exclusively heat bath fluctuations.

Forecasting atmospheric states. State-of-the-art models of the atmosphere are routinely used in weather forecasts. Formally, they are dynamical systems, and a forecast is the solution of an initial value problem for a finite time interval. By techniques called *data assimilation* one obtains the initial model state vector with about 10^8 components from a set of about 10^5 measurements of the current atmospheric state. This resembles the problem in dynamical systems theory called *shadowing*. We employ novel variational approaches in order to find better initial conditions with less computational effort compared to established methods.

Knowing that the model initial condition is only a rough estimate, weather services perform ensemble forecasts: They generate model trajectories for about 50-100 different initial conditions, which are obtained from the best guess by small systematic perturbations. This set of different forecasts for the same quantity at the same place and time allows one to assess the uncertainty of a forecast. We investigate what the proper interpretation of such an ensemble is. We could show that the spread of such ensembles, i.e., the diversity of the outcomes, is on average too small, since real measurements (the verifications) lie outside the ensemble too frequently. Such over-confident forecasts are a particular problem for the prediction of extreme weather, whose probability is generally underestimated. Our analysis is done on 5 years of operational forecast data from the ECMWF in Reading.

In Summer 2009, jointly with Prof. Fraedrich from the department of meteorology at University of Hamburg we organised a mpi**pks** international workshop on "Dynamics and Statistics of Climate and Weather", during which open issues of atmospheric fluctuations were discussed.

Nonlinear stochastic processes. Stochastic processes are very flexible models for non-equilibrium phenomena, hence they play a prominent role in several projects of our group. In low dimensions, the interplay of nonlinearity and stochasticity can produce interesting phenomena. We were particularly interested in hopping between metastable states when there is no potential barrier. Quite generally, the well established Kramers hopping rate is defined only for systems with a potential, which are a very small sub-class of interesting multi-stable systems. One alternative mechanism for meta-stability is of dynamical origin: regular islands in chaotic Hamiltonian systems can be understood as constraints due to conservation laws which are valid only in a part of the phase space. Being barriers to transport across them, they also induce multi-stability when Hamiltonian systems are driven by noise. We are studying such phenomena through the concept of random symplectic maps and iterated function systems. We could show that another non-potential source for metastability, namely state dependent diffusion coefficients with "hot" areas, can be translated into hopping dynamics.

Long range correlations. Quite generally, long range temporal correlations are an interesting issue, since they might be easily misinterpreted as trends. Correlations can even be so strong that empirical time averages will never converge. We were studying such phenomena in highly intermittent dynamical systems, where the conversion into continuous time random walks (CTRW) lead to a complete characterisation of the long time behaviour. In summer 2011, together with colleagues from Bar Ilan, London, Vienna, we will organise a seminar and workshop at mpi**pks** entitled "Weak chaos, infinite ergodic theory, and anomalous dynamics" which also covers the dynamical origin of long range temporal correlations.

Extreme events. We continue our efforts to understand properties of extreme events. On the path towards the classification of natural phenomena, we are currently testing whether it makes sense to distinguish between "turbulence like" extreme events and "SOC-like" ones. SOC, *self organised criticality* is a mechanism suggested in 1987 by Bak et al. as an explanation of power laws in nature. The tails of power laws are an evident manifestation of extreme events which are orders of magnitudes larger than the bulk of events, but not all extremes are of this type.

In prediction of extremes, we distinguish between detailed models (such as weather forecasting systems) and coarse grained models. Since the prediction of events is a classification problem (the occurrence of the event is a binary variable), coarse graining might be possible without a dramatic loss of information. Indeed, our data based prediction schemes perform quite well and in the case of the *Abelian sandpile model* they are as good as predictions using knowledge about the internal micro-state of the system. In the context of dynamical systems, *symbolic dynamics* is a well established concept, which might lead to a formal justification of the success of coarse grained forecast. However, this also shows the difficulties: Coarse graining might destroy Markov properties and thereby introduce long range correlations.

With funds of the Volkswagenstiftung and together with Prof. Kurths from the Potsdam Institute for Climate Impact Research PIK we organised an international workshop on extreme events in Potsdam last

September. The very same foundation supports a joint research project on *Extreme Events in Excitable Systems: Harmful Algal Bloom and Epilepsy*, in collaboration with groups from Potsdam, Oldenburg, and Bonn.

Cooperations

- Center for Dynamics at the TU Dresden: Holger Kantz is member of the board of directors of this newly founded center which will enhance the scientific interchange on dynamics in the Dresden area.

- Roland Ketzmerick, Physics Department, Technical University of Dresden (stochastically driven Hamiltonian systems).

- London School of Economics: Jochen Bröcker, post-doc in our group, is a *visiting research fellow* of the Centre for the Analysis of Time Series at LSE, main collaborator L.A. Smith, (probabilistic weather prediction and reliability, provides also access to ECMWF data).

- Georg Mayr, Meteorology Department, University of Innsbruck (prediction of surface winds and power output of wind farms). Jochen Bröcker will obtain his Habilitation at Uni Innsbruck.

- Ulrike Feudel (Oldenburg), Helmut Hillebrand (Oldenburg), Klaus Lehnertz (Bonn), Jürgen Kurths (PIK Potsdam) (Extreme events in excitable media).

1.9 Junior Research Groups

Emmy Noether Junior Research Group: Many-body effects in mesoscopic systems
(Head: Dr. Martina Hentschel)

The Emmy-Noether group "Many-body effects in mesoscopic systems" works at the mpi**pks** since April 2006. The research area of the group is electronic and optical mesoscopic systems. The phenomena investigated include many-body effects in quantum dots and theoretical as well as application oriented questions in the field of quantum chaos in optical microcavities. During the period 2009/10, the research was carried out by two PhD students (funded, as the group leader and one Postdoc, by the Emmy-Noether Programme of the DFG) and two to four Postdocs funded by the mpi**pks** Visitors Program. The group receives additional funding from the DFG Research Group 760 "Scattering Systems with Complex Dynamics" whose approval was renewed in April 2010. The group leader was awarded a two-year fellowship in the "Fast Track Programme" of the Robert-Bosch Foundation (that supports 20 young women scientists across Germany) in September 2008 and the Hertha-Sponer Prize of the German Physical Society (DPG) for 2011. The group's research results have been presented on a number of international conferences and workshops. The group leader and two Postdocs have organized the international workshop "Optical Microcavities: Quantum Chaos in Open Systems Meets Optical Resonators" that took place at the mpi**pks** May 17-21, 2010. It should be mentioned that the group leader was in maternity and parental leave, respectively, for most of the time period covered by this statement (precisely 3/4 of the time) after the birth of her two children.

Many-body effects have always been a core interest in condensed matter physics. The objective of the group is their investigation in electronic systems, where the finite number of particles in the system, its small size, intrinsic mesoscopic fluctuations and, very importantly, the existence of a system boundary, give rise to new physical behaviour. For example, in the mesoscopic X-ray edge problem, we have found that many-body effects such as Anderson orthogonality catastrophe are somewhat stronger in integrable than in chaotic quantum dots. Reasons are (quasi-)degeneracies of the energy levels and the change of the system character from integrable to pseudointegrable under the influence of a sudden, localized perturbation. For the photoabsorption cross section, we have found correlations of the wave function near the system boundary to play a crucial role and to alter the many-body response from a so-called rounded edge in the metallic case (where the electrons are described by Bloch waves that do not see any system boundary) into a peaked-edge in the mesoscopic regime. Other research topics are the Kondo effect in mesoscopic systems and graphene. For the latter we have also studied the photoabsorption cross section and found additional singularities related to the existence of the Dirac point and edge states.

In the area of **optical microcavities**, the second research area of the group, the focus has been on the investigation of deviations from ray-wave correspondence and on the experimentally relevant issue of achieving unidirectional emission from optical microcavities. This goal was achieved in collaboration with Jan Wiersig (University of Magdeburg) in cavities of so-called **Limaçon** shape (deformed disk shape) where we predicted directional emission (PRL 2008). This idea was very soon verified by four independent experimental groups. Deviations from the naively expected ray-wave correspondence occur when the wavelength becomes of the order of characteristic system length scales. Including these wave-inspired corrections (they are known as Goos-Hänchen shift and Fresnel filtering) into the ray picture can explain most of the observed deviations from ray-wave correspondence and leads, moreover, to new behaviour such as non-Hamiltonian dynamics. While the naive ray picture proved to be almost surprisingly useful even in small structures, deviations from ray-wave corresppndence do now become important in the smallest available microresonators.

Perspectives The group will continue the investigation of electronic and optical mesoscopic systems under special consideration of the characteristic differences due to complex wave phenomena that occur at small scales. One focus will be the dependence of the photoabsorption cross section and the Kondo effect on the density of states, that can to a certain extent, be customized in the mesoscopic regime, for example in graphene via edge-state engineering resulting from the breaking of symmetries at the system boundary. The motivation to study graphene-like photonic crystals is the possibility to directly manipulate (perturb) the honeycomb-lattice structure in table-size microwave billiards experiments and thereby to directly study this breaking of edge symmetries. Another research topic will be the interplay of different

many-body effects in quantum dots. Eventually, questions of quantum chaos in optical microcavities, including very small cavities as well as the effects of nonlinear materials and lasing cavities, will remain another focus of the group's research interests.

Collaborations

The group is well connected to the national and international community, comprising both theoretical and experimental collaborations:

- Continuation of the collaboration with Harold Baranger (Duke University, USA) and Denis Ullmo (Orsay, France) that was initiated during the group leader's Postdoc time at Duke University (Durham, USA) 2002-2004.
- Collaboration with Francisco Guinea (Madrid, Spain) on graphene.
- Collaboration with Eduardo Mucciolo (University of Central Florida, Orlando, USA) on the mesoscopic Kondo box.
- Collaboration with Dirk Morr (Chicago, USA) on the Kondo effect in graphene.
- Scientific exchange with Jeroen van den Brink (IFW Dresden) on X-ray edge physics.
- Cooperation with Jan Wiersig (University of Magdeburg), Roland Ketzmerick and Arnd Bäcker (both Technical University of Dresden) within the DFG Research Group 760 "Scattering systems with complex dynamics".
- Collaboration with the (experimental) groups of Karl Leo (Technical University of Dresden) and Oliver Schmidt (IFW Dresden).
- Collaboration with the (experimental) group of Federico Capasso (Harvard University, Cambridge, USA) on the far-field characteristics of microlasers with different (spiral, Limaçon, triangular) shape.
- Collaborations with the (experimental) groups of Hans-Jürgen Stöckmann (University of Marburg) and Achim Richter (Technical University of Darmstadt) are continued on varying topics, at present especially the Goos-Hänchen shift and graphene-like photonic crystals.
- Regular contacts and exchange with the groups of Takahisa Harayama (ATR Wave Engineering Laboratories, Kyoto, Japan), Chil-Min Kim (Paichai University, Daejon, Korea), and Hui Cao (Yale University, USA

Junior Research Group: Computational Nonlinear and Relativistic Optics
(Head: Dr. Stefan Skupin)

The Junior Research Group *Computational Nonlinear and Relativistic Optics* started to operate in fall 2007 at the mpi**pks**. In April 2009, the group leader Stefan Skupin became an appointment as *Carl Zeiss* Junior Professor for *Computational Photonics* at the Friedrich Schiller University in Jena. Due to this second engagement, Stefan Skupin is only two days per week present at the mpi**pks**, and it became necessary to appoint Mickael Grech as a long-term Post-Doc and assistant group leader. The group currently hosts two PhD students, Christian Köhler and Fabian Maucher. Moreover, Yiqi Zhang spent one year in the group as an exchange student (11/2009–10/2010, MPG-CAS Doctoral Promotion Program). Eduardo Cabrera Granado visited the group for one year as a Post-Doc (03/2010–02/2011), and the visitors program enabled several shorter visits of other senior scientists.

Computational physics is a fast growing discipline, and recent progress in computer technology makes it possible to solve large scale numerical problems which were not tractable at all only a decade ago. More and more super-computers become available for fundamental science (see, e.g., the new AIMS cluster of the mpi**pks** at RZG) and allow the simulation of whole physical experiments. This development offers a unique opportunity to conduct novel and innovative research.

Novel ultrashort light sources from laser induced plasma dynamics In the past decade, the range of wavelengths which is accessible by exploiting frequency conversion from an optical pump has grown dramatically. Remarkably, many methods to obtain extremely high or extremely low frequencies make use of, in one way or the other, nonlinear processes in laser-induced plasma. One famous example is high harmonics generation (HGG), where frequencies thousands times larger than the frequency of the pump pulse are generated due to recollision dynamics of free electrons with parent ions. More recently, it was demonstrated that by using light induced plasma dynamics, it is possible to produce frequencies just in the opposite part of the spectrum, namely in THz range, hundreds of times smaller than the optical pump frequency. Besides, in so-called femtosecond filaments, the interplay between the atomic nonlinearity and plasma defocusing leads to self-guiding, pulse self-compression and, last but not least, generation of new frequencies. Recent investigations suggest the possibility to produce ultrashort pulses in the ultraviolet (UV) and vacuum ultraviolet (VUV) range by exploiting spatio-temporal reshaping in filaments .

Thus, laser induced plasma dynamics can be used to design novel light sources in an extremely wide range of frequencies. However, the theoretical and numerical modeling of the underlying spatio-temporal dynamics is quite involved. For example, as far as extremely low frequencies in THz range are concerned, even the mechanism of THz emission is still subject to discussion. However, in a recent paper we were able to show excellent agreement between experimental and numerical THz signals. It turns out that a simple macroscopic current model correctly describes the THz generation process. Together with the forward Maxwell equation (FME) for the fast optical field this model provides a unifying framework for the whole frequency range starting from THz up to VUV. We believe that this ansatz has a huge potential to investigate general processes of nonlinear frequency generation from (multi)-frequency optical pumps. Apart from this FME model, which allows to simulate large propagation distances, we use finite difference time domain (FDTD) calculations to get "exact" results for small volumes or in reduced dimensionality.

Reliable sources of ultrashort high energy pulses in the VUV as well as in the THz range are exceptionally important for ultrafast spectroscopy. Ultrashort pulses in the VUV range allow to visualize dynamics of small molecules, whereas THz pulses are suitable for detection of molecular vibrations in large molecules. THz generation based on laser-induced plasma dynamics in an asymmetric light field created by two-color pulses is very attractive due to its tunability, high output energy and broad spectrum. One of our goals is to exploit and develop further our theoretical model for THz pulse generation including the propagation dynamics of the pump pulse. Full space-time resolved simulation of real-world situations and a quantitative comparison with experiments will allow us to understand better the mechanism of THz generation. Our model allows us to consider different setups including the conventional plasma-spot in tightly focused geometries, as well as a metallic waveguide to guide both THz and pump pulses. In the VUV range, standard methods of pulse generation provide durations down to 100 fs only. Very recently new methods based on filamentation in gas were realized allowing to achieve durations less than 15 fs , but with considerably small pulse energies in the nJ range. We plan to investigate the potential of such methods to achieve larger energies and even shorter pulse durations. In this respect, we are going to exploit a pulse self-shortening scenario in filaments in context of four wave mixing (FWM) and third harmonic generation (THG) with a signal in the VUV range. Generally, FWM in filaments is phase-mismatched. However, we see a possibility to achieve phase matching by using pump and idler pulses propagating noncollinearly, as well as quasi-phase-matching in filaments using periodically modulated pressure created by a gas jet passing through appropriately arranged nozzles.

On this topic, we collaborate with Luc Bergé (CEA/DAM, Arpajon, France), the group of Thomas Elsaesser (MBI, Berlin), and Ihar Babushkin (WIAS, Berlin).

Nonlinear localized waves in nonlocal media The propagation and dynamics of localized nonlinear waves is a subject of great interest in a range of physical settings, stretching from nonlinear optics to plasmas and ultracold atomic gases. The structure and stability of nonlinear optical modes is determined by the interplay of the radiation field with the functional form of the material nonlinearity. In the case of optical beams, the nonlinear response can be described in terms of the induced change in the refractive index n which is often approximated as a local function of the wave intensity. However, in many real physical systems the nonlinear response is spatially nonlocal which means that the refractive index depends on the beam intensity in the neighborhood of each spatial point. This occurs, for instance, when the nonlinearity is associated with some sort of transport processes such as heat conduction in media with thermal response, diffusion of charge carriers or atoms or molecules in atomic vapors. It is also the case

in systems exhibiting a long-range interaction of constituent molecules or particles such as in nematic liquid crystals or dipolar Bose-Einstein condensates (BEC).

Nonlocality is thus a feature of a large number of nonlinear systems leading to novel phenomena of a generic nature. For instance, it may promote modulational instability in self-defocusing media, as well as suppress wave collapse of multidimensional beams in self-focusing media. Nonlocal nonlinearity may even represent parametric wave mixing, both in spatial and spatio-temporal domain where it describes formation of the so called X-waves. Furthermore, nonlocality significantly affects soliton interaction leading to formation of bound states of otherwise repelling bright or dark solitons. It has also been shown that nonlocal media may support formation of stable complex localized structures, like rotating multihump and vortex ring solitons.

Currently, we are working on a scheme for the creation of three-dimensional bright solitons in a BEC. The approach is based on optical dressing of a groundstate atom BEC to highly excited Rydberg states. We were able to identify an appropriate range of Rydberg states that provides sign-definite attractive nonlinearities, and thus prevents condensate collapse as occurring in dipolar gases. We want to investigate not only the existence of stable self-trapped "condensate bullets", but the intrinsic anisotropy of the nonlocal interaction offers also an intriguing possibility to transfer angular momentum to the condensate and create, e.g., vortices.

On this topic, we collaborate with the group of Thomas Pohl (mpi**pks**), Wieslaw Królikowski (ANU, Canberra, Australia), and Mark Saffman (University of Wisconsin, USA).

Laser based charged particle acceleration High power laser-pulse interaction with plasmas offers a unique opportunity to study matter under extreme conditions of temperature and pressure. Current laser systems (with intensities $> 10^{18}$ W/cm^2 and soon beyond $> 10^{22}$ W/cm^2) allow to access the so-called relativistic regime of laser-plasma interaction. This interaction regime is characterized by the emission of various energetic particles (electrons, ions and also neutrons and positrons) and intense radiations (with frequencies ranging from THz to the gamma domain). These new sources of particles and radiations offer a vast range of applications.

Our research at the mpi**pks** is devoted to laser-based ion acceleration and its applications. Multi-MeV ion beams generated during the interaction of an intense laser pulse with a plasma can indeed initiate a thermonuclear reaction in the so-called fast-ignitor scenario for inertial confinement fusion. Due to their good laminarity, collimation and short duration, they are also used for time-resolved radiography in plasma experiments. Last but not least, high-quality ion beams may also be used for medical applications such as isotope creation and hadron-therapy.

Different mechanisms of ion acceleration have been proposed depending on whether ions originate from the front side (irradiated by the laser) or the rear side of the target. At the target rear side, ion acceleration occurs in the strong electrostatic field resulting from charge separation due to hot electrons escaping into vacuum. This mechanism, referred to as target normal sheath acceleration (TNSA), is the dominant process of ion acceleration for currently available (moderately relativistic) laser intensities. TNSA provides ion beams with interesting properties and relatively large efficiency of energy conversion (a few percent) from the laser pulse to the ions. However, the resulting ion beams have a characteristic broad spectrum with a sharp cut-off at maximal energy.

Multispecies (multilayered or homogeneous) solid targets have recently attracted a lot of attention as they may allow for a better control of the ion spectrum. We have proposed a new acceleration mechanism for the generation of high-quality (small energy and angular dispersion, $\Delta E/E \lesssim 10$ % and $\Delta\theta \lesssim 5°$, respectively) energetic (> 100 MeV) ion beams. This mechanism relies on the complete electron removal from a nanometric double-layer target by an intense ($> 10^{21}$ W/cm^2) laser pulse. Its potential application to hadron-therapy has also been considered. Scaling laws derived from analytical modeling as well as multidimensional (1D, 2D and 3D) particle-in-cell (PIC) simulations suggest that petawatt laser pulses are required for this application.

Our study of acceleration mechanisms alternative to TNSA also leads us to investigate the so-called radiation pressure acceleration (RPA) regime. In this scenario, ions are accelerated by direct transfer of momentum from the laser photons to the ions. The whole target is accelerated to potentially relativistic velocities as a compact quasi-neutral bunch. While this acceleration scheme may allow for the generation of intense quasi-monoenergetic ion bunches, the mechanisms responsible for energy dispersion are not yet well understood and are currently under investigation.

On this topic, we collaborate with the group of Erik Lefebvre (CEA/DAM, Arpajon, France) and Vladimir Tikhonchuk (CELIA, Bordeaux, France). The experimental investigation of ion acceleration and its applications (e.g., to proton radiography in plasma experiments) is done in collaboration with the group of Julien Fuchs (LULI, Palaiseau, France). Collaboration with Roland Sauerbrey and Ulrich Schramm (Forschungszentrum Dresden Rossendorf) is also acknowledged.

*Joint research program **mpi**pks and MPI-CPfS*

Over the past decade, a number of emergent phases in electronic systems have been the subject of combined experimental and theoretical interest. These novel phases ultimately arise from the strong Coulomb repulsion between electrons and the interplay between itinerant and local degrees of freedom. As a result, the way a many particle system can evolve from one phase to another has attracted considerable attention as a new paradigm for addressing the universal features of correlated quantum systems. The joint research group of the **mpipks** and the MPI-CPfS combines the expertise in Experimental solid state physics and chemical metals science of the MPI-CPfS with those on theoretical quantum many particle physics of the condensed matter research field of **mpipks** to address these universal features. The group of Dr. Stefan Kirchner, "Collective Phenomena in Solid State and Materials Science", is located at both institutes. It was started in 2009 and is involved in research on both the theoretical and the experimental aspects of this research program. Joint seminars between the two institutes feature theorists working in the broad area of strongly correlated electron physics, superconductivity and magnetism.

Junior Research Group: Collective Phenomena in Solid State and Material Science
(Head: Dr. Stefan Kirchner)

The joint junior research group of the Max Planck Institutes for the Physics of Complex Systems and for Chemical Physics of Solids began its work in February 2009. Research interests of the group center around strongly correlated electron systems with a current emphasis on quantum criticality in rare earth intermetallic compounds.

Phase transitions connect different states of matter and are ubiquitous. If the temperature vanishes at which the transition occurs, a quantum phase transition takes place. Such a transition can be continuous or discontinuous depending on whether the order parameter that characterizes the phase transition is continuous or not. Quantum criticality occurs as matter is tuned through a continuous zero-temperature phase transition and is found to affect the properties of matter in a wide temperature and parameter range fanning out from the zero-temperature critical point. So far, the existence of quantum critical points has been established beyond reasonable doubt only in heavy fermion systems although growing evidence exists that quantum criticality also governs the phase diagram of other strongly correlated materials, like e.g. the high-temperature cuprate superconductors. In the traditional approach to quantum criticality, the critical regime is described in terms of a Ginzburg-Landau-Wilson functional of the order parameter and its fluctuations where the order parameter is a physical quantity characterizing the ordered side of the critical point. Quantum mechanics enters in this approach only in increasing the effective spatial dimensions in which the Ginzburg-Landau-Wilson functional is defined. As a result, this classical theory in elevated dimensions predicts mean field behavior for many systems. In the context of magnetic quantum criticality, the classical Ginzburg-Landau-Wilson approach is known as the spin-density wave theory. Experimental and theoretical work for heavy fermion systems has established the existence of at least one other class of quantum critical points. This additional class of quantum critical points defies a description in terms of a Ginzburg-Landau-Wilson functional. Characteristic to all quantum critical points is the diverging correlation length as criticality is approached. This divergence is at the heart of the scale-invariant energy spectrum and the origin of 'universality' i.e. the phenomenon that the power law divergence of physical quantities is largely independent of physical details of the system. At present, neither a field theoretic formulation for the new class of quantum critical points is known nor a general classification of quantum critical points into universality classes is available.

The lack of any intrinsic scale at criticality suggests that quantum critical points are particularly susceptible to external perturbations as any perturbation has to be considered large compared to the (vanishing) intrinsic scales. Thus, understanding the effects of non-equilibrium correlations near quantum phase transitions seems of eminent practical relevance with respect to guidance of experimental work since

experimental probes lead to perturbations of the system under consideration. Quantum mechanics links statics and dynamics already at the equilibrium level of a quantum phase transition and makes it necessary to treat both on equal footing. This invalidates approaches that have been successfully used for classical dynamical phase transitions.

Intermetallic rare earth compounds are extended lattice systems where the competition between localized and itinerant degrees of physics gives rise to a complex behavior and a plethora of competing ground states where the relevant energy scales emerge out of the bare couplings that determine the high-temperature behavior. As a consequence, theoretical models like the so-called Kondo lattice model are effective models designed to describe the universal aspects of the problem. Thermodynamic and (bulk) transport measurements, i.e. the traditional bulk measures that are available at low temperatures are more and more augmented by local probes that have become available, e.g. neutron scattering techniques or most recently scanning tunneling microscopy for heavy fermions. These novel experimental tools give access to the microscopic coupling constants that enter theoretical models but in turn require effective theories that go beyond the universal aspects of the problem. With these developments in the broad area of instabilities in strongly correlated electron systems in mind, the joint junior research group 'Collective Phenomena in Solid State and Materials Science' focuses on the following topics:

- Development of effective theories for lattice problems to understand the emergent phases near electronic instabilities and obtaining a better microscopic modeling of local degrees of freedom and the effect of bond and site disorder. Of particular experimental relevance will be to address when quantum critical fluctuations can lead to Cooper pairing and hence to superconductivity.

- Addressing the numerical observation of symmetry enhancement near quantum criticality and developing the critical field theory for critical Kondo destruction. This critical field theory will have to capture the recently observed finite temperature scaling properties of the magnetotransport properties as well as the zero-temperature jump in the Fermi volume.

- Any experimental measurement creates a perturbation to the system. For a small perturbation the systems will react to it in a way that is compatible with the equilibrium fluctuation spectrum. This is the content of the fluctuation-dissipation theorem. In a quantum critical state the situation is more subtle due to its scale-invariant spectrum and the range of applicability of the fluctuation-dissipation theorem is a priori unclear. Understanding the effect of non-equilibrium drives as e.g. bias voltage or temperature gradients on the critical physics of appropriate quantum systems is therefore an issue of immense pratical relevance.

External Collaborations

In addition to the joint projects between the mpi**pks** and the MPI-CPfS, there exist several projects with external collaborators. Research projects currently exist with the group of

- Prof. Dr. Laurens Molenkamp from Universität Würzburg on the realization of the Bose-Fermi Anderson model in self-assembled II-VI semiconductor quantum dots.

- Prof. Dr. Qimiao Si from Rice University, Houston and Prof. Dr. Kevin Ingersent, University of Florida at Gainesville. The long-term goal of the collaboration with Qimiao Si and Kevin Ingersent and the members of their groups is the construction of the critical field theory of the particular unconventional quantum critical point that recently were observed in a number of intermetallic rare earth compounds. We try to tackle this problem by a two-pronged approach. On the one hand, we obtain a microscopic understanding of the physics near zero-temperature instabilities in certain models. This has so far been accomplished for the spin-isotropic Bose-Fermi Kondo model and the so-called pseudogap Bose-Fermi Anderson model. On the other hand, symmetry considerations can be used to pose important constraints on the underlying critical field theory. We e.g. recently argued that critical Kondo destruction is accompanied by an enhanced conformal symmetry, absent in the bare model. This is reminiscent of the symmetry restoration that occurs e.g. in the U(1) Thirring model, which restores the SU(2) symmetry dynamically.

- Prof. Dr. Dirk Morr from the University of Illinois at Chicago. Together with D. Morr and his group we pursue the question of how site disorder influences the quantum critical properties of the Kondo lattice. In addition, we intend to develop a theoretical framework for 'quasiparticle interference imaging' based on a SU(N) approach that is likely to be relevant to upcoming scanning tunneling microscopy measurements on doped $YbRh_2Si_2$. Quasiparticle interferences have recently been utilized in the hidden order compound URu_2Si_2 by the Davis group to trace the evolution of the band structure across the hidden order transition (A. Schmidt et al., *Nature* **465**, 570 (2010)).

- Prof. Dr. Hans Kroha from Universität Bonn. While a number of numerical tools exist to treat the short-time evolution of strongly correlated systems, the long-time limit of non-stationary problems has not received much attention. Together with the group of Hans Kroha, we aim at developing techniques for the long-time limit of periodically driven strongly interacting systems.

- Prof. Dr. Carlos Bolech who is currently at the University of Cincinnati and Prof. Dr. Enrique Munotz Tavera from the Pontificia Universidad Católica in Valparaiso, Chile. In this project we center our attention on steady-state transport through single-molecule single-electron transistors. The goal is to identify the origin of different voltage scaling coefficients seen in different experiments that are at variance with expectations of universality.

*Joint research program **mpi**pks and MPI-CBG*

The joint research program 'Physics of Biological Systems' between the Max Planck Institute for the Physics of Complex Systems and the Max Planck Institute of Molecular Cell Biology and Genetics strengthens the collaborations between these two institutes in Dresden. The objective of the program is to develop physical techniques - both experimental and theoretical - for analyzing biological systems. The program was started in 2004, and three Junior Research Groups at both institutes participate. The group of Dr. Thilo Gross (Dynamics of Biological Networks) is located at the **mpipks** and works on structural and dynamical aspects of complex biological networks. The group of Dr. Iva Tolić-Nørrelykke (Interior Design of the Cell) is located at the Max Planck Institute of Molecular Cell Biology and Genetics and studies how the cell organizes its interior over its lifetime. The group of Dr. Stephan Grill (Motor Systems) is located at both institutes and addresses cell-scale emergent physical properties and the collective function of molecular machines. A number of collaborations, joint group-meetings, and a seminar series on the Physics of Biological Systems allow for high levels of interaction between these and other groups within both institutes. This program continues to provide a unique research environment bringing together experimental biology and theoretical physics to shed light on the physical principles that underlie living systems.

Junior Research Group: Dynamics of Biological Networks
(Head: Dr. Thilo Gross)

In biology, networks appear in many different contexts and on many different scales, ranging from gene-regulation to societies. Our knowledge of the structure of these networks advances rapidly because of the two great revolutions of our time; progress in experimental biology continues to elucidate the networks on the molecular level, meanwhile the widespread use of novel forms of electronic communication provides data on human interactions. Although the structure of many important networks is thus being uncovered, the functioning and failure of these networks is often linked to their dynamical rather than structural properties. Efficient tools are therefore needed to make predictions on the dynamics that can be sustained by a network with a known or purported structure. The group dynamics of biological networks uses insights from nonlinear dynamics and statistical physics to develop new approaches to network dynamics. While the tools of nonlinear dynamics were primarily developed for application to low-dimensional systems, networks are inherently high-dimensional. For applying these tools one therefore either has to extend the tools of nonlinear dynamics or find proper low-dimensional descriptions of networks. In our work we follow both of these approaches two different contexts.

Generalized Models. Loosely speaking, a generalized model is a system of differential equations in which terms appear that are not restricted to specific functional forms. In comparison to conventional modeling approaches, generalized models reveal only limited information, but do so with higher degrees of generality

and efficiency. They are therefore well suited to describe systems in which the topology, the specific pattern of interactions, is known, but the exact nature of these interactions has not yet been determined.

In the past two years, the approach of generalized modeling, developed by members of the group, has been increasingly adopted by other labs. We took this as an incentive to extend the mathematical basis of generalized modeling and formally proved the correctness of the key steps in the generalized modeling procedure. Furthermore, we extended the approach of generalized modeling to new classes of systems, including delay-differential equations. Finally, we applied the approach of generalised modeling to new applications including intra-guild competition in ecology, the regulation of bone remodeling, stoichiometric constraints in producer-grazer systems, and signalling cascades in cells.

Adaptive Networks. The second main area of research is the investigation of *adaptive networks*. On these networks a dynamical process takes place while simultaneously the topology of the network evolves in time. The interplay of dynamics ON the network and dynamics OF the network gives rise to several forms of self-organization. While almost all real world networks are adaptive, the dynamics of this class of systems have only very recently come into the focus of rigorous investigations. Because of their ubiquity adaptive networks are currently attacked from many different direction and with tools different disciplines have established. Recently, common themes have begun to appear in several studies and a unified theory seems to be within reach.

In the past two years important advances in the understanding of adaptive network dynamics have been made. A major focus of our work is therefore presently to transport these insights back into applications, where they can be used for making predictions on real-world systems. Examples include for instance a recent study of the adaptive self-organisation that tunes biological neural networks to a critical state, where information processing is maximally efficient. In parallel we extend and refine modeling approaches to adaptive networks, with the aim of representing systems from applications more directly in adaptive network models.

Junior Research Group: Interior Design of the Cell
(Head: Dr. Iva Tolić-Nørrelykke)

How does a living cell organize its interior? Spatio-temporal organization is crucial for life at all levels of complexity, from macromolecules to cells, organs, and organisms. We are a team of biologists and physicists investigating the dynamics of spatial order inside the cell. We use the fission yeast *Schizosaccharomyces pombe* as a model system because it has a simple symmetrical cell shape, a small number of microtubules, and highly developed genetics. We combine experimental methods (laser scanning microscopy, laser cutting, optical tweezers, mutants), advanced image analysis, and theoretical research at the interface of physics and biology. Our main research activities are:

Nuclear Oscillations. At the onset of meiosis (sexual reproduction) in fission yeast, two cells of opposite mating types fuse at their tips forming a banana-shaped zygote. Subsequently, the two nuclei of the parental cells fuse into one, which starts to oscillate from one end of the cell to the other. These oscillations have a period of about ten minutes and last for several hours. The oscillations are crucial for proper chromosome pairing, recombination, and spore viability. Similar chromosome movements have been observed in a variety of other organisms, where they also play a role in chromosome pairing and recombination. Nuclear oscillations are dependent on astral microtubules that radiate from the spindle pole body and on cytoplasmic dynein, a minus-end directed microtubule motor. Using laser ablation of specific microtubules, we have shown that the nuclear movement is driven by pulling forces exerted along the leading microtubules. By imaging GFP-tagged dynein motors, we found that dyneins dynamically redistribute from one part of the cell to the other. We observed single dyneins as they diffuse in the cytoplasm and attach to a microtubule. Once bound to the microtubule, dyneins perform one-dimensional diffusion along the microtubule, which may be their strategy to search for anchor proteins at the membrane. By combining quantitative live cell imaging with a theoretical model, we found that dyneins linking the microtubule to the membrane detach from the membrane in response to load forces they experience. This mechanically regulated self-organization generates asymmetric patterns of dyneins and, consequently, of forces required for nuclear movement. Our work therefore demonstrates that spatio-temporal pattern formation within a cell can occur as a result of mechanical cues, which differs from conventional molecular signaling, as well as from self-organization based on a combination of biochemical reactions and diffusion.

Search for Kinetochores. Accurate chromosome segregation during cell division is necessary for genomic stability. It is crucial to prevent aneuploidy, which is associated with development of cancer as well as a variety of birth defects. In order to get segregated, chromosomes have to connect to microtubules of the mitotic spindle through specialized structures called kinetochores. At the beginning of mitosis, microtubules have to capture the kinetochores. A central question is how microtubules find kinetochores. A pioneering idea that could explain this process is based on microtubule dynamics (Mitchison and Kirschner, 1984). In this search-and-capture scenario, the microtubules are assumed to grow in random directions from the centrosomes. If a microtubule does not interact with a kinetochore, it will undergo catastrophe and shrink back to the centrosome. New microtubules are nucleated, each of them having a chance to reach a kinetochore. At some point, a lucky microtubule will capture a kinetochore and become stabilized by this interaction. Eventually, all kinetochores will get captured. This mechanism, however, relies on a large number of microtubules and their high dynamicity. We hypothesize that so-far unknown mechanisms may exist to increase the efficiency of kinetochore capture. To study how microtubules search for kinetochores we use fission yeast, where we can follow the dynamics of each astral microtubule during its lifetime, due to a small number of microtubules. We found that kinetochores can be captured by microtubules performing random angular movement. By using live cell imaging, we observed that astral microtubules pivot around the spindle pole body. By studying the relationship between the microtubule angular movement and microtubule length, we found that this movement is most likely driven by thermal fluctuations. In addition, we found that kinetochores and astral microtubules, by performing random movement, explore a comparable fraction of space. Finally, by introducing a theoretical model, we show that the process of kinetochore capture can be explained by the observed random movement of astral microtubules and of the kinetochore.

Alignment of the Mitotic Spindle. In all eukaryotic cells, correct segregation of the genetic material during cell division requires proper positioning and alignment of the mitotic spindle with respect to the cell division plane. Our previous work has shown that in fission yeast, the spindle is aligned by interphase microtubules during early mitosis, and by astral microtubules and cell shape during late mitosis. However, the mechanisms that control spindle alignment in mid-mitosis have remained unknown. Lack of such a control may lead to extensive spindle rotation and misalignment, which in turn results in chromosome mis-segregation if spindle elongation is impaired. Our work has revealed that the association of mitochondria with the spindle poles reduces spindle rotation. In wild type, spindles with associated mitochondria did not rotate as much as free spindles. In a mutant of the centrosomin-related protein Mto1, mitochondria were less associated with the spindles, which rotated more than in wild type. We propose that there is a symbiotic relationship between mitochondria and the mitotic spindle, where close association between the two organelles facilitates the positioning of both: while the spindle helps to segregate mitochondria equally among the nascent daughter cells, mitochondria decrease spindle rotation and thus promote spindle alignment.

The Role of Kinesin-8 in Nuclear Centering. Centering of the cell nucleus is important for proper organization of the intracellular space, as well as for positioning of the growth regions and the division plane. Forces responsible for nuclear centering in fission yeast interphase cells are generated by 3-5 bundles of microtubules, which extend along the major axis of the cell. Each bundle consists of 2-4 microtubules with their minus ends associated with the nucleus, and the plus ends pointing towards the cell ends. Microtubule length is regulated by the kinesin-8 motors Klp5 and Klp6, which walk towards the plus end of the microtubule and promote microtubule catastrophe (a switch from growth to shrinkage). When the plus end of a growing microtubule reaches the cell end, it generates a pushing force on the nucleus, but how the cell regulates these forces in order to center the nucleus remains unknown. Here we tackle this problem by using a combination of live cell imaging, cell manipulations by laser ablation and optical tweezers, and a theoretical model. By comparing the nuclear positioning in wild-type cells and in mutant cells deleted for Klp5, we found that in wild type the distribution of the position of the nucleus is narrower than in the mutant. To explain this effect we developed a model for nuclear centering: The model includes dynamic microtubules and plus end directed motors. The microtubule pushing force is described by a force-velocity relationship. We could reproduce the difference in nuclear centering observed in the Klp5 deleted cells in comparison with wild type only by assuming that Klp5 motors change the force-velocity curve. We propose that cells, in order to position organelles, employ kinesin-8 motors to regulate the microtubule pushing forces.

Aging. Aging and eventual death has fascinated humans since ancient times, yet a central question remains unanswered: Is aging inherent to all living organisms? In unicellular organisms, replicative aging

is defined by a slow-down of cell division as the cells repeatedly divide, caused by inheritance of aging factors such as damaged proteins. We show that the cells of fission yeast do not exhibit replicative aging. We performed a pedigree analysis of microcolonies growing from a single cell. First, in contrast to observations in aging unicellular organisms, slowly dividing mother cells of fission yeast did not give rise to slowly dividing daughter cells. Second, the final cell divisions prior to cell death, when replicative aging should be most pronounced and thus division slowest, were not slower than average. Finally, no slow-down of division was observed in cells that repeatedly inherited the old or new cell pole for more than 30 divisions, old or new spindle pole body, a larger or a smaller part of the cytoplasm. Moreover, damaged proteins from the mother cell, visualized by a GFP-tagged chaperone Hsp104, were distributed randomly between the daughter cells. Together our results suggest that a fission yeast colony does not accumulate damage in a lineage of cells and thus does not exhibit aging. In contrast to most organisms, which segregate damage to aging cells in order to produce offspring with high replicative potential, fission yeast may be following a different life strategy that relies on maintenance of the replicative potential of all cells. This highlights fission yeast as a potential cellular model for human non-aging cells, such as cancer, germ, and stem cells.

Cooperations

Frank Jülicher, mpi**pks**: Modeling of nuclear oscillations and centering

Nenad Pavin, University of Zagreb, Croatia, and mpi**pks**: Modeling of nuclear oscillations and centering, search for kinetochores

Thilo Gross, mpi**pks**: Aging and protein aggregation in symmetrically dividing cells

Benjamin Lindner, mpi**pks**: Search for kinetochores

Stefan Diez, MPI-CBG, Dresden: *In vitro* reconstitution of nuclear oscillations

Frank Bradke, MPI of Neurobiology, Martinsried: The role of centrosomes in neuronal growth

Juraj Gregan, University of Vienna: Tension on mitotic chromosomes

Junior Research Group: Motor Systems

(Head: Dr. Stephan W. Grill)

Our group is interested in how molecular machines, the workhorses of the cell, function collectively to give rise to the complex dynamical processes observed in living organisms. The whole is greater than the sum of the parts. In this spirit we pursue an understanding of how molecular mechanisms give rise to specific behaviors that emerge at length and time scales relevant for processes at the cell biological level, using a combined experimental and theoretical approach. The main focus of our lab concerns the dynamics of the actomyosin cytoskeleton and its relation to molecular mechanisms. We also investigate transcription of DNA into RNA and the relation to molecular events that occur in the machinery that is involved.

Cytoskeletal Systems. To date, systematic approaches that link physical mechanisms at the molecular scale to emergent behaviours at the cellular scale are missing. We bridge this gap, and combine theory and experiment to investigate the interplay between cellular mechanics and regulatory biochemistry in the context of cell polarization in *Caenorhabditis elegans* embryos.

We are interested in how the actomyosin cytoskeleton behaves at a coarse-grained and cell-scale level. We investigate the cell cortex in the one cell stage *C. elegans* embryo, which undergoes large-scale actomyosin cortical flow prior to its first mitosis in order to polarize the cell. We characterize cortex structure and dynamics with imaging techniques and with biophysical techniques, such as cortical laser ablation and quantitative photo-bleaching experiments. We develop and employ novel theoretical approaches to describe the emergent cell scale mechanical behaviour in terms of an active complex fluid. Finally, we utilize approaches from molecular biology and genetics to understand how these emergent mechanical properties are influenced by molecular activities.

A particular focus lies in approaches to understand the interplay between regulatory biochemistry, operating through PAR polarity proteins, and cell-scale cytoskeletal mechanics. We investigate this interaction, which is crucial to the development of all animals, by studying pattern formation in active fluids. Here, active stress is regulated by diffusing molecular components. Nonhomogeneous active stress profiles create patterns of flow which transport stress regulators by advection. For example, a single diffusing species

that up regulates active stress, can generate steady flow and concentration patterns. This work describes a novel mechanism of pattern generation. It extends the original work of Alan Turing describing how two chemical species diffuse and react with one another to generate spatial patterns, to include active mechanical stresses, deformation and transport of the material in which the chemical species diffuse.

We apply this general approach to understand how mechanics and biochemistry interact in the process of polarization of the *C. elegans* embryo. We use optical techniques to characterize the motility of specific proteins that are part of the associated regulatory biochemical pathways. We investigate their abilities to form patterns in the framework of reaction-diffusion. We find that this mass-conserved system can self organize and switch from a stable unpolarized state into a polarized state in response to stimuli. Importantly, flows of the actomyosin cortex generate perturbations in the spatial distributions of the proteins that are part of the regulatory pathways. If sufficiently large, these perturbations trigger polarization of an otherwise stable unpolarized state. These findings describe a novel mechanism by which cortical flows are able to localize the components that specify an axis within the cell, which is an essential process in the development of each and every animal.

Transcriptional Systems. RNA polymerase is the molecular machine responsible for reading out the genetic code stored within DNA in the form of an RNA transcript. This transcript is later used for translation into the precise amino acid sequence that forms the protein product, which is of course encoded by the sequence of DNA that was originally read out. Since the production of each and every protein in a cell commences with this process of information transfer, RNA polymerase represents a central control point for all cellular functions and behaviors. We investigate how this machine moves along the DNA template, and how it ensures that a minimum number of copy mistakes is made. We ask if a large part of the irregular behavior observed in transcription is a direct consequence of the need for rapid production of long high-fidelity transcripts. By extending established theoretical proofreading schemes to include transcript shortening, we build a quantitative stochastic model coupling transcriptional proofreading and chain elongation. Through this we elucidate the precise interplay between transcriptional pauses, fidelity, polymerization rate, and nucleotide consumption. This reveals a mechanism whereby slow and irregular transcription at the level of individual polymerases leads to astronomical gains in the production rate and nucleotide efficiency with which long and high-fidelity transcripts can be produced. These theoretical investigations are complemented by the construction of a high-resolution dual-trap optical tweezer apparatus, which is complete. We currently utilize this microscope to test theoretical predictions regarding the transcriptional progress of polymerase molecules, by monitoring and manipulating one molecule at a time.

The group is jointly appointed to the MPI-CBG and mpi**pks**, was started in 2006, and has grown to full size over the past couple of years. Stephan Grill received the ARCHES Prize of the German Ministry of Education and Research in 2009, the European Molecular Biology Organization (EMBO) young investigator award in 2010, and the Paul Ehrlich- und Ludwig Darmstaedter-Nachwuchspreis for biomedical research in 2011.

Cooperations

Ohad Medalia, University of Zurich: Ultrastucture of the actomyosin cortex

A. A. Hyman, MPI-CBG: Cortical polarization in *C. elegans*

J. Howard, MPI-CPfS: Single cell perturbation experiments

F. Jülicher, mpi**pks**, Dresden: Active Polar Gels

C. Müller, European Molecular Biology Laboratory, Grenoble Oustation, France: Transcription by RNA Polymerase III

J. M. R. Parrondo, Universidad Complutense de Madrid, Spain: Irregular dynamics for transcriptional proofreading

1.10 Advanced Study Groups

Advanced Study Group 2010: Unconventional Magnetism in High Fields
(Convenor: Dr. Mike Zhitomirsky)

The Advanced Study Group (ASG) "Unconventional Magnetism in High Fields" was installed for a five-month period from April to September, 2010 with the aim to investigate novel field-induced phenomena in geometrically frustrated and quantum magnets. The ASG activity was coordinated with the Division of Condensed Matter and the research group "New States of Quantum Matter." A second goal was to promote scientific collaboration with experimental groups from the Dresden High Magnetic Field Laboratory (HMD), the Max Plank Institute for Chemical Physics of Solids (MPI-CPfS), and the Institute for Solid State and Material Research (IFW). The group members were Andrey Chubukov (University Wisconsin-Madison), Peter Holdsworth (ENS, Lyon), Frederic Mila (EPFL, Lausanne), and Mike Zhitomirsky (C.E.A., Grenoble). In addition the ASG hosted 30 long- and short-term visitors. A special seminar series was organized at the mpi**pks** with more than 25 presentations given by our members and visitors, as well as by invited speakers from the neighboring institutes. A. Chubukov was also one of the scientific coordinators of the workshop on "Emergent Quantum States in Complex Correlated Matter" that took place at the mpi**pks** on August 23–27, 2010. Principal directions of research were as follows:

Quantum spin-nematic state. Enhanced quantum fluctuations may destroy conventional long-range magnetic order and stabilize a spin analog of liquid crystals—a state with partially broken rotational symmetry characterized by tensor order parameter. Such a new illusive state of matter has attracted a lot of theoretical interest in the past, but has never been discovered so far in real materials. Motivated by a number of recently studied frustrated magnetic materials we explore a new root to the spin-nematic phase based on the formation of bound magnon pairs in quantum antiferromagnets with competing antiferro- and ferromagnetic interactions [1], see also the research part 2. The bound magnon states are formed in the fully polarized phase in high magnetic fields and undergo a Bose condensation transition with decreasing field prior to the conventional single-magnon condensation. The resulting condensate of magnon pairs has direct similarities with the Cooper pair condensate in superconductors. In addition, the pair condensate remains invariant under π-rotation about the field direction reflecting the quadrupolar nature of its order parameter. The developed theory predicts presence of the spin-nematic phase in the frustrated chain material $\mathrm{LiCuVO_4}$. Very recent high-field experiments have indeed found a new phase in this compound above 40 T. We have further examined the stability of bound magnon pairs in a variety of frustrated models including planar magnetic systems, which are now extensively studied at MPI-CPfS.

Monopole dynamics in spin ice. The fractionalization of magnetic dipoles into free and deconfined magnetic charge (monopoles) is a direct consequence of the extensive ground state degeneracy, which constitutes a vacuum for the quasi-particle excitations. We have modeled the ac susceptibility measurements on the spin ice material $\mathrm{Dy_2Ti_2O_7}$ by the diffusive dynamics of this Coulomb gas of quasi particle interactions [2]. In parallel with these developments novel experiments have been devised to measure the magnetic charge of the quasi-particles using the Wien effect. We provided theoretical support for a Wien effect experiment [3] in which the magnetic response of a crystal of $\mathrm{Dy_2Ti_2O_7}$ to a small magnetic field (1 to 10 Gauss only) was measured in a SQUID magnetometer specially designed to deal with very low fields. The results were interpreted in analogy with the dielectric response of a leaky capacitor, with magnetic relaxation due to both bound and free magnetic charges. Through this quantitative analysis we were able to confirm the predicted value of the magnetic charge associated with a Monopole excitation and illustrate the validity of the Wien effect for this magnetic Coulomb gas system. Finally, we continued projects dedicated to the topological properties of the vacuum of spin ice state. We have previously shown that, applying a bond distortion, reducing the symmetry of the manifold of vacuum states to Z_2 leads to a multicritical mean field phase transition. We began investigating the finite size scaling behavior of this transition, with particular interest in the identification of Gaussian fluctuation terms [4]. This system maps onto the six-vertex model, which in two dimensions is integrable. The transition has not previously been interpreted in terms of mean field and Gaussian fluctuations.

Unconventional phases of cold atomic gases in optical lattices. Lattice spin systems in a magnetic field can be directly mapped onto the hard-core boson models due to the equivalence between $SO(2)$ and $U(1)$ symmetry groups. Generalization of the effective spin interaction from the conventional $SU(2)$ to the $SU(3)$ symmetric potential was undertaken in [5]. It further allows the use of spin language to

describe the physics of three-flavor fermionic atoms in optical lattices. A number of surprising results, such as the three-sublattice ordered pattern on a bipartite lattice and the different role played by quantum and thermal fluctuations were obtained. Enhanced symmetries in the cold atomic gases were also the main topic of the effective field-theoretical study in [6], where the presence of multipolar states was established for spin-3/2 fermions near the half-filling.

Theoretical models for frustrated magnetic materials. The frustrated pyrochlore material $\mathrm{Er_2Ti_2O_7}$ exhibits a unique nonplanar magnetic structure. Based on the nature of the lowest-energy crystal-field levels we derive an effective theoretical model for $\mathrm{Er_2Ti_2O_7}$: a quantum spin-$1/2$ XY antiferromagnet on a pyrochlore lattice [7]. The analytical calculations for this model show that zero-point fluctuations select the experimentally observed magnetic structure out of infinitely degenerate manifold of classical ground states. Theoretical support was also provided for the ultrasonic experiments on the spinel antiferromagnet $\mathrm{CdCr_2O_4}$ in high magnetic fields [8].

The fractional magnetization plateau and new high-field phases in the triangular antiferromagnet $\mathrm{Cs_2CuBr_4}$ provide further interesting example of the order from disorder phenomenon in magnetism. Theoretical description of this material requires extension of the previous results to the case of the spatially anisotropic lattice. The anisotropic triangular antiferromagnet was theoretically studied using symmetry analysis and the semiclassical large-S expansion near the saturation field H_s and close to $\frac{1}{3}H_s$ [9]. The nontrivial behavior was found for a range of parameters including presence of a classically unstable incommensurate planar "fan" state, a non-coplanar double-spiral phase, and two non-coplanar cone phases with and without broken Z_3 symmetry.

One additional research topic in this direction was the investigation of the effect of the Dzyaloshinskii-Moriya (DM) interaction in strongly frustrated magnets. Although the DM term is nominally weak, at most a few percent of the dominant exchange interaction, its role can be significant in frustrated magnets, where the ground state is highly degenerate at the classical level and where there is a high density of low-energy, excitations close to condensation. The effect of the DM interaction was studied for the spin-$1/2$ kagome antiferromagnet [10], realized in herbertsmithite, and for the orthogonal dimer material $\mathrm{SrCu_2(BO_3)_2}$ [11]. The joint project with the ESR group at HMD was devoted to the investigation of magnetic excitations in copper pyrimidine dinitrate, a spin-$1/2$ antiferromagnetic chain with both alternating g-tensor and the DM interactions. A transition from the sine-Gordon region (with soliton-breather elementary excitations) to a spin-polarized state (with magnon excitations) was identified at $H_s \approx 48.5$ T. This interpretation is further confirmed by the quantitative agreement with the numerical DMRG results for a spin-$1/2$ Heisenberg chain with a staggered transverse field, over the entire field range of the experimental data.

Unconventional spin dynamics in high fields. Surprisingly enough, the dynamical properties of all quantum antiferromagnets undergo rather dramatic transformation in strong magnetic fields even at zero temperature. This is related to the field-induced spontaneous magnon decays, which are determined by cubic anharmonicities in the effective boson Hamiltonian. There is a deep analogy between cubic nonlinearities in the magnon Hamiltonian of a noncollinear antiferromagnet and the presence of similar interaction terms in a superfluid boson systems. An interesting aspect of the dynamics in two-dimensional quantum spin systems is the decay enhancement due to Van Hove singularities in the two-particle density of states. A self-consistent regularization scheme was developed for a model example of the square-lattice Heisenberg antiferromagnet, which exhibits decay dynamics in the vicinity of the saturation field [13]. General aspects of magnon-magnon and magnon-phonon interactions on the thermal transport, including the role of spontaneous decays, were treated in [14].

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Advanced Study Group 2010: Quantum thermodynamics of finite systems
(Convenor: Prof. Dr. Gerhard C. Hegerfeldt)

Members: J. Gonzalo Muga (Universidad del Pas Vasco, Spain), Larry Schulman (Clarkson University, USA), Bernard Gaveau (Universit Paris VI, France), Giulio Casati (Universit degli Studi dell' Insubria, Italia), Rafael Sala-Mayato (Universidad de La Laguna, Spain)

The Advanced Study Group took place from June to September 2010. The composition of the group changed with time and as a consequence the research persued and the emphasis put on different research topics also changed with time.

From the start of the ASG, Gaveau, Schulman and the convenor were present. The two former continued to wrestle with their thermodynamics research on power, small engines and entanglement. Interpreting the "study" mandate broadly, there was an intense interaction for a week with a visitor from Athens, Antigone Nounou, a philosopher with physics background and interests in gauge fields and the Aharonov-Bohm effect. Antigone Nounou is one of those participating in a current debate in the philosophy community on the *reality* of gauge fields. During her visit to the mpi**pks** she gave a rousing seminar on "explanation", "rousing" in the sense that some of those who attended were roused from skepticism and self-assurance, to realize that it can sometimes be difficult to know what we mean as explanation. The reality debate can likewise be difficult for the physicist to appreciate, but in any case the question she raised challenged Schulman's notion of how to deal with multiple connectness in the path integral. The outcome was a preprint, co-authored by Gaveau, Nounou and Schulman, in which the original homotopy ideas retain their validity in the context of the time-dependent Aharonov-Bohm effect. There was also overlap with the convenor's recent explanation of the Aharonov-Bohm effect through forces.

While the advanced study group was in session quite a number of workshops and conferences were held at the mpi**pks**, and of course the participants of the ASG took the opportunity to attend some of the lectures. In a workshop on BEC at the mpi**pks** there was a talk by J. Schmiedmayer (Vienna) reporting experimental work relating to thermalization for atoms in traps. This was of obvious interest for us, and during discussions with him he suggested inviting I. Mazets from his group as a visitor to the ASG. The latter's visit led to an intense interchange on thermalization in quantum optics.

As regards the number of members and visitors present, August was the busiest month. The members Gonzalo Muga, Larry Schulman, Bernard Gaveau, Rafael Sala-Mayato and the convenor were joined toward the end of August by Giulio Casati. The visitors in August included Yair Ezer, Erik Kosloff, Erik Torrontegui, David Guery-Odelin, Andreas Ruschhaupt, Daniel Alonso, and Günter Mahler who visited for three weeks.

The collaboration of A. Ruschhaupt and G. Muga with G. Mahler, with his expertise, clarified a thermodynamical description of one-way barriers and atom diodes. The overlap with Casatis group was also stimulating, as they propose heat-one-way barriers. These are mostly classical devices, and the challenge was to find a quantum physical implementation.

During an informal talk by R. Sala-Mayato on the problems he was investigating with G. Muga the convenor remarked on a connection to the measuring problem as formulated by von Neumann and later somewhat differently by Lüders. Out of this remark has grown a collaboration on how to possibly distinguish experimentally between these two approaches.

In the last month of the ASG, the thermoelectric effect and the associated thermodynamic efficiency, written in terms of the so-called figure of merit ZT, was examined in great detail in joint discussions by Casati and participants of the ASG. In particular the increase of ZT was investigated. The understanding of the possible microscopic mechanism leading to an increase of ZT is at present quite limited. These common sessions took place every day and lasted several hours each day. The main point is that dynamical nonlinear systems may provide a new approach to the problem and may allow to unveil the physical mechanisms which may lead to high thermoelectric efficiency. As a result of these discussions several lines of future research have been proposed, discussed and determined. Research along these lines is now in progress as a collaboration among different scientists who have participated in the study group.

Participants of the ASG established fruitful interactions with other researchers of the mpi**pks** and with members of the Technical University of Dresden, in particular with Masudul Haque, Ingrid Rotter and Mark Mineev-Weinstein from the mpi**pks** as well as with Alexander Eisfeld and Roland Ketzmerick from the university.

The breadth of the topics treated in the Advanced Study Group is best illustrated by listing the seminars given by participant and local scientists:

Larry Schulman: "Clusters from higher order correlations"

Ingrid Rotter: "The role of exceptional points in quantum systems"

Mark Mineev-Weinstein: "Universality and Mathematical Structure of Laplacian Growth"

Antigone N. Nounou: "Scientific models and the Aharonov-Bohm effect"

Gerhard Hegerfeldt: "A fresh look at the Aharonov-Bohm effect: A physical understanding through the forces in action"

Noam Erez: "Heating and cooling by measurement: Zeno meets Lindblad"

Ronnie Kosloff: "Introduction to reciprocating Quantum Refrigerators"

Gonzalo Muga: "Shortcuts to adiabaticity"

Igor Mazets: "Thermalization and correlations in quasi-1D ultra-cold atomic gases"

Daniel Alonso: "Decoherence in a quantum harmonic oscillator monitored by a Bose-Einstein condensate"

Andreas Ruschhaupt: "Atom Diode – a laser-based device for uni-directional atomic motion"

Günter Mahler: "On the emergence of irreversibility"

Bernard Gaveau: "Work and power for stochastic dynamics"

Giuliano Benenti:"Microscopic mechanism for increasing thermoelectric efficiency"

Tomaz Prosen: "Transport in quantum spin chains far from equilibrium"

Martin Horvat: "Some recent developments in the classical theory of thermo-electricity"

Carlos M. Monasterio: "On the thermoelectric efficiency and anomalous heat and charge transport"

Keiji Saito: Generating Function Formula of Heat Transfer in Harmonic Networks

Stefano Lepri: "Wave rectification in nonlinear dynamical systems"

Marko Znidarich: "Quantum nonequilibrium steady states: An exact solution"

Giulio Casati: Thermoelectric efficiency

In summary, the Advanced Study Group has been an ideal framework for making important progress on generic aspects of Quantum Thermodynamics of Finite Systems and on a number of specific objectives. The participants thank the Max Planck Institute for the Physics of Complex Systems for making this endeavor possible. The research started in this summer will lead to quite a number of publications which are presently being prepared.

Advanced Study Group 2008/2009: Quantum Aggregates
(Convenor: Prof. John S. Briggs)

The aim of the ASG was to advance the theory of the spectra and dynamics of quantum aggregates with special emphasis on aggregates of large organic molecules including the photosynthetic unit and aggregates of ultra-cold atoms in traps. These topics were singled out, partly on account of my own background in both atomic and organic molecule physics, but also because of the presence at **mpi**pks of the groups of Dr. Eisfeld and Dr. Pohl who work in precisely these two areas. Indeed throughout the five-month existence of the ASG there was a close collaboration of the Members and Visitors with these groups. Drs. Eisfeld and Pohl, and their co-workers, were present at all seminars and discussions organized within the ASG. The group began its activity on 12^{th} October 2008 with Members Briggs and Kleber in attendance. All visitors gave seminars on each and every visit. The first was J.Macek, a world expert in atomic theory, already in late October. At the same time V.Malyshev visited and a collaboration with Dr. Eisfelds group was initiated. In November the first Visitor working in the field of cold atoms, I. Lesanovsky was welcomed to Dresden. Again a collaboration with Dr. Pohls group ensued. A major activity took place from 10 to 15 November when several Visitors were simultaneously present and a round of discussions culminated in a mini-conference including contributions ranging from biology to solid-state physics. The programme is attached.

In January attention turned to cold atoms with the visit of M.Weidemueller and co-worker Ch. Hofmann for one week. Here, apart from Weidemuellers seminar there were daily meetings on the subject of cold Rydberg atoms. The weeks following, January 21 - 29 saw a repeat of the November brainstorming week with five Visitors present to discuss theoretical work on the transfer of electronic excitation on molecular aggregates. The resumption of activity in March saw the arrival of Member P.Reineker, an expert on the physics of vibronic coupling on aggregates. Another world leading authority on vibronic coupling, V.May made another visit in March and this provided a great stimulus to the work of the ASG. Perhaps the high point of the ASG was right at the end, April 21 - 24, when the Workshop on Quantum Aggregates was attended by all Visitors and several other leading scientists in the field.
At the final discussion round-table on Friday 24 April it was agreed unanimously that the interdisciplinary activity had been enriching scientifically for all concerned. In particular both Visitors and other participants at the Workshop expressed the wish that a larger conference should be held soon and an ongoing research programme in the field of Quantum Aggregates be established in Germany with the aim of emphasizing the unity of theoretical approaches in the diverse types of quantum aggregates studied during the course of the ASG. A proposal for a DFG Schwerpunktprogramm has been submitted and a decision is expected in early 2011.

Publications and Collaborations During the course of the ASG several collaborations were initiated between Members,Visitors and members of staff of mpi**pks** with the aim of submitting joint papers for publication.

The following publications arose out of the ASG:

1. J.Roden, G.Schulz, A.Eisfeld and J.S.Briggs, Energy Transfer on a Vibronically-Coupled Quantum Aggregate. Chem. Phys. 131, 044909 (2009).
2. J. H. Macek, J. B. Sternberg, S. Y. Ovchinnikov, and J. S. Briggs, Theory of Deep Minima in (e,2e) Measurements of Triply Differential Cross Sections Phys. Rev. Lett. 104, 033201 (2010)
3. Eisfeld, A.; Vlaming, S. M.; Malyshev, V. A. & Knoester, J. Excitons in Molecular Aggregates with Lévy-Type Disorder: Anomalous Localization and Exchange Broadening of Optical Spectra Phys.Rev.Lett. 105, 137402 (2010)
4. Philipp O.J. Scherer , Sighart F.Fischer, Coherent excitations in photosynthetic systems, in "Theoretical Molecular Biophysics", Springer 2010, p.269.
5. I.Lesanovsky, Th. Pohl and A.Eisfeld, Coherent Ionic propagation on Cold Atom Aggregates.(to be submitted)
6. Roden, J., Eisfeld, A., Dvorak, M., Bünermann, O. & Stienkemeier, F. (2011) "Vibronic Lineshapes of PTCDA Oligomers in Helium Nanodroplets" J. Chem. Phys. In press
7. Roden, J., Strunz, W. T. & Eisfeld, A. (2011) "Non-Markovian quantum state diffusion for absorption spectra of molecular aggregates" J. Chem. Phys. In press
8. C.Warns, I.J. Lalov and P.Reineker, Donor/acceptor molecular aggregates: Vibronic spectra of mixed Frenkel and charge-transfer excitons. Jour.Luminescence 129,1840 (2009).
9. V. May: Beyond the Förster Theory of Excitation Energy Transfer: Importance of Higher-Order Processes in Supramolecular Antenna Systems, in: Villy Sundström (ed.), "Solar Energy Conversion" (special issue) Dalton Trans. 45, 2009, 10086.DOI: 10.1039/B908567J
10. G. Kyas and V. May: Density Matrix Based Microscopic Theory of Molecule Metal-Nanoparticlei Interactions: Linear Absorbance and Plasmon Enhancement of Intermolecular Excitation Energy Transfer J. Chem. Phys. 134, 034701 (2011).
11. J. Megow, B. Röder, A. Kulesza, V. Bonacic-Koutecky, and V. May: A Mixed Quantum-Classical Description of Excitation Energy Transfer in Supramolecular Complexes: Förster Theory and Beyond, in Theodor Förster commemorative issue, ChemPhysChem (in press).
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13. Eisele, D. M.; Knoester, J.; Kirstein, S.; Rabe, J. P.; Vanden Bout, D. A., Individual nanotubular J-aggregates with highly uniform exciton fluorescence on solid substrates, Nature Nanotechnology, 4, 658 (2009).
14. Lyon, J. L.; Eisele, D. M.; Kirstein, S.; Rabe, J. P.; Vanden Bout, D. A.; Stevenson, K. J, UV-vis Spectroscopy and Cyclic Voltammetry Investigations of Tubular J-Aggregates of Amphiphilic Cyanine Dyes, ECS Transactions 16(28), 77-84 (2009).

Chapter 2

Selection of Research Results

2.1 Photo Activated Coulomb Complexes

CHRISTIAN GNODTKE, ALEXEI MIKABERIDZE, ULF SAALMANN, JAN M ROST

We introduce Coulomb complexes and investigate their properties [1]. They offer analytical insight into the highly non-linear dynamics of multiphoton absorption by many electrons in a large molecule or cluster as a result of irradiation with an intense laser pulse. Coulomb Complexes explain the shape of the photo electron spectrum for moderate laser intensity as found in the experiment and deliver a transparent understanding of high energy wings in the electron spectrum observed in xenon clusters [2].

Multiphoton absorption occurs when matter is illuminated by intense light fields. Historically, it was discovered in atoms where one bound electrons can absorb many photons giving rise to phenomena such as high harmonic generation (HHG) and above threshold ionization (ATI).

In extended systems, such as clusters or quantum dots, a delocalized electron cloud can form a nanoplasma which absorbs efficiently many photons through (classical) resonant coupling [3]. For two-component systems where the center material has lower ionization potential than the hull (e.g, a xenon cluster embedded in a helium droplet), dramatic "catalytic" effects can occur: While the pristine helium cluster is transparent for radiation of $I = 7 \times 10^{14}\mathrm{Wcm}^{-2}$ or less with photons of 1.2 eV energy, a dozen xenon atoms in the center is sufficient to remove *all* electrons from their bound orbitals of up to 10^5 helium atoms. This happens since (owing to the linear polarization of the light) a cigar-shaped electron plasma is formed as sketched in Fig. 1. It remains resonant along the laser polarization with the frequency of the light for a long time [4].

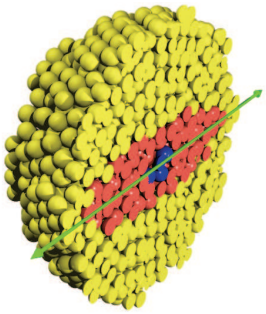

Figure 1: Schematic cut through a xenon cluster (blue) embedded in helium (yellow and red), where red indicates ionized helium and therefore the cigar-shaped nanoplasma. The green line is the laser polarization, after [4].

For higher photon frequencies of the order of the ionization potential of atoms ($\sim$ 12 eV), a new absorption mechanism becomes relevant: inverse Bremsstrahlung [5]. Increasing the photon energy even further to XUV frequency (100 eV) and beyond up to X-rays, the multiphoton light-matter coupling changes drastically its character compared to 1.2 eV photons. Now, multiphoton absorption is realized by different atoms absorbing one photon each. During the short time when the laser pulse rises a separation of positive (ions) and negative charge (electrons) is realized. The latter remain partially bound to the ion cloud as a relatively cold plasma. The Coulomb forces among all charged particles completely dominate the dynamics and induce general properties to such "Coulomb Complexes" (CC), irrespectively of the exact nature of their atomic constituents.

Photo activation of Coulomb Complexes Since the Coulomb forces dominate the dynamics we only need to describe the number of electrons $N(t)$ photo ionized during a laser pulse. Assuming a Gaussian envelope for the pulse with peak intensity I_0, half width $T = 2\tau(\ln 2)^{1/2}$ and atomic single ionization with a cross section σ_ω, we get $N(t) = N_\infty/2[1 + \mathrm{erf}(t/\tau)]$, where $N_\infty = N_A\sigma_\omega I_0\tau/\omega$ with N_A atoms in the CC. The separation of charges with N_∞ negative electrons leads to a positive background charge $Q = N_\infty$. For simplicity we assume here a homogeneous charge distribution and a spherical shape of the original cluster of atoms with radius R so that the potential created is that of sphere with constant charge density, trivially Coulombic $U(r > R) = -Q/r$ outside the cluster and

$$U(r \le R) = -\frac{Q}{2R}(3 - (r/R)^2) \qquad (1)$$

inside. All N electrons eventually activated in a random sequence at random atomic positions inside the cluster exert their electrostatic (Coulomb) forces from the beginning in order to avoid discontinuities upon photo activation. The latter means operationally in our approach that the electron to be activated switches from infinite mass to its natural mass and starts to move. For now, we also assume the laser pulse to be such that the ions are static during the pulse so that the background potential does not change. This restriction can be lifted in future studies.

Analytical properties of Coulomb complexes The main motivation behind our formulation of Coulomb complexes is to work out analytical properties. They remain buried in simulations which, of course, describe specific situations more accurately. One of them is the

sequential emission shape (SES) of a Coulomb complex, namely that the photo electron spectrum has a characteristic plateau (see Fig. 2). It has been observed in the experiment [6] as well as in simulations [7] but without an understanding of its origin. For a CC the plateau can be easily derived: Sequential emission implies that an electron which leaves the CC of charge Q' does not influence the escape of the next electron which sees a charge $Q'' = Q' + 1$. Since its not known from which position in the CC the electron with final energy E is released, one has to integrate over all possible initial positions in the volume V of the CC,

$$dP/dE(Q') = V^{-1} \int_V d^3r \delta(E - \epsilon - U(r)) \,. \qquad (2)$$

The final energy distribution dP/dE is obtained by integrating over all charges Q' in (2),

$$dP/dE = V^{-1} \int_0^Q dQ' \int_V d^3r \delta(E - \epsilon - U(r)) \,. \qquad (3)$$

Interchanging the sequence of integration and realizing that $U(r)$ is linear in Q' (see (1)), the emergence of a plateau for dP/dE is obvious. It is limited to energies E for which the δ-function in (3) can be fullfilled.

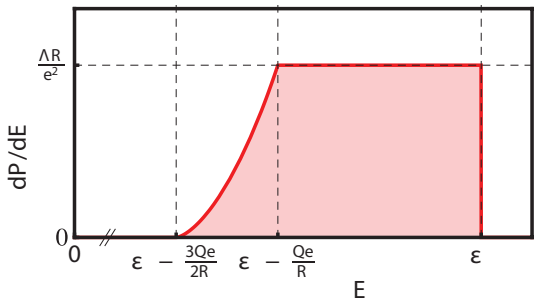

Figure 2: Analytical electron spectrum dP/dE for a CC with radius R, charge Q and excess energy ϵ; Λ is a universal constant $\Lambda = 3^{3/2} \ln(2 + \sqrt{3}) - 6$ and e is the elementary charge.

The CC reveals another analytical property: The parameters involved in photo activation of large systems are not independent of each other namely the triple (R, ϵ, T) characterizing a CC of radius R, atomic excess energy after photoabsorption ϵ and pulse length T also describes a one-parameter family of CCs with $(\eta^{-1}R, \eta\epsilon, \eta^{-3/2}T)$, with $\eta > 0$ as illustrated in Fig. 3.

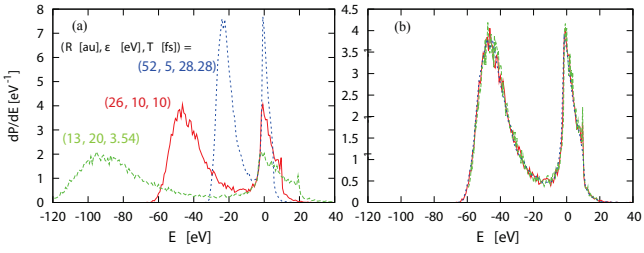

Figure 3: Electron spectra dP/dE for different Coulomb complexes (R, ϵ, T) as given in (a) and related by the scaling parameter $\eta = 1, 2, 1/2$; (b) the rescaled spectra $\eta^{-1} dP(\eta E)/dE$, after [1].

The double peak structure in Fig. 3 always emerges for a typical CC with the peak at negative energies representing the trapped nanoplasma and the peak for $E > 0$ but below the photo line at $E = \epsilon$ (spike at 10 eV) representing direct escape events.

Understanding experiments with Coulomb Complexes Thomas Möller and his group at the TU Berlin performed an experiment with xenon and Argon clusters under light of 90 eV photon enery at the free electron laser FLASH in Hamburg with puzzling result: In general one would expect photo electron signal from a cluster of atoms at the atomic photo line and red shifted since electrons ionized later have to overcome the already existing ion charges upon escape which slows them down. While this was indeed observed in argon, xenon clusters exhibit a wing of photo electrons with energies blue shifted from the atomic line. This wing grows for increasing intensity.

With the help of the Coulomb complex we could show that this wing develops for xenon due to the fact that a large number of photons are activated in a very short time due to photo absorption close to the giant resonance frequency xenon (90 eV). This results in energy changing collisions of the electrons in the continuum before they leave the CC and therefore to some electrons which are faster than produced by atomic photo ionization. If the density of photo activated electrons is reduced (which can be achieved by either reducing the laser intensity or using another element with lower photo cross section, e.g., argon), the blue wing vanishes and the dynamics approaches the limit of sequential emission [2]. Indeed, such electrons are already visible in the typical CC spectrum of Fig. 3 with a small probability beyond the spike of the atomic photo line at 10 eV.

US and JMR thank the KITP in Santa Barbara for hospitality and support of this work.

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2.2 Molecular bond by internal quantum reflection

WEIBIN LI, ELIAS DIESSEN, THOMAS POHL, JAN M ROST

Recently, the existence of ultralong range molecules has been demonstrated experimentally [1]. Reproducing theoretically the measured spectral lines of the Rb_2^* Rydberg molecule quantitatively [2], turned out to be much more difficult than anticipated with the benefit of a few surprises on the way: (i) The spectrum of excited Rb_2^* is due to internal quantum reflection (IQR) stabilizing the molecule against fast decay into $Rb_2^+ + e^-$. (ii) The experiment did not only generate Rydberg dimers but also trimers. (iii) The homonuclear Rb_2^* molecule has a permanent dipole moment [3].

Proposed with a simple consideration [4] and supported by extensions to trimers [5] and borromean dimers [6], the measurement of the entire excitation spectrum of a long range Rydberg dimer motivated us to investigate the spectrum theoretically. The difficulties encountered as well as the properties (i) and (iii) are related to the fact that the low energy collision $Rb+e^-$ has a p-wave shape resonance which means that one has to include not only s-wave scattering but also the p-wave scattering to describe the collision of the electron at position $\mathbf{r}$ with the ground state atom at $\mathbf{R}$.

Theoretical approach The hamiltonian reads

$$H = \mathbf{p}^2/2 - 1/r + V \equiv H_0 + V(\mathbf{r}, \mathbf{R}) \qquad (1)$$

with the additional pseudo potential due to the ground state atom

$$V(\mathbf{r}, \mathbf{R}) = 2\pi\delta(\mathbf{r} - \mathbf{R}) \left(A_s(k) + 3A_p(k)^3 \overleftarrow{\nabla} \cdot \overrightarrow{\nabla} \right) , \quad (2)$$

where $A_s(k)$ and $A_p(k)$ are the energy dependent scattering lengths for s- and p-wave scattering and k is semiclassically defined through the energy of the isolated Rydberg atom $E_n = k^2/2 - 1/R$. Since the potential is energy dependent, a formally correct solution must proceed via the construction of a Green function [2] which produces for fixed $\mathbf{R}$ molecular potential curves $U(R)$, see Fig. 2.

To get the spectrum (Fig. 1) of the Rydberg molecule, one needs to solve the vibrational Schrödinger equation with $U(R)$ which is far from the standard routine for two reasons: First, we are at a highly excited manifold and when the two atoms come together, the molecule decays into $Rb_2^+ + e^-$. Hence one has at $R = 0$ an open boundary condition whose specific nature cannot be determined within the present description. However, what comes as a rescue is the form of the potential: Due to the p-wave resonance it exhibits a steep cliff like shape falling about three orders of magnitude (see inset of Fig. 2) compared to the modulation depth of the potential shown in Fig. 2. This allows one to treat the vibrational motion as a resonance which can decay *inward* as compared to the usual situation of decay when the particles move away from each other. The simplest way to determine the resonance positions is the stabilization method of Hazy and Taylor [7] where one artificially encloses the system in a box with variable size. Here we only put an inner limit R_0 of the box (the outer one is provided by the potential well). The corresponding energies of the bound states are shown in Fig. 3. One clearly sees the resonances as the lines connecting the avoided crossings. The widths can be determined either by binning (Fig. 2b) or from the Wigner time delay [8] (Fig. 1c) in good agreement with each other.

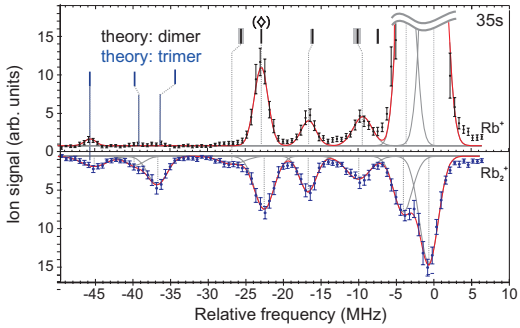

Figure 1: Spectrum for Rb with principal quantum numbers $n = 35$. Frequencies are measured with respect to the atomic transition $5s_{1/2} \rightarrow ns_{1/2}$. The upper parts show the atomic ion spectrum Rb^+ (black) and the lower ones the spectra of the molecular ions Rb_2^+ (blue). Calculated binding energies (table 1) are indicated by vertical lines, for the dimer in black, for the trimer in blue.

Dimers and trimers The positions of the resonances agree well with the experimental ones, see table 1. The situation is similar to other manifolds $n = 36, 37$, also measured in the experiment. The experimental lines missing in the theoretical dimer spectrum are in fact spectral lines of a trimer, formed with two ground state and the Rydberg Rb atoms. The ground state energy E_{00} is to a very good approximation twice the dimer, $E_{00} = 2E_0$, and the missing lines are different excitations of the trimer in its two dimer-like legs. Hence, we can infer from our theoretical analysis that the experiment did not only produce dimers but also trimers in single photon association [2]. The energy spectrum of the latter is very well approximated by the sum of two dimer energies $E_{\nu'\nu} = E_{\nu'} + E_\nu$.

$-E_{ij}$ [MHz]	theory	exp.: Rb_2^+	exp.: Rb^+
E_3	7.8	—	—
E_2	10.7	9.9(7)	8.9(7)
E_1	16.5	16.6(5)	16.5(5)
E_0 ♢	23.1	22.4(5)	22.8(5)
E_{-1}	25.9	26.3(7)	—
E_{12}	33.8	26.3(7)	—
E_{10}	39.6	39.6(12)	—
E_{00}	46.2	45.0(8)	45.5(8)

Table 1: Binding energies oft the 35s dimer E_ν and trimer $E_{\nu'\nu}$ (in blue) of Rb, measured from the atomic $n = 35$ Rydberg line. The experimental positions are given with uncertainties and correspond to the two different decay channels in Fig. 1. The diamond indicates the "ground state" in the outer well, labeled as $\nu = 0$.

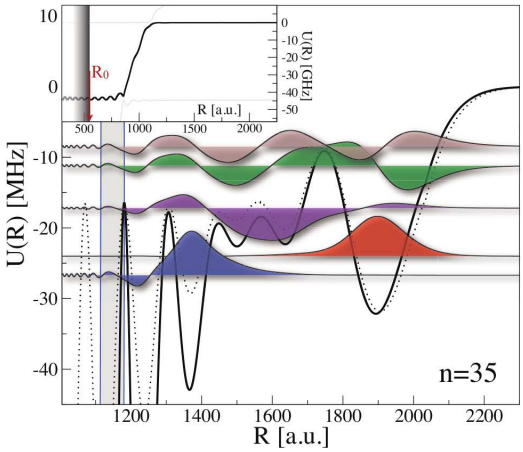

Figure 2: Molecular potential curve for $n = 35$ obtained from the Green function calculation (solid line) and from a model potential (dotted line) taking V in Eq.(2) as a perturbation with an effective scattering length $A_s^{(\mathrm{eff})}$ to reproduce the outermost potential well. The grey area around $R \approx 1200$a.u. marks the region of quantum reflection where the WKB-approximation is not valid. The baseline of the shown molecular wave functions corresponds to their respective vibrational energies. The inset demonstrates the rapid potential drop at the avoided crossing and illustrates the variable inner boundary condition R_0 used for stabilization plot of Fig.3.

Life time of dimer states To experimentally double check the decay rates γ_{IQR} of the states controlled by IQR as predicted in Fig. 3 is not straightforward, since the dimers are embedded in an ultracold gas of Rb atoms. Collisions lead to loss of dimers reducing their lifetime in addition to the finite lifetime of the Rydberg atom. The γ_{IQR} are only an additive contribution to the widths due to these decay mechanisms. However, the γ_{IQR} can be extracted by measuring experimental linewidths $\gamma_{\mathrm{exp}}(\rho)$ as a function of atomic density which allows to separate the collision induced life time by extrapolating the (linear) dependence on atomic density to $\rho = 0$. Moreover, by comparing $\gamma_{\mathrm{exp}}(\rho)$ for a state stabilized by IQR with the width for the ground state E_0, which is stable against the molecular decay, one can deduce from the experiment γ_{IQR}. Since the procedure is quite involved, experimental data has been obtained only for the ground state E_0 of 35s and E_1. The residual experimental decay rate $\gamma_1 = 3.3(12) \times 10^4 \mathrm{s}^{-1}$ is slightly larger than $\gamma_1 = \tau_1^{-1} \equiv (d\theta/dE)^{-1} = 2.47 \times 10^4 \mathrm{s}^{-1}$ calculated from the Wigner time delay (see Fig. 3) as discussed in [9], where also the theoretical decay widths for the other states are given.

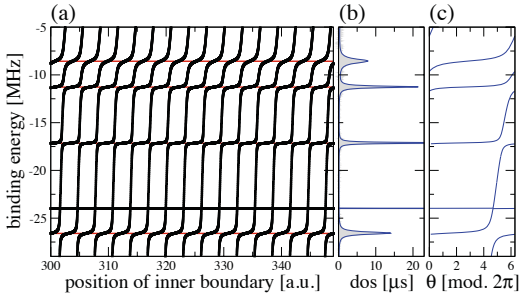

Figure 3: Stabilization plot with the vibrational energies as a function of the position R_0 of the inner boundary (see Fig.2). The density of states (dos) obtained by binning the data of (a) and shown in (b), reveals the energies and widths of the molecular resonances, in perfect agreement with the corresponding results from the Wigner time delay (c).

Dipole moment of the $^3\Sigma(5s - 35s)$ dimer molecule A homonuclear molecule as discussed here with Rb_2^* does normally not possess a permanent dipole moment, whose signature is a linear Stark effect in a small electric field. However, the Rydberg dimer does show a linear Stark effect pointing to a dipole moment of about 1 Debye experimentally as well as theoretically [3]. The reason for this unusual property is again the p-wave scattering resonance which mixes to the dominant 35s atomic Rydberg wavefunction other Rydberg components allowing for the formation of a dipole moment.

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2.3 Modular Entanglement in Continuous Variables

CLEMENS GNEITING, KLAUS HORNBERGER

Is it possible to deduce entanglement from an interference pattern, to perform an "entangled Young experiment", following the famous single-particle interference experiments? In view of the great success and compelling power of single-particle interference experiments for demonstrating the wave-particle duality of material particles, it is natural to ask whether it is also feasible to establish *entanglement* in the motion of material particles by means of *nonlocal* matter wave interference. To be more specific, suppose we hold a two-particle state $\Psi(x_1, x_2)$ which gives rise to a nonlocal interference pattern when subjected to joint position measurements,

$$|\Psi(x_1,x_2)|^2 = w(x_1-x_0)w(x_2+x_0)\cos^2\left(2\pi\frac{x_1-x_2}{\lambda}\right), \tag{1}$$

where the envelope $w(x_1 - x_0)$ localizes particle 1 with an uncertainty $\sigma_x \gg \lambda$ in the vicinity of x_0, and similarly particle 2 around $-x_0$. Obviously, the interference pattern describes correlations in the relative coordinate $x_{\text{rel}} = x_1 - x_2$ of the two particles. But are these correlations necessarily a signature of entanglement? In the case of "EPR states" (e.g. squeezed Gaussian states), entanglement can be deduced from the reduced fluctuations in both the relative coordinate x_{rel} and the total momentum $p_{\text{tot}} = p_1 + p_2$, since the canonically conjugate operator pairs x_j, p_j ($[\mathsf{x}_j, \mathsf{p}_j] = \mathrm{i}\hbar$), $j = 1, 2$, set lower limits to these fluctuations for separable states [1, 2]. In the situation described by (1), in contrast, it is not the relative coordinate that is "squeezed", but its value modulo λ.

In this contribution we show how this observation can be employed to derive an entanglement criterion. The key is to identify *modular variables* [3] as the appropriate pair of "conjugate" observables. The criterion is rooted in a state-independent additive uncertainty relation (UR) for these variables, which remedies the problems arising from the operator-valued commutator appearing in the Robertson UR. We construct a class of non-Gaussian states, denoted *modular entangled states*, which offer natural and robust generation protocols and violate this criterion. The interference pattern in (1) is shown to represent only the weakest form of nonlocal correlations exhibited by this class.

Multi-slit interference To discuss the prerequisites of particle interference and its relation to the modular variables it is instructive to recapitulate the single-particle case first. Ideally, the (transverse) state immediately after passing an aperture of N slits is described by a superposition of N spatially distinct state components determined by the shape of the slits,

$$\langle x|\psi_{\text{ms}}\rangle = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}\langle x+nL|\psi\rangle, \tag{2}$$

where L denotes the slit separation. The particular shape of the single-slit wave function $|\psi\rangle$ is irrelevant for our discussion provided its spatial width σ_x satisfies $\sigma_x \ll L$. This guarantees that the envelope of the resulting fringe pattern varies slowly on the scale of a single fringe period and thus encloses a large number of interference fringes. Note that the state (2) can equally be read as a longitudinal superposition of comoving wave packets.

The subsequent dispersive spreading of the N wave packets during the free propagation to the screen results in their overlap and interference, yielding in the far-field limit the characteristic interference pattern on the screen. In terms of the initial state (2), this position measurement at asymptotic times corresponds to a formal momentum measurement of $p = m(x - \langle\psi_{\text{ms}}|\mathsf{x}|\psi_{\text{ms}}\rangle)/t$. The probability distribution

$$|\langle p|\psi_{\text{ms}}\rangle|^2 = |\langle p|\psi\rangle|^2 F_N\left(\frac{pL}{h}\right) \tag{3}$$

exhibits the fringe pattern $F_N(x) = 1 + (2/N)\sum_{j=1}^{N-1}(N-j)\cos(2\pi jx)$. In case of $N = 2$ Eq. (3) reduces to the sinusoidal fringe pattern of the double slit, whereas for $N > 2$ one obtains the sharpened main maxima and suppressed side maxima characteristic for multi-slit interference. This reflects a tradeoff between the number of superposed wavepackets N and the uncertainty of the phase of the interference pattern, in analogy to the tradeoff between the variances of a conjugate variable pair. A similar tradeoff exists between number of fringes $M \approx \sigma_p L/h \approx L/\sigma_x$ covered by the envelope of the interference pattern and the width-to-spacing ratio $\sigma_x/L \approx 1/M$.

Modular variables These mutual relationships between the multi-slit state (2) and the resulting interference pattern (3) are captured best by splitting the position (momentum) operator into an integer component N_x (N_p) and a modular component $\bar{\mathsf{x}}$ ($\bar{\mathsf{p}}$) [3],

$$\mathsf{x} = \mathsf{N}_x\ell + \bar{\mathsf{x}} \quad ; \quad \mathsf{p} = \mathsf{N}_p\frac{h}{\ell} + \bar{\mathsf{p}}, \tag{4}$$

where $\bar{x} = (x + \ell/2)\mathrm{mod}\ell - \ell/2$ and $\bar{p} = (p + h/2\ell)\mathrm{mod}(h/\ell) - h/2\ell$. For the multi-slit state (2) the adequate choice of the partition scale is given by $\ell = L$. The probability distribution (3) can then be written as $|\langle p = N_p h/L + \bar{p}|\psi_{\text{ms}}\rangle|^2 \approx |\langle p = N_p h/L|\psi\rangle|^2 F_N(\bar{p}L/h)$,

which indicates that the modular variables isolate different characteristic aspects of interference: the periodic fringe pattern is described by the modular momentum $\bar{p}$, its envelope by the integer momentum N_p. Similarly, N_x describes the distribution of wave packets in (2) and $\bar{x}$ their (common) shape.

The modular variables $\bar{\mathsf{x}}$, $\bar{\mathsf{p}}$ have the remarkable property that they commute, $[\bar{\mathsf{x}}, \bar{\mathsf{p}}] = 0$, despite originating from conjugate observables [3]. On the other hand, the tradeoff between the number of superposed wave packets N and the phase of the interference pattern is now reflected by a "conjugate" relationship between the integer position N_x and the modular momentum $\bar{\mathsf{p}}$, as expressed by a non-vanishing *state-dependent* commutator $[\mathsf{N}_x, \bar{\mathsf{p}}]$. Similarly, the tradeoff between the width-to-spacing ratio σ_x/L and the number of covered fringes is described by a non-vanishing state-dependent commutator $[\bar{\mathsf{x}}, \mathsf{N}_p]$ of the modular position $\bar{\mathsf{x}}$ and the integer momentum N_p.

Modular entangled states We are now prepared to move on to entangled states of two material particles. Ultimately, we are interested in states that reveal their entanglement by a nonlocal interference pattern in position, similar to (1). To this end, we introduce two-particle *modular position entangled* (MPE) *states*, which are defined by superposing correlated pairs of (counterpropagating) wave packets of different velocities (instead of different spatial positions),

$$|\Psi_{\text{mpe}}\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} |\psi_{x_0,(N_0+n)h/\lambda}\rangle_1 |\psi_{-x_0,-(N_0+n)h/\lambda}\rangle_2, \tag{5}$$

where $\langle x|\psi_{x_0,p_0}\rangle = \phi(x-x_0)\exp(\mathrm{i}p_0(x-\bar{x}_0)/\hbar)$ denotes a (well-behaved) wave packet that is localized in phase space around (x_0, p_0). N_0 represents an arbitrary base integer momentum. Distinctness of the wave packets requires that their momentum width σ_p is smaller than their separation in momentum space, $\sigma_p \ll h/\lambda$, or, equivalently, $\sigma_x \gg \lambda$. For clarity we assume that the particles are spatially separated, positioned at $\pm x_0$. Such states could be generated (to good approximation) by the sequential coherent dissociation of a diatomic molecule [4]. Performing position measurements on each side, the non-separable structure of (5) gives rise to an interference pattern in the relative position $x_{\text{rel}} = x_1 - x_2$, $|\langle x_1, x_2|\Psi_{\text{mpe}}\rangle|^2 = |\phi(x_1-x_0)|^2|\phi(x_2+x_0)|^2 F_N((x_1 - x_2)/\lambda)$ (with $\bar{x}_{0,1} = \bar{x}_{0,2}$), or, equivalently, to a squeezing in the modular relative position $\bar{x}_{\text{rel}} = \bar{x}_1 - \bar{x}_2$.

Modular entanglement criterion The correlations in the modular relative position $\bar{x}_{\text{rel}}$ and the total integer momentum $N_{p,\text{tot}} = N_{p,1} + N_{p,2}$ exhibited by the MPE states (5) can be exploited to demonstrate the underlying entanglement. In analogy to [1], we consider the sum of variances, $\langle(\Delta \mathsf{N}_{p,\text{tot}})^2\rangle_\rho + \langle(\Delta \bar{\mathsf{x}}_{\text{rel}})^2\rangle_\rho/\ell^2$. Using the Cauchy-Schwarz inequality one can show that a separable state of motion, $\rho = \sum_i p_i \rho_{1i} \otimes \rho_{2i}$, implies $\langle(\Delta \mathsf{N}_{p,\text{tot}})^2\rangle_\rho + \langle(\Delta \bar{\mathsf{x}}_{\text{rel}})^2\rangle_\rho/\ell^2 \geqslant \sum_{i,j} p_i \{\langle(\Delta \mathsf{N}_{p,j})^2\rangle_i + \langle(\Delta \bar{\mathsf{x}}_j)^2\rangle_i/\ell^2\}$, with $j = 1, 2$. In contrast to [1], we cannot use the Robertson UR to estimate the remaining sums of variances, since the expectation value of the state-dependent commutator $[\bar{\mathsf{x}}, \mathsf{N}_p]$ vanishes when evaluated for an MPE state (5). However, one can establish a state-independent *additive uncertainty relation* for the modular EPR variables, $\langle(\Delta \mathsf{N}_{p,j})^2\rangle + \langle(\Delta \bar{\mathsf{x}}_j)^2\rangle/\ell^2 \geqslant c_{\mathsf{N}_p,\bar{\mathsf{x}}} > 0$. Using this, we immediately get the desired criterion,

$$\langle(\Delta \mathsf{N}_{p,\text{tot}})^2\rangle_\rho + \frac{1}{\ell^2}\langle(\Delta \bar{\mathsf{x}}_{\text{rel}})^2\rangle_\rho \geqslant 2c_{\mathsf{N}_p,\bar{\mathsf{x}}}, \tag{6}$$

which must be satisfied by any separable state. The constant $c_{\mathsf{N}_p,\bar{\mathsf{x}}}$ is given by the smallest eigenvalue of the operator $\mathsf{A}_j = \mathsf{N}_{p,j}^2 + \bar{\mathsf{x}}_j^2/\ell^2$, which evaluates numerically as $c_{\mathsf{N}_p,\bar{\mathsf{x}}} \cong 0.0782351$.

The MPE states (5) violate the separability criterion (6) for any $N \geqslant 2$. Indeed, the resulting variances read $\langle(\Delta \mathsf{N}_{p,\text{tot}})^2\rangle_{\text{mpe}} = 0$ and $\langle(\Delta \bar{\mathsf{x}}_{\text{rel}})^2\rangle_{\text{mpe}} = \frac{\lambda^2}{6}(1 - S(N))$, (again with $\ell = \lambda$) where the monotonically increasing squeezing function $S(N) = (6/\pi^2)\sum_{j=1}^{N-1}(N - j)/Nj^2 < 1$ evaluates as, e.g., $S(2) = 0.30$, $S(4) = 0.55$, $S(10) = 0.76$ and $S(100) = 0.96$. This proves the possibility to deduce entanglement from a nonlocal interference pattern. Note that one can achieve perfect squeezing in the limit $N \to \infty$.

Conclusion We presented a scheme to provide and detect entanglement in the motion of two free material particles. Elementary position measurements at macroscopically distinct sites give rise to a nonlocal interference pattern; the non-separability then follows from reduced fluctuations in adapted modular variables. In this sense, the scheme allows one to "deduce entanglement from interference", and hence to illustrate the wave-particle duality on a new level including quantum mechanical nonlocality. The scheme is sufficiently generic and robust to admit various experimental realizations; one scenario would, e.g., gradually dissociate an ultracold diatomic Feshbach molecule [4]. In addition, it is clear that the entanglement criterion is applicable to any bipartite continuous variable system with conjugate operator pairs, e.g. quadrature amplitudes of field modes, and could thus offer a valuable alternative to existing entanglement detection schemes.

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2.4 Rotons and Supersolids in Rydberg-Dressed Bose-Einstein Condensates

NILS HENKEL, REJISH NATH, THOMAS POHL

We study the behavior of a Bose-Einstein condensate in which atoms are weakly coupled to highly excited Rydberg states. Since the latter have very strong van der Waals interactions, this coupling induces effective, nonlocal interactions between the dressed groundstate atoms, which, opposed to dipolar interactions, are isotropically repulsive. Yet, one finds partial attraction in momentum space, giving rise to a roton-maxon excitation spectrum and a transition to a supersolid state in three-dimensions.

The search for Supersolids Since introduced by Landau [1], the notion of a roton minimum in the dispersion of quantum liquids has been pivotal to understanding superfluidity in helium. This later led to the prediction of a peculiar solid state, simultaneously possessing crystalline and superfluid properties. In such a supersolid [2], the particles that must supply the rigidity to form a crystal, at the same time provide for superfluid nonviscous flow. Forty years after its conjecture, this apparent contradiction continues to attract theoretical interest and has ushered in an intense search for experimental evidence [3] in solid ^{4}He, whose interpretations are currently under active debate [4].

Here, we demonstrate how three-dimensional roton excitations may be realized in atomic Bose-Einstein condensates (BECs), introducing an alternative system to study supersolidity [5]. The supersolid phase transition is shown to arise from effective interactions, realized through off-resonant optical coupling to highly excited nS Rydberg states giving rise to an effective soft-core interaction potential for the groundstate.

Effective interactions The system is composed of N atoms, each possessing a ground state $|g_i\rangle$ and an excited nS Rydberg state, denoted by $|e_i\rangle$. The two states are optically coupled with a two-photon Rabi frequency Ω and detuning Δ (see Fig.1a). Within a many-body perturbation expansion, the resulting Born-Oppenheimer potential surface is found to be

$$W_G(\mathbf{r}_1,...,\mathbf{r}_N) = \sum_{i<j} \frac{\tilde{C}_6}{r_{ij}^6+R_c^6} \qquad (1)$$

The effective potential $U(r_{ij}) = \tilde{C}_6/(r_{ij}^6 + R_c^6)$ is exemplarily shown in Fig.1b. The peculiar shape of U is easily understood within a simple two-atom picture: For far-distant atomic pairs, a small fraction $(\Omega/2\Delta)^2$ is independently admixed to each groundstate atom, such that $U(r_{ij})$ is of vdW-type with an effective coefficient $\tilde{C}_6 = (\Omega/2\Delta)^4 C_6$. At smaller distances, however, the interaction shift $V_{ee}(\mathbf{r}_{ij})$ renders dressing to the doubly excited $|E_{ij}\rangle$ states ineffective, such that the effective potential approaches a constant value. Typically, R_c can take on rather large values of a few μm.

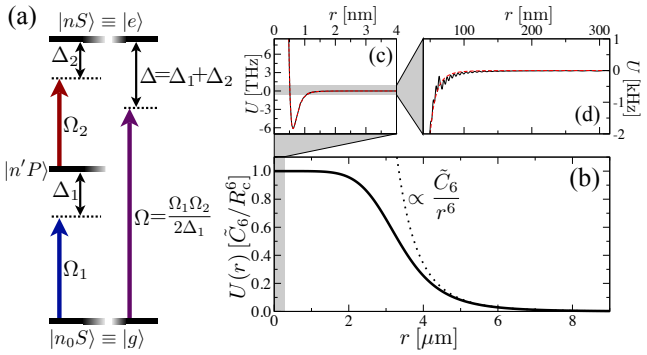

Figure 1: (a) Schematics of the considered three-level atom, illustrating the laser coupling between the atomic groundstate $|n_0S\rangle$ and the Rydberg state $|nS\rangle$. For $\Delta_1 \gg \Omega_1$, the system reduces to an effective two-level atom, with the states $|g\rangle \equiv |n_0S\rangle$ and $|e\rangle \equiv |nS\rangle$ coupled with a two-photon Rabi frequency Ω and detuning Δ. (b) Effective potential resulting from the off-resonant coupling to the strongly interacting Rydberg states for $n = 60$ and $\Delta = 50$MHz. Panels (c) and (d) provide an enlarged view of the potential showing the contributions from both groundstate-Rydberg atom and groundstate-groundstate atom interactions (solid line) as well as the sole contribution from the latter (dashed line).

Excitation spectrum For small $\tilde{C}_6$ the BEC ground state corresponds to a homogeneous superfluid with density ρ_0. Its elementary excitations with wave number $\mathbf{k}$ and corresponding energy ϵ are calculated from the corresponding Bogoliubov-de Gennes equations. Upon appropriate length and energy scaling (see Fig.2), the dispersion is determined by a single dimensionless parameter $\alpha = \rho_0 M\tilde{C}_6/\hbar^2 R_c$, parametrizing the interaction strength. Due to the inner potential plateau at $r < R_c$, the momentum space potential $\tilde{U}$ has negative attractive contributions around $k = k_{rot} \sim 2\pi/R_c$, such that the spectrum develops a roton minimum at $k = k_{rot}$ (see Fig.2) for sufficiently large $\alpha > \alpha_{rot} \approx 4.8$. The corresponding roton gap δ decreases with increas-

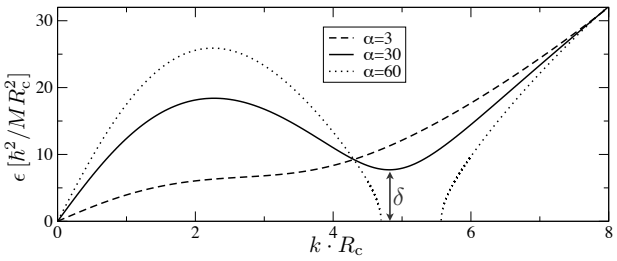

Figure 2: Dispersion relation $\epsilon(k)$ for different values of the interaction parameter α. The arrow indicates the roton gap δ.

ing α and ultimately vanishes at $\alpha_{\rm inst} \approx 50.1$ (see Fig.3a), marking the onset of a roton instability, at which density modulations may grow without energy cost.

Crystal formation We performed three-dimensional simulations, using a mean-field approach. Our calculations of the ground state energy show that at a critical value of $\alpha_{\rm suso} \approx 30.1$, one finds a transition to a stable supersolid. This first-order transition precedes the roton-instability and takes place at a finite roton gap. To demonstrate experimental feasibility of forming such supersolid states, we studied the time evolution, starting from a homogenous BEC. As a specific example, we discuss the BEC dynamics for a simple time dependence of α, shown in Fig. 3a. The sudden parameter quench at $t = 0$ causes relaxation towards a short-range ordered, "glassy" state [c.f. Fig. 3b]. As α is decreased close to the phase transition some of the structures vanish entirely, leading to a mixed phase in which extended superfluid fractions of nearly constant density coexist with density-modulated domains [c.f. Fig. 3c]. The latter increase in time [c.f. Fig. 3d], and ultimately merge to form sizable „crystallites"of regular density modulations [c.f. Fig. 3e].

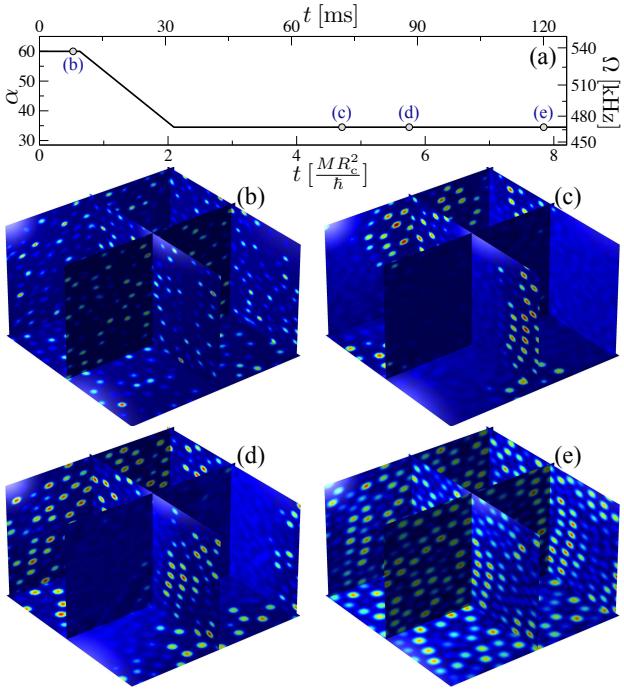

Figure 3: Snapshots of the BEC dynamics for a time-varying interaction parameter $\alpha(t)$ shown in (a). Panels (b)-(e) show the density along orthogonal slices through the simulation box at times indicated in (a). The upper and right axes in (a) show the actual time and Rabi frequency for a ^{87}Rb BEC with $n = 60$, $\Delta = 50$MHz and $\rho_0 = 2 \cdot 10^{14}$cm^{-3}.

Experimental feasibility For the calculations of Fig. 3 we chose a particular example of coupling to $60S$ Rydberg states in a ^{87}Rb condensate, for which Rydberg excitation has recently been demonstrated [6]. For typical laser parameters and BEC densities the dynamics proceeds on a timescale of $\sim 100\mu$s. This must be compared to the lifetime of Rydberg states, which is generally limited by spontaneous decay of the involved excited states and by auto-ionization of close Rydberg atom pairs. In the present case, the latter is strongly suppressed due to the interaction blockade of doubly excited states. Rydberg state decay, due to spontaneous emission and black-body radiation, is more significant with typical rates on the order of 10ms^{-1}. However, since the Rydberg state is only weakly populated by the far off-resonant coupling to the groundstate, the resulting effective decay rate can be decreased to much smaller values, yielding an effective lifetime on the order of seconds. The additional decay of the intermediate $n'P$ state (c.f. Fig.1a) finally decreases the effective lifetime to about 0.5s.

Conclusion The possibility to unambiguously realize supersolid states in atomic BECs opens up a range of new studies, from investigations of thermal effects to supersolid formation in finite systems and their dynamical response to perturbations, such as trap rotations. Generally, the described setting offers new avenues for the realization of complex nonlocal media, where the sign, shape, and strength of interactions can be tuned through proper choice of the addressed Rydberg state and the applied laser parameters, and even permits local spatial control of nonlocal interactions via tightly focused beams. For example, attractive interactions can be realized via D-state dressing of alkaline atoms or coupling to Strontium Rydberg S-states [7], which was recently shown to promote the formation of stable bright solitons, i.e. three-dimensional self-trapping of Bose-Einstein condensates [8].

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2.5 Electromagnetically Induced Transparency in Strongly Interacting Ultracold Gases

SEVILAY SEVINÇLI, CENAP ATES, THOMAS POHL

The effect of electromagnetically induced transparency (EIT) [1] in light-driven multi-level systems continues to play a pivotal role in quantum and nonlinear optics. Enabling slow light propagation and thus long photon interaction times at low loss levels [2], EIT media provide a promising route to applications in optical communication and quantum information science. Optical nonlinearities, however, typically arise from higher order light-atom interactions, such that realizations of such applications at very low light intensities [3] remain challenging. In this respect, recent experimental studies of EIT in cold Rydberg gases [4, 5] are opening up new perspectives for nonlinear optics on a few photon level [6]. The exaggerated properties of Rydberg atoms and, in particular, their strong interactions, suggest that nonlinear phenomena can be greatly enhanced in ultracold Rydberg gases.

Here, we study the correlated many-body dynamics of cold Rydberg gases optically driven in an EIT configuration, from which we obtain the nonlinear optical response in the presence of arbitrarily strong atomic interactions [7]. Our calculations reveal a universal behavior of the nonlinear susceptibility and provide a good description of recent measurements of the nonlinear optical absorption of ultracold Rydberg gases.

The underlying Rydberg-EIT level scheme is shown in Fig.1. The signal laser couples the ground state $|1\rangle$ to a low lying state $|2\rangle$ with Rabi frequency Ω_1. State $|2\rangle$ is coupled by a strong control laser ($\Omega_2 > \Omega_1$) to a highly excited Rydberg state $|3\rangle$. In addition, the intermediate state $|2\rangle$ radiatively decays with a rate γ, whereas spontaneous decay of the long-lived Rydberg level can safely be neglected. For resonant driving, each atom settles into a dark state, $|d_i\rangle \sim \Omega_2|1_i\rangle - \Omega_1|3_i\rangle$, which is immune to the laser coupling and radiative decay [1]. Consequently, the complex susceptibility χ_{12} of the lower transition vanishes and the medium becomes transparent.

In the presence of van der Waals interactions

$$U = \sum_{i<j} U_{ij}|3_i3_j\rangle\langle 3_i3_j| = \sum_{i<j} \frac{C_6}{|\mathbf{r}_i - \mathbf{r}_j|^6}|3_i3_j\rangle\langle 3_i3_j| \quad (1)$$

between atoms in the Rydberg state $|3\rangle$ the situation becomes more complex. Note that the van der Waals coefficient $C_6 \sim n^{11}$ strongly increases with the atom's principal quantum number n. For typical values $n \sim 60$ this yields an enhancement of about 10^{11} compared to interactions in low-lying states, implying a drastically

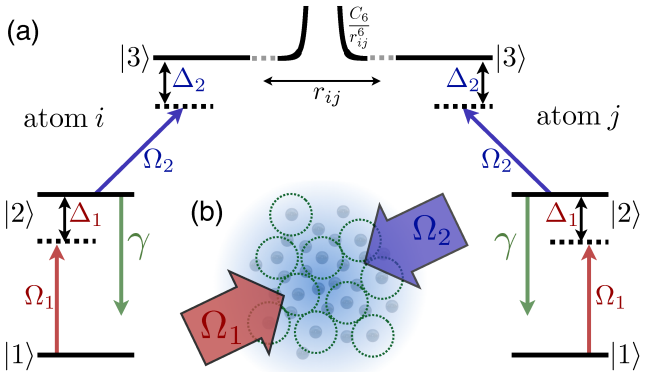

Figure 1: (a) Illustration of the considered three-level ladder scheme. Two laser fields successively couple the states $|1\rangle$, $|2\rangle$ and $|3\rangle$. For isolated atoms, EIT is realized on two-photon resonance $\Delta_1 = -\Delta_2$. In a cold gas of Rydberg atoms (b), the van der Waals interaction shift C_6/r_{ij}^6 modifies this ideal transparency and leads to a nonlinear optical response of the medium.

different excitation dynamics. On the one hand, the resulting level shifts lead to a strong suppression of Rydberg excitation, due to an excitation blockade of close atoms [8]. On the other hand, the interactions perturb the atomic dark states [5], and admix the dissipative intermediate state [9]. To account for these effects, we start from the von Neumann equation

$$i\dot{\rho}^{(N)} = [H_0 + U] - i\mathcal{L}[\rho^{(N)}]\,, \quad (2)$$

for the N-body density matrix $\hat{\rho}^{(N)}$ of the gas. Here $\hat{H}_0$ describes the laser-driven, independent atom dynamics and the Lindblad operator $\mathcal{L}$ accounts for spontaneous decay of the intermediate state.

To obtain the steady state populations of eq.(2), we transform it to a many-body rate equation for the diagonal elements $\rho_{\alpha\alpha}^{(i)}$ of the single-atom reduced density matrices for the ith atom. This gives a set of N coupled rate equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\rho_{11}^{(i)}\\ \rho_{22}^{(i)}\\ \rho_{33}^{(i)}\end{pmatrix} = \begin{pmatrix}-a_{11}^{(i)} & a_{12}^{(i)} & a_{13}^{(i)}\\ a_{21}^{(i)} & -a_{22}^{(i)} & a_{23}^{(i)}\\ a_{31}^{(i)} & a_{32}^{(i)} & -a_{33}^{(i)}\end{pmatrix}\begin{pmatrix}\rho_{11}^{(i)}\\ \rho_{22}^{(i)}\\ \rho_{33}^{(i)}\end{pmatrix}, \quad (3)$$

where the rate coefficients $a_{\alpha\beta}^{(i)}$ are straightforwardly obtained as a function of the laser parameters, with interactions entering through the effective detuning $\Delta_2^{(i)} = \Delta_2 - \sum'_{j\neq i} U_{ij}$. The sum only runs over atoms in the Rydberg state, such that the individual atomic transition rates become dynamical variables that depend on the entire many-body state of the system. Although this rate equation still covers the exponentially large number of all 3^N many-body states, it can be efficiently

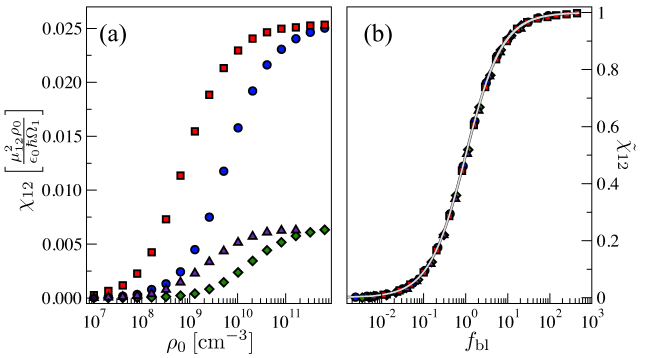

Figure 2: (a) Nonlinear absorption coefficient $\mathrm{Im}[\chi_{12}]$ as a function of the density of Rubidium atoms for $\Omega_2 = 2$MHz and $\gamma_{12} = \gamma_{23} = 0$. The different symbols correspond to different principal quantum numbers and probe Rabi frequencies: $\Omega_1 = 1$MHz, $n = 50$ (squares), $\Omega_1 = 0.5$MHz, $n = 50$ (circles), $\Omega_1 = 1$MHz, $n = 70$ (triangles) and $\Omega_1 = 1$MHz, $n = 70$ (diamonds). (b) After proper scaling [cf. eqs.(6) and (5)] all data points follow the simple universal scaling relation eq.(7) (line).

solved via classical Monte-Carlo sampling, which yields the fully correlated N-body state-distribution of the particles, and in particular the average level populations $\rho_{\alpha\alpha} = N^{-1}\sum_i \rho_{\alpha\alpha}^{(i)}$. Since $\mathrm{Im}(\rho_{12}) = \frac{\gamma}{\Omega_1}\rho_{22}$ the Monte-Carlo approach also allows to determine the imaginary part of the complex optical susceptibility

$$\chi_{12} = \frac{2\mu_{12}^2\rho_0}{\epsilon_0\hbar\Omega_1}\rho_{12}\,, \tag{4}$$

where μ_{12} is the dipole moment of the probe transition and the real part of χ_{12} can be obtained from the absorption spectrum using the Kramers-Kronig relations.

The density dependence of the absorption is shown in Fig.2a. The observed saturation at high densities can be understood from simple arguments. At very high densities, the presence of a single Rydberg atom blocks excitation of a large number of adjacent atoms. As a consequence the majority of atoms acts as effective two-level systems. Taking the limit $\Delta_2^{(i)} \to \infty$ the high-density steady state value of ρ_{12}, hence, approaches

$$\mathrm{Im}[\rho_{12}^{(\infty)}] \;=\; \frac{\Omega_1\gamma}{\gamma^2 + 2\Omega_1^2}\,. \tag{5}$$

It thus appears reasonable to employ the derived high-density limit as a natural scale for χ_{12}. In addition we can use the excitation blockade [8] to rescale the gas density, i.e. the abscissa in Fig.2a. Comparing the Rydberg atom density $\rho_{\mathrm{ryd}} = \rho_0 N^{-1}\sum_i \rho_{33}^{(i)}$ obtained from the Monte Carlo calculation to the corresponding value $\rho_{\mathrm{ryd}}^{(0)}$ for vanishing interactions one obtains the fraction

$$f_{\mathrm{bl}} = \frac{\rho_{\mathrm{ryd}}^{(0)}}{\rho_{\mathrm{ryd}}} - 1 \tag{6}$$

of suppressed Rydberg excitations. Re-expressing ρ_0 through eq.(6) and scaling the probe beam absorption by eq.(5), yields a universal dependence of $\tilde{\chi}_{12} = \chi_{12}/\chi_{12}^{(\infty)}$ on the laser parameters, atomic density and interaction strength. We have verified this behavior for a wide range of parameters, some of which are exemplified in Fig.2. Indeed, all data points collapse on a single curve (c.f. Fig.2b) described by

$$\tilde{\chi}_{12} = \frac{f_{\mathrm{bl}}}{1 + f_{\mathrm{bl}}}\,. \tag{7}$$

This simple formula nicely illustrates the effects of excitation blocking on the optical susceptibility of the Rydberg-EIT medium: For $f_{\mathrm{bl}} < 1$ one finds a nonlinear absorption proportional to the blockade fraction, which, however, saturates at the two-level limit $\chi_{12}^{(\infty)}$ for $f_{\mathrm{bl}} \gtrsim 1$, i.e. at the onset of a strong excitation blockade. Since $f_{\mathrm{bl}} \sim \Omega_1^4$ for weak Rydberg excitation this implies a finite cubic nonlinearity, as observed in [5].

In conclusion we have shown that the correlated level dynamics of laser-driven Rydberg gases yields strong photon-photon interactions, manifested in a nonlinear intensity dependence of the optical susceptibility. Beyond providing an intuitive understanding of the basic mechanism behind the optical nonlinearities, the presented approach is consistent with our previous quantum calculations in low-density gases [9] and yields excellent agreement with recent experimental measurements [10] of the nonlinear absorption of cold Rubidium Rydberg gases [5]. In addition, the revealed universal behavior may be valuable for future experimental efforts, by permitting quick estimates of optical nonlinearities and allowing to determine the medium absorption from pure population measurements. While we have primarily focussed on nonlinear absorption phenomena the developed approach can also be used to study the optical response of far-detuned EIT media and, thus, to explore prospects for realizing strong coherent photon-photon interactions. In future work, our present approaches will be extended to study interaction effects on the slow-light propagation and ultimately the many-body dynamics of multi-photon pulses on a quantum level, i.e. to explore prospects for realizing strongly interacting quantum gases of photons via Rydberg-Rydberg interactions.

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2.6 Delayed Coupling Theory of Vertebrate Segmentation

LUIS G. MORELLI, SAÚL ARES, FRANK JÜLICHER

Vertebrate segmentation The body plan of all vertebrate animals has a segmented organization that is reflected in the repeated arrangement of vertebra and ribs. This structure forms during the development of the organism by a process called segmentation. The segments —called somites— form sequentially along a linear axis, one by one, with a precisely controlled timing, see Fig. 1. The timing of vertebrate segmentation is set by a genetic clock. This clock is realized by oscillations of the levels of certain proteins in individual cells [1]. The genes encoding for these proteins are called cyclic genes. Their expression changes periodically in time. The genetic oscillations of cells in the tissue are coordinated by molecular signaling systems that introduce a coupling of neighboring cellular oscillators. This gives rise to a collective spatio-temporal pattern which consists of waves that travel and eventually stop and arrest in a periodic arrangement of somites. Signaling gradients ranging over larger distances control the slow down and arrest of the cellular oscillators and guide spatio-temporal patterns during segmentation. The segmentation process can be studied on different levels of organization that range from molecular and cellular to tissue length scales. We have developed a theoretical description of somitogenesis based on a coarse grained representation of cellular oscillators as phase oscillators. Our study of the collective self-organization of coupled genetic oscillators during segmentation highlight the importance of time-delays in the coupling [2]. These time-delays arise because of the slow dynamics of signaling processes that couple neighboring cells. The resulting *delayed coupling theory* can be compared to quantitative experiments. This allows us to identify key principles of cellular coordination during vertebrate morphogenesis.

Delayed coupling theory The spatio-temporal patterns of genetic oscillations are described by coupled sets of phase oscillators which are arranged in space. The state of a single oscillator is characterized by the phase $\theta_i(t)$, where i labels the oscillator. The dynamic equations for the phases are given by [3]

$$\dot{\theta}_i(t) = \omega_i(t) + \frac{\varepsilon_i(t)}{n_i} \sum_j \sin\left[\theta_j(t-\tau) - \theta_i(t)\right] \quad (1)$$

where the sum is over all neighbors j of cell i. Here, ε denotes the coupling strength and τ is the time delay involved in coupling. We solve these equations in one or two-dimensional space with moving boundary at one end of the system. The posterior boundary is extended towards one side by the addition of new oscillators at a rate v/a, where v is an extension velocity and a the distance between neighboring cells. We consider a frequency profile which is moving together with the expanding end. Therefore, the intrinsic oscillation frequency ω_i for a given oscillator varies with time.

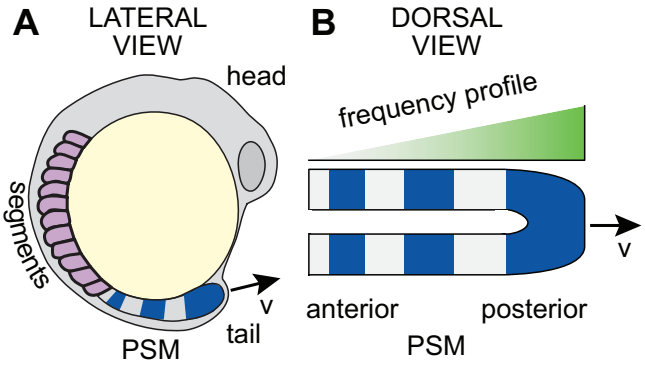

Figure 1: (A) Schematic lateral view of a zebrafish embryo showing formed segments (purple) and waves of gene expression (blue) in the unsegmented tissue, the presomitic mesoderm (PSM). The tail grows with velocity v. (B) From a dorsal view the PSM is a U-shaped tissue. A frequency profile along the PSM causes faster genetic oscillations in the posterior PSM.

Collective modes Our theory makes key predictions regarding the effects of coupling and coupling delays on the collective oscillator patterns. After an initial transient dynamics, the system settles in a spatio-temporal limit cycle with collective frequency Ω which obeys the relation

$$\Omega = \omega_A - \varepsilon \sin(\Omega\tau). \quad (2)$$

This frequency is governed by the autonomous frequency ω_A of the fastest oscillators at the posterior side, modified by effects of coupling described by the coupling strength ε. This implies that changes in coupling strength would lead to changes in oscillation period and thus in variations of the wavelength of cyclic gene expression patterns as well as the resulting segment length, see Fig. 2. Furthermore, the theory predicts the existence of dynamic instabilities. When the coupling delays approaches half of the autonomous period of the fastest oscillators, the locally synchronous waves are disrupted because the coupling becomes effectively "antiferromagnetic", i.e. it favors antiphase of neighboring oscillators. Both predictions have been confirmed experimentally [4]. Our theoretical predictions have led to the discovery of the first mutants with altered collective period, so called period mutants, see Fig. 3A. Furthermore, treating embryos with the drug DAPT, which inhibits the signaling system involved in cell-cell coupling leads to concentration dependent increases in oscillation period that can be understood quantitatively, see Fig. 3B.

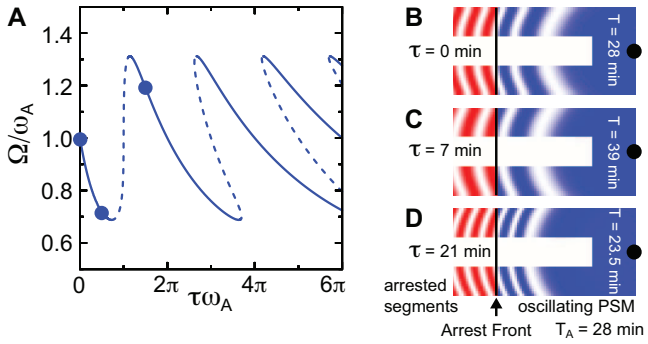

Figure 2: A time delay in the oscillator coupling affects the collective frequency, the wavelength of gene expression patterns and segment length. (A) Dimensionless collective frequency Ω as a function of time delay τ of coupling for coupling strength $\varepsilon/a^2 = 0.07$ min^{-1}, and intrinsic frequency $\omega_A = 0.224$ min^{-1}. Solid lines: stable solutions of Eq. (2). Dashed lines: unstable solutions of Eq. (2). Blue dots correspond to the three cases shown in panels (B-D). (B-D) Snapshots of numerical solutions of the model given by Eq. (1) in a two-dimensional geometry for different time delays as indicated. Color intensity indicates the value $\sin\theta$ of the phase θ.

Dynamic instabilities and the effects of fluctuations

Our theory reveals that regions of stable collective oscillations are separated by unstable modes if the time-delay of coupling is varied. This suggests that changes of coupling delay can lead to a disruption of the wave pattern at the limit between stable and unstable regions. We have tested these predictions in experiments, where coupling delays were reduced by overexpression of the mindbomb (*mib*) gene. Above a critical level of Mib overexpression, wave patterns are lost and embryos die.

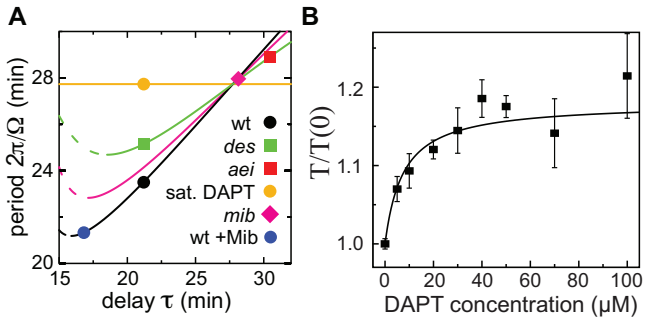

Figure 3: (A) Collective period Ω as a function of time delay τ for different coupling strengths (solid lines). The symbols indicate operating points for wild-type and different mutants as indicated. At saturated DAPT concentration no coupling exists (yellow). The blue circle corresponds to Mib overexpression discussed in Fig. 4. (B) Experimentally determined collective period $T = \Omega/2\pi$ (symbols) as a function of DAPT concentration, which is a drug that influences coupling strength. The theoretical prediction of the delayed coupling theory is shown as a solid line.

If the instability is approached, starting from stable patterns, we observed precursors of the dynamic instability in the fluctuations of the pattern. In the vicinity of the instability, correlation functions of oscillator phase change their shape as the wave patterns becomes increasingly noisy. The same signatures of the approach to instability are also found in numerical simulations of the system if we introduce noise terms. We can quantitatively compare correlation functions obtained in Mib overexpression experiments with noisy simulations of our model, see Fig. 4.

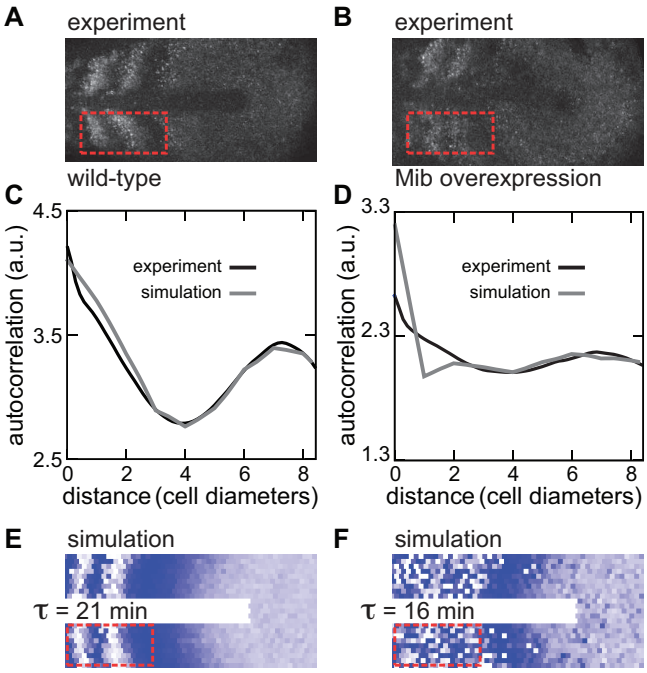

Figure 4: Coupling delays regulate the stability of the segmentation clock. (A,B) Representative experimental patterns of the cyclic gene *dlc* in wild-type (A), and Mib overexpression (B) conditions. Data courtesy of A.C. Oates and L. Herrgen. (C,D) Average autocorrelation function of spatial patterns in regions indicated by red boxes in (A,E) and (B,F) respectively. (E,F) Snapshots of numerical simulations of the model given by Eq. (1) with noise for wild-type parameters (E) and shorter coupling delay (F).

Discussion

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2.7 Reorientation of Large-Scale Polar Order in Two-Dimensional Tissues

DOUGLAS STAPLE, MATTHIAS MERKEL, FRANK JÜLICHER

Planar cell polarity. During the development of an organism from a fertilized egg, cells multiply by cell division and organize in space to form complex morphologies. An important situation is the formation of epithelia which are sheet-like, two-dimensional packings of cells. Cells often exhibit a structural polarity in the plane of the epithelium. Cell polarity implies that a vectorial asymmetry exists and the cell morphology defines a direction in the plane of the epithelium, see Fig. 1. Typically, the polarity of individual cells is locally aligned and large-scale patterns of cell polarity emerge during the development of an epithelium [1]. The mechanisms by which cell polarity patterns are dynamically reorganized are unknown. Furthermore, a fundamental problem is to understand how patterns of planar cell polarity (PCP) that are ordered on large scales emerge at early stages of development.

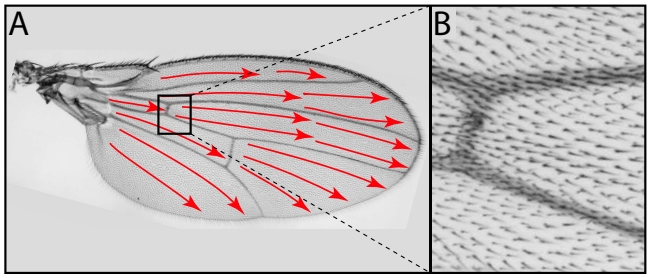

Figure 1: (A) Hair pattern on the adult wing of the fly exhibiting large-scale order with wing hairs pointing towards the distal end of the wing. Arrows indicate the hair orientation in different regions. (B) Higher magnification of region in (A) reveals individual wing hairs. (Experimental images courtesy of Suzanne Eaton, MPI-CBG.)

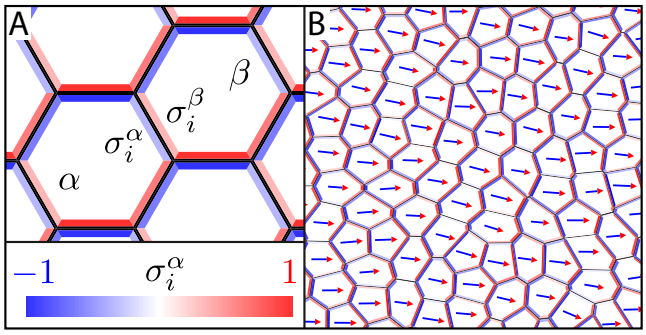

Figure 2: (A) Schematic representation of the distribution of planar cell polarity (PCP) proteins along cell bonds. Distal and proximal proteins are shown in red and blue, respectively. In a vertex model cell shapes are described by a polygonal network of cell bonds. We describe levels of polarity proteins on a bond i by variables σ_i^α, where α is a cell index. (B) The distribution of polarity proteins defines a polarity vector in each cell, represented by an arrow. In simulations of the vertex model, we find that large-scale polar order emerges during growth.

Genetic and cell biological studies have revealed that a family of proteins called PCP proteins play a key role in the dynamic organization of polarity patterns. Mutants in these proteins lead to the formation of polarity defects such as swirls [1]. These PCP proteins are recruited along the junctions between neighboring cells where they form complexes and aggregates that span from the membrane of one cell to its neighbor. Furthermore, within a given cell, subsets of these proteins are typically located at opposite sides of the cell, implying a polar pattern of PCP proteins in the cell, see Fig. 2.

The wing of the fruit fly Drosophila provides an important model system for the study of epithelia and the development of planar polarity patterns. The precursor of the wing in the larvae and the pupa undergoes dynamic remodeling processes. The patterns of cell polarity in the wing epithelium become apparent in the orientation patterns of hairs that grow on the adult wing, see Fig. 1. In close collaboration with experimentalists, we have quantified the planar polarity patterns in the fly wing at different stages of development, and have identified principles underlying the reorientation of planar polarity patterns. In particular, we find that cell rearrangements and cell flows play a key role in guiding polarity reorientation.

Polarity patterns and cell flows. Using flies expressing fluorescently labelled PCP proteins, we measure the polarity patterns on the single cell level. The signatures of cell polarity can be characterized by a nematic, which is a traceless symmetric tensor. Locally averaged PCP patterns obtained by this method are shown in Fig. 3. This analysis revealed for the first time that large-scale polarity exists already at early pupal stages of the fly wing, see Fig. 3A. We find that this initial pattern is subsequently reoriented in a process that takes about one day. It eventually leads to the previously known polarity pattern of wing hairs in the adult wing, see Fig. 3B. During this reorientation process the tissue is remodeled by cell rearrangements. We have quantified these movements by measuring the time-dependent cell flow field $\mathbf{v}(\mathbf{r},t)$, see Fig. 3C. Inhomogeneities of the cell flow give rise to local rates of rotation $\omega = (\partial_x v_y - \partial_y v_x)/2$, compression $C = (\partial_x v_x + \partial_y v_y)/2$ and shear. Shear is characterized by a traceless symmetric velocity gradient tensor:

$$\begin{pmatrix} S_1 & S_2 \\ S_2 & -S_1 \end{pmatrix} = k_s \begin{pmatrix} \cos 2\theta_s & \sin 2\theta_s \\ \sin 2\theta_s & -\cos 2\theta_s \end{pmatrix}, \qquad (1)$$

which defines a shear axis at an angle θ_s and a shear rate k_s. In general, flow profiles are expected to reorient polarity and we developed theoretical approaches to study these phenomena.

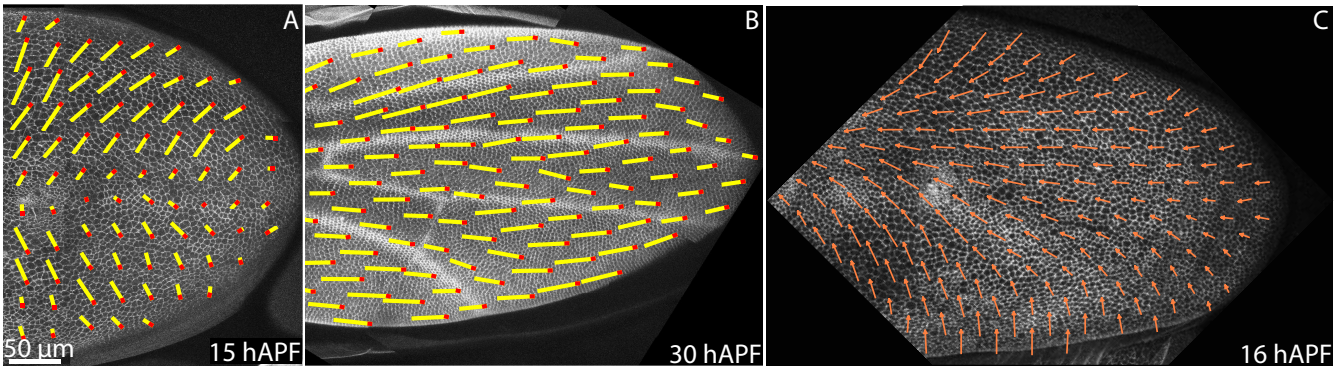

Figure 3: (A and B) Patterns of nematic and vectorial order in planar cell polarity (PCP) protein distributions quantified from microscope images of developing fly wings in the pupal stage. The magnitude and axis of nematic order averaged over groups of cells is represented by yellow bars at early times (A) and later times (B). Times is given in hours after puparium formation (hAPF). (C) Pattern of cell flow computed from time-lapse experimental images. Local averages of cell velocity are indicated by arrows.

Theory of planar cell polarity dynamics. We describe the dynamics of cell polarity reorientation on two different scales: the cellular scale and a hydrodynamic continuum limit. On the cellular scale, we use a vertex model for cell shapes and cell mechanics [2,3] in which we introduce bond variables σ_i^α to describe PCP distributions [4], see Fig. 2. Each bond i possesses two variables σ_i^α and σ_i^β that correspond to proteins on bond i in adjacent cells α and β, respectively. The dynamics of cell bond variables is governed by a potential function

$$E = J_1 \sum_i \sigma_i^\alpha \sigma_i^\beta - J_2 \sum_{\{i,\,j\}} \sigma_i^\alpha \sigma_j^\alpha - J_3 \sum_\alpha \boldsymbol{\epsilon}^\alpha \cdot \mathbf{Q}^\alpha, \quad (2)$$

as $d\sigma_i^\alpha/dt = -\gamma \partial E/\partial \sigma_i^\alpha$, where t is time and γ is a kinetic coefficient. Here the parameter J_1 describes interactions that favor alignment of the polarities of adjacent cells and the parameter J_2 describes interactions that stabilize polarity within each cell. The coupling strength of cell polarity (represented by the PCP nematic $\mathbf{Q}^\alpha$) to cell elongation (described by the tensor $\boldsymbol{\epsilon}^\alpha$) is denoted J_3.

Using this model, we identify a simple and general mechanism to generate large-scale polar order, see Fig. 2B. This is achieved by starting from a small number of cells with random PCP variables and then slowly growing the network by repeated cell division. At early times polarity orders in small networks and this order is maintained during growth. Interestingly, depending on the parameter regime, no topological defects in the orientation pattern are generated by this process. Furthermore, we have studied the influence of shear on PCP order, and have shown that shear generally reorients planar polarity in the vertex model [4].

The reorientation of a polarity field in an inhomogeneous flow is most easily understood in a continuum description, valid on large scales [4,5]. Considering for simplicity a homogeneous polarity pattern, the angle of polarity θ changes dynamically as

$$\frac{\partial \theta}{\partial t} = \nu k_s \sin 2(\theta - \theta_s) + \omega. \quad (3)$$

This implies that both local shear and rotation reorient polarity. The effects of shear are captured by a dimensionless phenomenological coefficient ν. Solving Eq. (3) for the measured flow field in the fly wing, we show that most of the observed reorientation of cell polarity patters can be accounted for by the effects of local rotations and shear. This comparison between theory and experiment allowed us to estimate $\nu \simeq -3$. A negative value of ν implies that polarity preferentially aligns with the shear axis.

Discussion. We have shown that the dynamic organization of polarity patterns in tissues results from the collective behaviors of many cells both in terms of cell flow and polarity. The emergence of large-scale order can be facilitated by growth processes that allow the system to suppress topological defects in the orientation field, which usually exist in large two-dimensional polar systems. The flow-induced reorientation of polarity patterns reported here show that general hydrodynamic concepts developed originally to describe liquid crystals also apply in living systems.

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2.8 Coupling Virtual and Real Hair Bundles in a Hybrid Experiment

KAI DIERKES, FRANK JÜLICHER, BENJAMIN LINDNER

Active amplification in hearing. Humans possess an extraordinary ability to detect complex sound stimuli and to analyze their spectral and temporal fine structure. It has been recognized that the human sense of hearing relies on an active nonlinear process boosting vibrations within the cochlea [1], i.e. the inner ear organ responsible for the coding of auditory signals into patterns of neural activity. Spontaneous otoacoustic emissions, i.e. sounds emanating from the ear canal even in the absence of any external auditory stimulus, constitute a striking manifestation of this active amplifier. As of today, its exact biophysical implementation, however, remains elusive.

Two processes on a cellular scale have been suggested to play the key role in auditory amplification [2]. On the one hand, there is the ability of outer hair cells to undergo length changes in response to modulations of their transmembrane potential (electromotility). On the other hand, hair bundles, which also constitute the universal mechano-transducers in the inner ear, can generate active forces and even perform spontaneous oscillations (hair-bundle motility).

The hair-bundle amplifier. The hair bundle is a tuft of a few tens to a few hundreds stiff finger-like protrusions, termed stereocilia, emanating from the surface of specialized sensory hair cells. Upon deflection, minute geometric rearrangements within the hair bundle lead to the opening and closing of mechanically gated ion channels. In this way, the hair bundle transduces mechanical stimuli (deflections) into electrical signals (ionic currents).

Next to operating as mere transducers, hair bundles from the bullfrog's sacculus have been shown to exhibit many features reminiscent of the auditory amplifier. Even in the absence of external stimulation, hair bundles can perform noisy spontaneous oscillations [3]. The forces necessary for these oscillations to occur are produced by calcium-regulated molecular motors, which operate on the inside of stereocilia. Most importantly, hair bundles can amplify weak periodic stimuli in a frequency-dependent manner [4]. In particular, for intermediate driving amplitudes, a nonlinear decay of sensitivity is observed, similar to the one characteristic for cochlear responses [4].

However, noise limits the extent of amplification a single hair bundle can achieve [5]. Noise stems from thermal interactions with the bathing fluid, stochastic opening of the mechanically gated ion channels, and a fluctuating component of force production by molecular motors. The operation of a single hair bundle therefore does not suffice to quantitatively account for the operation of the whole cochlea.

Coupled hair bundles. Hair bundles *in vivo* are often found to be attached to overlying elastic structures, such as tectorial or otolithic membranes. This suggests the possibility that coupling of hair bundles plays a role to enhance the properties of hair-bundle mediated amplification.

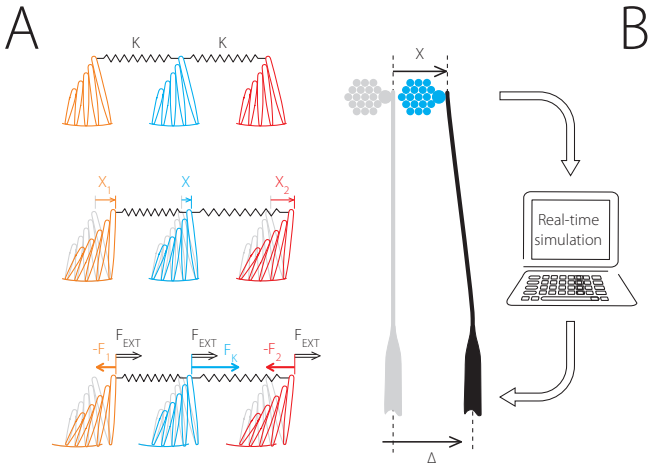

Figure 1: Coupling a hair bundle to two cyber clones by dynamic force clamp. (A) Schematic representation of a system of three coupled hair bundles. A hair bundle (blue) is connected to one neighbor on each side (orange and red) by identical springs. Relative movements of the hair bundles induce coupling forces. (B) Experimental realization. A single hair bundle is monitored. Two cyber clones, substituting the two flanking hair bundles in (A), are simulated on the computer. In real-time coupling forces and possibly also external periodic forces are computed and exerted by means of a glass fiber that was attached to the hair bundle's tip. We adjusted cyber-clone parameters such that our stochastic simulation would mimic the dynamics of the hair bundle used during the experiment, i.e. in particular its frequency, amplitude and quality of oscillation. Adopted from [9].

Contributions of our group. In earlier studies, we approached this hypothesis from a theoretical point of view. On the basis of an existing biophysical description of stochastic hair-bundle dynamics [5], we investigated the effect of elastic coupling [6]. In our simulations, we found that elastic coupling could induce synchronization among hair bundles and lead to an effective noise reduction. The latter manifested itself in an increased phase coherence of spontaneous oscillations and an enhancement of nonlinear amplification. In particular, we observed a sharpend frequency tuning and a pronounced increase in sensitivity to weak amplitude stimulation. An analysis of the response characteristics of a generic noisy oscillator helped to further understand the detrimental effect of noise in this particular context [7, 8].

Dynamic force clamp. In collaboration with J. Barral and P. Martin (Insitut Curie, Paris) we developed an experimental setup to adress the problem [9]. It was technically not feasible to interconnect biological hair bundles with elastic linkages. Therefore, we opted for a hybrid approach in which we coupled a biological hair bundle to two virtual hair bundles ("cyber clones") simulated in real-time on a computer (see Fig. 1). More specifically, in each time step (update rate 2.5kHz), we (i) monitored the position of the hair bundle, (ii) calculated the coupling forces acting on the hair bundle and the virtual cyber clones, (ii) exerted the force on the hair bundle by means of a flexible glass fiber, and (iv) integrated the stochastic differential equations describing cyber-clone dynamics (including the respective coupling forces) to generate the new positions of the virtual bundles. By means of this novel dynamic force clamp, we were thus able to emulate a situation in which a biological hair bundle under study was elastically coupled to two neighboring hair bundles of similar characteristics.

Main results. In a first set of experiments, we investigated the influence of coupling on the spontaneous activity of the three oscillators.In the absence of coupling, the oscillatory movements performed by the hair bundle and the two cyber clones were pairwise uncorrelated (see Fig. 2A, top), with increasing coupling strength, they became more and more correlated. Under strong coupling, near complete synchronization was observed (see Fig. 2A, bottom). At the same time, coupling brought about an effective noise reduction for the hair bundle and the two cyber clones. This was evidenced by a twofold increase in phase coherence of hair-bundle and cyber-clone oscillations, as reflected in their quality factor Q (not shown).

In a second set of experiments, we determined the effect of coupling on the response of the hair bundle to periodic stimulation. In particular, we were interested in its sensitivity $|\chi|$ in response to stimulation with a sinusoidal driving $F_{\text{ext}}(t) = A \sin 2\pi\nu t$, where ν denotes the characteristic frequency of oscillation. The external force was applied to hair bundle and cyber clones alike. Sensitivity was defined as $|\chi|(A,\nu) = |X_\nu/F_\nu|$, where X_ν and F_ν are the Fourier amplitudes of hair-bundle deflection and driving force at the frequency of stimulation, respectively. While coupling rendered sensitivity unchanged for strong driving amplitudes, for weak driving a twofold increase of sensitivity was observed (see Fig. 2B).

All measurements were in quantitative agreement with pure computer simulations of three coupled cyber clones.

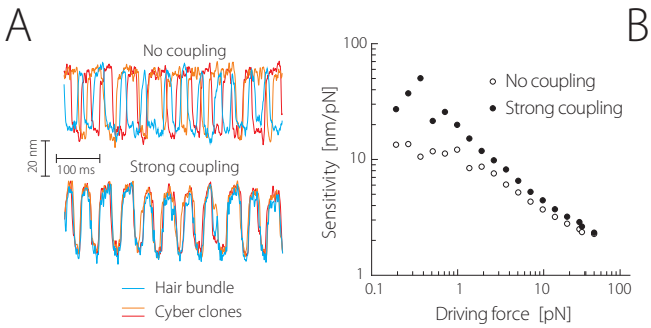

Figure 2: The effect of coupling on hair-bundle dynamics. (A) In the absence of coupling (top), hair-bundle (blue line) and cyber-clone (red and orange line) oscillations are pairwise uncorrelated. In the case of strong coupling (bottom), hair bundle and cyber clones move in synchrony. In (B), we plot hair-bundle sensitivity to sinusoidal stimulation as a function of the driving amplitude. While for strong driving amplitudes, coupling has no effect on sensitivity, for weak driving, coupling enhances sensitivity about twofold. Adopted and modified from [9].

Conclusion. Our numerical, analytical, and experimental results suggest that elastic coupling of active hair bundles can enhance the transmission and amplification of periodic stimuli by means of a noise reduction. Our work therefore supports the idea that small groups of coupled hair bundles constitute the essential oscillatory element in the active amplifier at work in the human ear.

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2.9 How Stochastic Adaptation Currents Shape Neuronal Firing Statistics

TILO SCHWALGER, BENJAMIN LINDNER

Channel noise and spike-frequency adaptation. Neurons of sensory systems encode signals from the environment by sequences of electrical pulses – so-called spikes. This coding of information is fundamentally limited by the presence of intrinsic neural noise. One major noise source is channel noise that is generated by the random activity of various types of ionic channels in the cell membrane. In other words, the current associated with a certain population of ion channels exhibits fluctuations unless the population is infinitely large. The fast currents that establish the spiking mechanism can be thus a source of such channel noise leading to a substantial variability of the neuronal response.

Besides these fast spike-generating currents, slow adaptation currents can also be a source of channel noise. Adaptation currents mediate a long-term drop of firing rate to a sustained stimulus, called spike-frequency adaptation (SFA). SFA is found in many neurons and profoundly shapes the signal transmission properties of a neuron by emphasizing fast changes in the stimulus but adapting the spiking frequency to slow stimulus components. The role of such spike-frequency adaptation for neural coding is, however, still poorly understood in the context of stochastic spike generation. In particular, the effects of different kinds of noise such as fast channel noise and slow adaptation channel noise on the neuronal spiking statistics is still largely unknown.

Stochastic and deterministic adaptation. To gain a better insight into the stochastic dynamics of adapting neurons we have analyzed the spiking activity of a noisy integrate-and-fire neuron model with an adaptation current (Fig.1). In the model, neural noise originates from either slow adaptation channel noise or fast channel noise. Surprisingly, the two noise sources lead to qualitatively different statistics of the inter-spike intervals (ISI), i.e. the intervals between two subsequent spikes [1]. The same difference in the ISI statistics is also observed in simulations of a more detailed Hodgkin-Huxley-type neuron model. These theoretical findings suggest that higher-order ISI statistics might help to experimentally distinguish adaptation noise from fast channel noise as the dominating intrinsic noise source of sensory neurons.

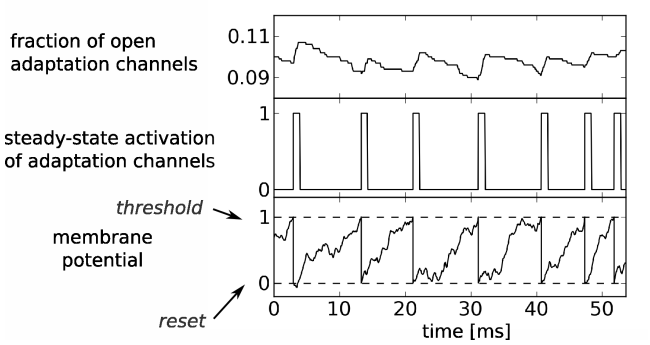

Figure 1: Illustration of the neuron model with a stochastic adaptation current. The membrane potential V (bottom panel) is driven by a constant base current, Gaussian white noise (modelling fast channel noise) and an inhibitory adaptation current. Whenever the membrane potential hits the threshold at $V = 1$ it is reset to the reset potential $V_{\text{reset}} = 0$. These threshold events define the spike times of the model. At the same time, adaptation channels can open during a short time window after each spiking event increasing or decreasing the open probability towards the steady state activation indicated in the middle panel. As a result the fraction of open channels, and thus the adaptation current, makes a random walk that increases immediately after each spike and decays in between spikes (top panel). This spike-triggered adaptation current inhibits in turn the dynamics of V realizing a negative feedback mechanism.

For the theoretical analysis we considered a perfect integrate-and-fire model with a voltage-gated adaptation current (similar to the M-type current) for two limit cases [1]:

1. *Deterministic adaptation.* The slow adaptation current is taken to be deterministic corresponding to a large (macroscopic) population of independent adaptation channels. The variability of the ISIs is solely caused by fast noise sources modeled by a white Gaussian noise.

2. *Stochastic adaptation.* The ISI variability is only due to the stochasticity of the adaptation current resulting from a finite number of slow adaptation channels.

From a mathematical point of view, both cases belong to the class of non-renewal models, because the slow adaptation current introduces memory of previous ISIs. Such processes are notoriously difficult to analyze. The non-renewal properties can be characterized by the serial correlation coefficient ρ_n of the ISI sequence $(\dots, T_{i-1}, T_i, T_{i+1}, \dots)$ defined by

$$\rho_n = \frac{\langle T_i T_{i+n}\rangle - \langle T_i\rangle^2}{\langle T_i^2\rangle - \langle T_i\rangle^2}. \qquad (1)$$

Hence, ρ_n measures the correlation between ISIs that are lagged by n.

Main results.

1. In the case of deterministic adaptation we find that the ISI density can be well approximated by an inverse Gaussian probability density. This density is equal to the first-passage-time density of a Brownian motion with a drift corresponding to a base current that is reduced by the adaptation (Fig. 2A). Furthermore, we have derived an analytical formula for the serial correlation coefficient ρ_n, which shows that neighboring ISIs are negatively correlated (Fig. 3). This characteristic feature has been numerically found in other neuron models with deterministic adaptation and fast fluctuations (e.g. [2, 3]) and has been experimentally observed for a variety of neurons (for reviews see [4, 5]).
2. A stochastic adaptation current can be approximated by a long-correlated colored noise process with effective parameters (reduced values of mean, noise variance, correlation time). As a consequence, the ISI densities become strongly skewed and peaked compared to an inverse Gaussian distribution (Fig. 2B) Another striking difference is, that the ISI correlations are positive and not negative as in the case of fast noise (Fig. 3). We have provided analytical formulas for the skewness, kurtosis and serial correlation coefficient of the ISIs that clearly explain these properties.

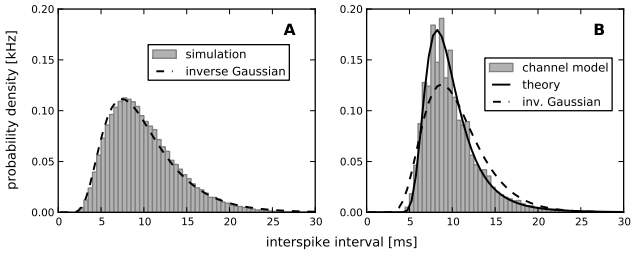

Figure 2: **(A)** Interspike interval (ISI) density for the case of deterministic adaptation. The gray bars display the result from a simulation of the model, the dashed line represents the inverse Gaussian distribution obtained from the theory. **(B)** ISI density in the case of stochastic adaptation. An inverse Gaussian distribution (dashed line) with the same mean ISI and the same variance does not fit the ISI density obtained from the simulation of the model with adaptation channels (gray bars). Circles depict simulation results of the diffusion approximation (Gaussian approximation) of the channel noise, the solid line shows our theoretical approximation.

Conclusions. We have put forward several novel analytical results that characterize the non-renewal spiking behavior of neurons with noise and stochastic or deterministic adaptation. Our analysis has revealed a striking difference of the ISI statistics depending on whether slow adaptation noise or fast current noise is dominating. These findings suggest an indirect way to determine the dominant source of noise on the basis of the ISI statistics. As an application, we have used our theoretical results to understand the origin of neuronal response variability of auditory receptor cells of locusts (collaboration with J. Benda, Munich). Preliminary analysis indicates that slow adaptation currents may indeed contribute to neuronal variability of this primary sensory neuron.

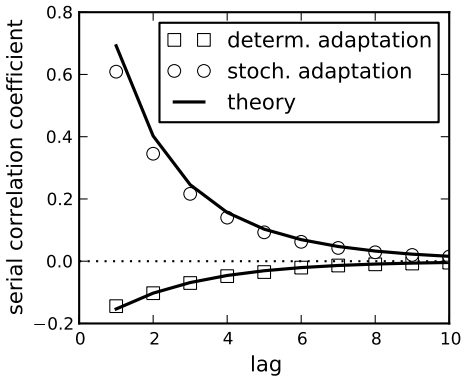

Figure 3: Serial correlation coefficient ρ_n as a function of the lag n. In the case of deterministic adaptation interspike intervals (ISIs) are negatively correlated, whereas in the case of stochastic adaptation ISIs become positively correlated.

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2.10 Experimental Manifestations of Magnetic Monopoles

L. D. C. JAUBERT, R. MOESSNER

In 2008, it was predicted that the magnetic material spin ice [1] should exhibit unusual quasiparticles which have properties of magnetic monopoles [2]: they experience mutual magnetic Coulomb forces; couple to an external magnetic field in the same way as electric charges couple to electric fields; are sources and sinks of the magnetic field **H**; and would show up in a SQUID-based monopole search experiment in the same way as (elementary) cosmic monopoles would.

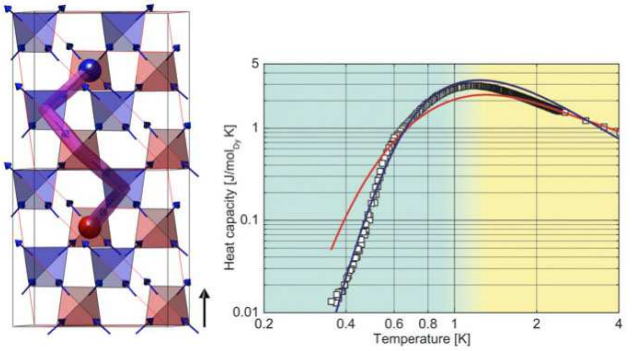

Figure 1: Left: The Ising spins in spin ice are constrained to point along the direction connecting the centres of the tetrahedra they belong to. The lowest energy for a tetrahedron is obtained for a two-in-two-out configuration, as illustrated. Applying a field, B || [001], results in a preference for aligning the tetrahedral magnetisation with the applied field direction. In the three dimensional pyrochlore, Dirac strings of flipped spins terminate on tetrahedra where magnetic monopoles reside. Right: The measured heat capacity per mole of $Dy_2Ti_2O_7$ at zero field (open squares) is compared with a Debye-Huckel theory for the monopoles (blue line) and the best fit to a single-tetrahedron (Bethe lattice) approximation (red line). The ice blue (yellow) backgrounds indicate the spin ice (paramagnetic) regimes, respectively.

The next logical step was to determine whether magnetic monopoles in fact do occur experimentally. To reach this goal, a number of potential signatures were considered, which probe different aspects of the physics of monopoles and the underlying magnetic Coulomb phase which acts as their vacuum [3–10].

Our work focused on several aspects. Firstly, the fact that these emergent monopoles are connected by flux strings which – unlike the Dirac strings of elementary monopoles – are observable; these "Dirac strings" have characteristic features due to their extended, one-dimensional, nature. Secondly, we considered the collective behaviour of the dilute liquid of monopoles at low temperature, which is quite analogous to that found in electrolytes, and should therefore share its universal properties. Finally, we have considered non-equilibrium phenomena probing the energy landscape which arises from interactions between the monopoles. This presents the possibility of probing the behaviour of pointlike topological defects in a three-dimensional magnet.

Crucially, the emergent monopoles in spin ice are deconfined: they can separate and move essentially independently. Thus, the equilibrium defect density is determined not by the cost of a spin flip but by the properties of the gas of interacting monopoles. In Fig. 1(right), the measured heat capacity is compared to Debye-Huckel theory [11], which describes a gas of monopoles with Coulomb interactions. This theory is appropriate to low temperatures, where the monopoles are sparse, and it captures the heat capacity quantitatively. At higher temperatures, spin ice turns into a more conventional paramagnet and the monopole description breaks down. Previous to our work, no analytical treatment of the low-temperature thermodynamics of spin ice had been available.

Monopole deconfinement is also reflected in the spin configurations: as two monopoles of opposite sign separate, they leave a tensionless string of reversed spins connecting them, a classical analogue of a Dirac string: in the theory of Dirac [12], these are infinitely narrow, unobservable solenoidal tubes carrying magnetic flux density (B-field) emanating from the monopoles. In our case, the strings are real and observable thanks to the preformed dipoles of the spins; strings can change length and shape, at no cost in energy other than the magnetic Coulomb interaction between their endpoints.

As the strings consist of magnetic dipoles, the method of choice for imaging them is magnetic neutron scattering. The application of a large magnetic field along one of the principal axes orients all spins. The resulting ground state is unique and free of monopoles. Upon lowering the field through a critical field h_S [13] sparse strings of flipped spins appear against the background of this fully magnetised ground state. In the absence of monopoles, such strings must span the length of the sample and terminate on the surface; otherwise, they can terminate on magnetic monopoles in the bulk. Each link in the string involves a spin being reversed against the field.

The panels in Fig. 2 show reciprocal space slices of the neutron scattering results at a field near saturation of $h = 5/7h_S$: cone-like scattering emanates from what was the position of the pinch points [4,7] in zero field.

These can be modeled by noting that the strings execute a random walk; when their density is small, interactions between them can be neglected to a first approximation, so that the spin correlations are those of a diffusion process with the z coordinate assuming the

role usually played by time:

$$C(x,y,z) \approx \frac{1}{z}\exp\left(-\gamma\frac{x^2+y^2}{z}\right) \quad . \qquad (1)$$

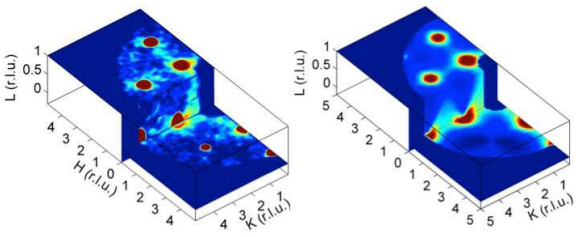

Figure 2: Magnetisation and diffuse neutron scattering with field applied along the [001] axis. Left: 3D representation of the single crystal neutron diffraction data from E2, HZB, at $5/7h_S$ and 0.7 K showing a cone of scattering coming from (020) Bragg peak. Right: Calculation of diffuse scattering characteristic of the weakly biased random walk correlations with bias of 0.53 : 0.47 and $\mathbf{B}_{int}||$ [001].

The scattering from a large ensemble of such walks has been calculated including all the geometrical factors for the neutron scattering cross section. As can be seen from the side-by-side comparison of the data and modelling, the string configurations account very well for the data and reproduce the cone of scattering observed (Fig. 2).

It turns out that the interactions between the strings – considered to be of a hard-core exclusion nature in the theory above – can elegantly be tuned by modulating the exchange constants in different directions of the pyrochlore lattice. By choosing exchange constants as displayed in Fig. 3, we obtain a very unusual "infinite order" phase transition out of the Coulomb into a fully ordered phase, at a critical temperature $T_c = 4\delta/(3\ln 2)$.

Mathematically, the system can be described using a transfer matrix to 'propagate' the strings along the [001] direction. This transfer matrix is block-diagonal in the number of strings, and one finds that (i) below T_c the magnetisation is saturated; and (ii) at T_c all sectors are equiprobable *and* all configurations within a sector are equiprobable, reflecting the absence of interactions between strings [14]. Indeed, at T_c, the transfer matrix exhibits a symmetry enhancement from U(1) to SU(2)! A consequence of the absence of interactions between strings is that the surface tension between oppositely magnetised domains vanishes and the domain wall width diverges as T_c is approached from below. At T_c^- the magnetisation profile away from the domain wall centre $M(y)$ is a function only of $y/L_\perp$. Below T_c the domain wall width $\ell_w^{-1} \propto (1-T/T_c)^{1/2}$ (Fig. 3). It is striking to find broad domain walls in an Ising magnet; they may be detectable using small angle neutron scattering.

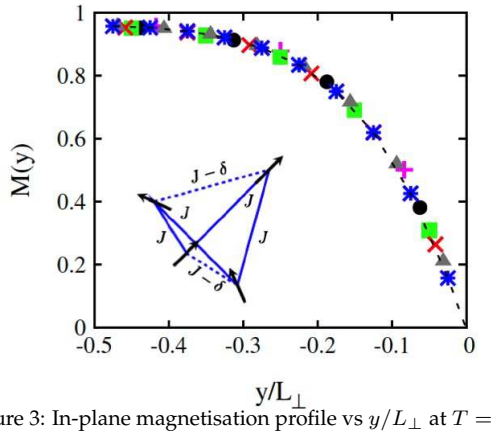

Figure 3: In-plane magnetisation profile vs $y/L_\perp$ at $T = 0.999T_c$ for plane size $L_\perp = \{6, 8, 10, 12, 16, 20\}$. Inset: A tetrahedron of the pyrochlore lattice with exchange J and $J-\delta$ as indicated: the dashed bonds lie in (001) planes. One of the two ground states for $\delta > 0$ is shown.

The natural way to generate the required degeneracy lifting in a magnetic compound is to apply uniaxial pressure along the [001] axis of a single crystal. To see this exotic "infinite-order" phase transition, pressures about a factor three larger then the ones studied so far [15] are necessary. We hope our work will stimulate further experimental efforts to realise this unusual transition.

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2.11 The Statistical Mechanics of Quantum Complexity: Random Quantum Satisfiability

A.M. LÄUCHLI, R. MOESSNER

The potential power of quantum computers motivates the intense effort in progress to understand and, eventually, build them. Much interest has naturally been focused on algorithms that outperform their classical counterparts. However, the development of a complexity theory for quantum computers suggests that we already know problems, those shown to be 'QMA-complete', whose worst case solutions will take even quantum computers a time exponential in problem size. These appropriately generalize the class of NP-complete problems–those which are easy to check but (believed to be) hard to solve on classical computers–to quantum computers [1,2].

The classic technique of complexity theory is "assigning guilt by association", i.e. by exhibiting the polynomial time equivalence of a new problem to a particular problem believed not to be amenable to efficient solution. For NP-complete problems this leads to the celebrated Cook-Levin theorem, which shows that the satisfiability problem with clauses in three Boolean variables (3-SAT) encapsulates the difficulty of the entire class [3]. While this is a powerful and rigorous approach, it has two limitations. It does not directly tell us why a problem has hard instances and it does not tell us what general features they possess.

Over the past decade joint work by computer scientists and statistical physicists has produced an interesting set of insights into these two issues for 3-SAT (and related constraint satisfaction problems). These insights have come from the study of instances chosen at random from ensembles where the density of clauses α acts as a control parameter. One can think of this as representing the study of typical, but not necessarily worst, cases with a specified density of clauses/constraints. Using techniques developed for the study of random systems in physics, it has been shown that the ensembles exhibit a set of *phase transitions* between a trivial satisfiable (SAT) phase at small α and an unsatisfiable (UNSAT) phase at large α (see *e.g.* [4–6]). These transitions mark sharp discontinuities in the organization of SAT assignments in configuration space as well as a vanishing of SAT assignments altogether. This information has provided a heuristic understanding of why known algorithms fail on random SAT when the solution space is sufficiently complex and in doing so has localized the most difficult members of these ensembles to a bounded range of α.

We have begun [7–9] an analogous program for quantum computation with the intention of gaining insight into the difficulty of solving QMA-complete problems. Specifically, we introduce and study random ensembles of instances of the quantum satisfiability (k-QSAT) problem formulated by Bravyi [11]. Like classical 2-SAT, 2-QSAT is efficiently solvable (*i.e.* it is in P), while for $k \geq 4$, k-QSAT is QMA_1-complete. Our central results are as follows. Firstly, we have obtained the complete phase diagram, including an explicit construction of satisfying states, for 2-QSAT (see Fig. 1). For $k \geq 3$-QSAT, we have established the existence of several phases (c.f. Fig. 2), and in particular we find a phase where there exists a basis of satisfying states made up solely of product states (a PRODSAT phase). It has since been established that there is, for sufficiently large k, always a transition out of this to a different, SAT– un-PRODSAT, phase.

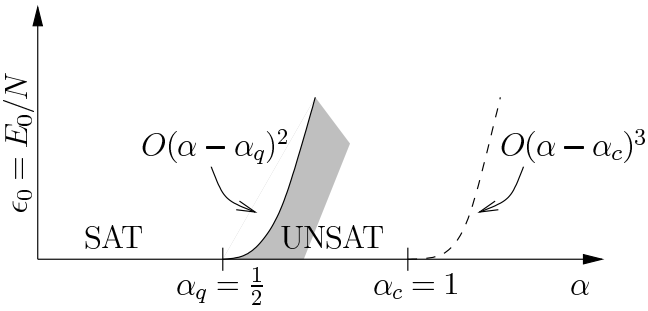

Figure 1: Phase diagram of 2-QSAT. The quantum SAT-UNSAT transition $\alpha_q = \frac{1}{2}$ coincides with the emergence of a giant component in the random graph, which lies at half the classical 2-SAT transition $\alpha_c = 1$ [12]. The solid (dashed) line marks an asymptotic upper bound on the quantum (classical) ground state energy density ϵ_0.

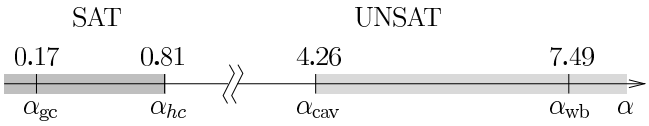

Figure 2: Phase diagram of 3-QSAT. For $\alpha < \alpha_{hc} \approx 0.81$, the problem is rigorously SAT. The UNSAT transition is bounded below by the weak bound $\alpha_{\mathrm{wb}} = -1/\log(1 - 1/2^k)$, but also (slightly less rigorously) by the classical cavity transition α_{cav} [6]. The giant component of the random graph emerges squarely in the SAT phase at $\alpha_{\mathrm{gc}} = \frac{1}{k(k-1)} \approx 0.17$.

In more detail, we study the following problem. Consider a set of N qubits. We first randomly choose a collection of k-tuples, $\{I_m, m = 1 \ldots M\}$ by independently including each of the $\binom{N}{k}$ possible tuples with probability $p = \alpha/\binom{N}{k}$. This defines an Erdös hypergraph with αN expected edges; we exhibit simple examples of these for $k = 2, 3$ in Fig. 3. In classical k-SAT, the next step is to generate an instance of the problem by further randomly assigning a Boolean k-clause to each k-tuple of the hypergraph. In key contrast to the classical case, where the Boolean variables and clauses

take on discrete values – true or false – their quantum generalizations are continuous: the states of a qubit live in Hilbert space, which allows for linear combinations of $|0\rangle$ ("false") and $|1\rangle$ ("true"). Thinking of a Boolean clause as forbidding one out of 2^k configurations leads to its quantum generalization as a projector $\Pi_\phi^I \equiv |\phi\rangle\langle\phi|$, which penalizes any overlap of a state $|\psi\rangle$ of the k qubits in set I with a state $|\phi\rangle$ in their 2^k dimensional Hilbert space. In order to generate an instance of k-QSAT the states $|\phi\rangle$ (of unit norm) is picked randomly in this Hilbert space.

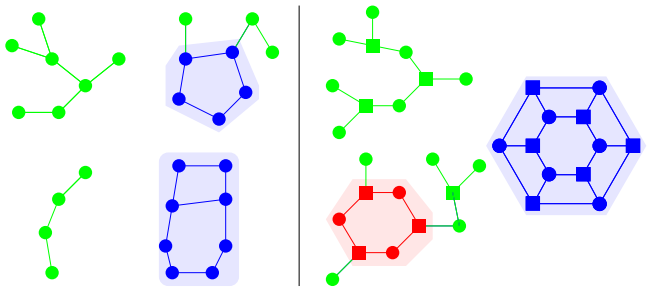

Figure 3: Examples of random (hyper-) graphs for 2-SAT (left) and 3-SAT. Left: The clusters, clockwise from bottom left, are chain, tree, clusters with one and two closed loops ("figure eight"). By our geometrisation theorem the shaded objects play a role in determining existence, and nature, of satisfying states. Right: Circles denote qubits, and squares denote clauses.

The sum of these projectors defines a positive semidefinite Hamiltonian

$$H = \sum_{m=1}^{M} \Pi_{\phi_m}^{I_m} \qquad (1)$$

and the decision problem for a given instance is, essentially, to ask if there exists a state that simultaneously satisfies all of the projectors, *i.e.* to determine whether H has ground state energy, E_0, exactly zero.

One of our most remarkable results is presented in the following. The ensemble of problems we study is random in two ways. Firstly, the interactions are represented by random graphs. Secondly, the projectors are drawn at random. It turns out that different realisations of the latter does not exhibit a variation in satisfiability. Specifically:

Geometrisation Theorem: Given an instance H of random k-QSAT over a hypergraph G, the degeneracy of zero energy states $\dim(\ker(H))$ takes a particular value D with probability 1 with respect to the choice of projectors on the edges of the hypergraph G.

This means that $\dim(\ker(H))$, which can be obtained from solving a "hard" *quantum* problem, appears as a property of a *classical* graph which, for $k \geq 3$, has as yet not been identified. For $k = 2$, an L-site tree has $D = L + 1$, whereas a cluster with one closed loop has $D = 2$, and $D = 0$ holds in the presence of more than one closed loop (Fig. 3).

Besides the question about existence, and the number D, of satisfying assignments, it is interesting to ask about their *nature*. We have found that, for $\alpha < \alpha_{\rm PS}$, there exists with probability 1 a satisfying assignment that is a product state of qubits: $|\Psi_{\rm PS}\rangle = \otimes_{i=1}^{N} |\psi_i\rangle$. In general, this holds when the interaction graph G permits a dimer covering of its clauses (Fig. 4).

Our first study has established basic features of phase structure and solution space of random k-QSAT. Beyond this, the study of this and related models remains an active and growing nascent part of quantum complexity theory. Particularly interesting questions involve the existence of a cascade of 'entanglement transitions' as well as the possibility of a quantum–PCP theorem establishing a rigorous notion of quantum glassiners.

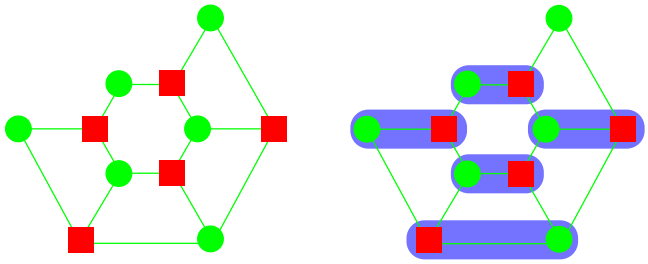

Figure 4: Example of a $k = 3$ interaction graph with $M < N$, circles (green) indicate qubits and squares (red) indicate clause projectors that act on adjacent qubits (left); a dimer (blue shaded) covering that covers all clauses (right).

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2.12 Entanglement Analysis of Fractional Quantum Hall States on Torus Geometries

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Introduction. The description of condensed matter phases using *entanglement measures*, borrowed from the field of quantum information theory, has led to a large body of work [1]. One situation where this interdisciplinary work has been particularly fruitful is in the study of topologically ordered states [2, 3]. Fractional quantum Hall (FQH) states of two-dimensional electrons in a magnetic field stand out as the only experimentally realized topologically ordered phases. These states have recently received renewed intense attention due to quantum computation proposals based on their topological properties. An intriguing feature of FQH states is that their edges have gapless modes, described by chiral Luttinger liquids.

Here we summarize studies of the *entanglement entropy* and the *entanglement sepctrum* in the most prominent FQH states, namely the Laughlin states, placed on a toroidal geometry [4,5].

Entanglement measures, topological order, and edge modes. A prominent measure of entanglement is the von Neumann entropy of entanglement, S_A, measuring the entanglement between a block (A) and the rest (B) of a many-particle system in a pure state. The entanglement entropy $S_A = -\mathrm{tr}\,[\rho_A \ln \rho_A]$ is defined in terms of the reduced density matrix, $\rho_A = \mathrm{tr}_B\,\rho$, obtained by tracing out B degrees of freedom from the system density matrix $\rho = |\psi\rangle\langle\psi|$, with $|\psi\rangle$ denoting a ground state wave function.

In one dimension the scaling behavior of the block entanglement entropy is well understood. In two dimensions (2D), no such generic classification exists. However, for topologically ordered states in two dimensions, the scaling of S_A contains topological information about the state:

$$S_A = \alpha L - n\gamma + \mathcal{O}(1/L), \qquad (1)$$

where L is the block boundary length, γ characterizes the topological field theory describing the state [2], while n counts the number of disconnected components of the boundary. The value of γ is related to the "quantum dimensions" of the quasiparticle types of the theory, $\gamma = \ln \mathcal{D}$, where $\mathcal{D}$ is the total quantum dimension. For Laughlin states at filling $\nu = 1/m$, $\gamma = \frac{1}{2}\ln m$.

It is also useful to study the complete spectrum of the reduced density matrix, obtained by a Schmidt decomposition of the ground state:

$$|\psi\rangle = \sum_i e^{-\xi_i/2} |\psi_i^A\rangle \otimes |\psi_i^B\rangle.$$

The $\{\xi_i\}$ form the *entanglement spectrum* (ES). The states $|\psi_i^A\rangle$ ($|\psi_i^B\rangle$) form an orthonormal basis for the subsystem A (B).

Very recently, ES studies have been used [3] to probe edge modes of FQH states. The entanglement between two partitions of an edgeless wavefunction may seem at first sight unrelated to edge physics. However, the entanglement spectrum can be regarded as the spectrum of an effective "entanglement Hamiltonian" confined to the A region of space, which typically contains similar physics as the original physical Hamiltonian, but is dominated by the boundary region between A and B. Since the region A does have a boundary, the low-lying spectrum would then show an edge structure, even though the total system has no edge. This construction of studying edge physics in ES works particularly well in situations where the bulk is gapped but edges are gapless, which is the case for FQH states. Refs. [3] analyzed the ES of FQH states on the sphere with hemispheric partitioning. The Virasoro multiplet structure of the conformal field theory (CFT) describing the edge appears in the low-lying part of the ES.

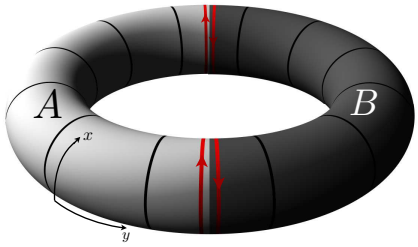

Figure 1: Torus setup for block entanglement computations. The lowest Landau level is spanned by orbitals which in Landau gauge are centered along the circles shown. The arrows indicate the chiralities of the virtual 'edges' created by the block partitioning.

The torus geometry. The torus geometry (Fig. 1) gives us access to new physics and new analysis tools, compared to the spherical geometry used, e.g., in [3,7]. The two circumferences of the torus (L_1, L_2 in the x,y directions) are continously variable parameters which allow a sensitive analysis of the scaling behaviors.

The natural partitions of the torus are cylinder-like segments with two disjoint edges. The ES thus contains the physics of a combination of two separate conformal edges. This leads to 'towers' in the ES spectrum, when plotted against appropriate quantum numbers. Even in cases where the two edges have different spectra, the two spectra combine to form towers. The two-edge picture provides enormous predictive power, as the assignment of only a few edge mode energies enables us to construct the remaining ES.

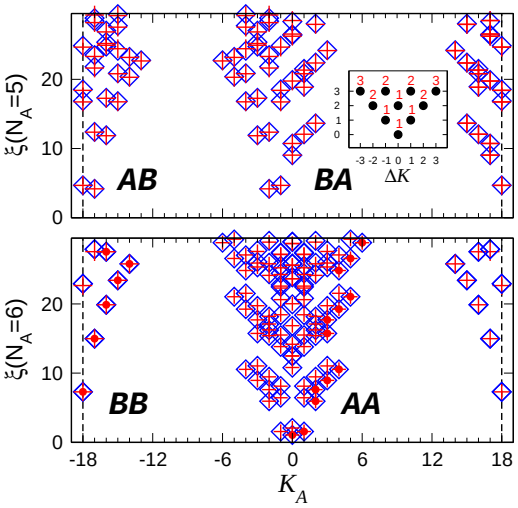

Figure 2: Entanglement spectrum for Laughlin state at $\nu = 1/3$, with 12 particles and $L_1 = 10$, plotted against block momentum K_A. The blue squares represent numerically obtained data. The assigned edge modes are labeled by green dots while the combinations of those edges are marked by red crosses. The script letters are microscopic identifiers for the two edges combining to form each tower. The striking correspondence of the red crosses with numerical data shows that our algorithm based on the two-edge picture allows the reconstruction of the entire entanglement spectrum using only the postions of the green dots. The inset shows a CFT tower formed by two ideal chiral edges, the states labeled with their degeneracies.

The torus geometry also allows us to adiabatically connect to the "thin torus" limit, which is exactly solvable [6] and has as ground states the "Tao-Thouless" crystalline states. Many features of the ES can be understood starting from these simple states. The CFT tower structure persists even very close to the thin-torus limit, which by itself is an uncorrelated product state.

Also, the toroidal geometry has a natural continuous variable, the aspect ratio, which provides far greater control and accuracy in calculations of γ, compared to the spherical case where such calculations have been tried previously [7].

Tower structure and CFT identification. Numerical ES are shown in Fig. 2 for a 12-particle Laughlin state. A prominent feature is that the ES consists of 'towers'. Most of the towers are symmetric, while some are skewed. We interpret each tower as a combination of chiral modes of two edges (two block boundaries). An *ad hoc* assignment of a small number of (Virasoro) energies provides the necessary input for constructing each tower.

The number of independent modes of a chiral $U(1)$ CFT at momentum k is given by the partition function $p(k) = 1, 1, 2, 3, 5, 7, 11, ...$ for k = 0,1,2,.... When two *linearly* dispersing chiral modes combine, one expects an ideal tower of states like the one shown in Fig. 2 (inset). The observed towers in the numerical ES can be explained by postulating the individual edge spectra to have split degeneracies while preserving the Virasoro counting. Two such modified edge spectra can be combined to construct towers which are less degenerate than the ideal case of Fig. 2 (inset).

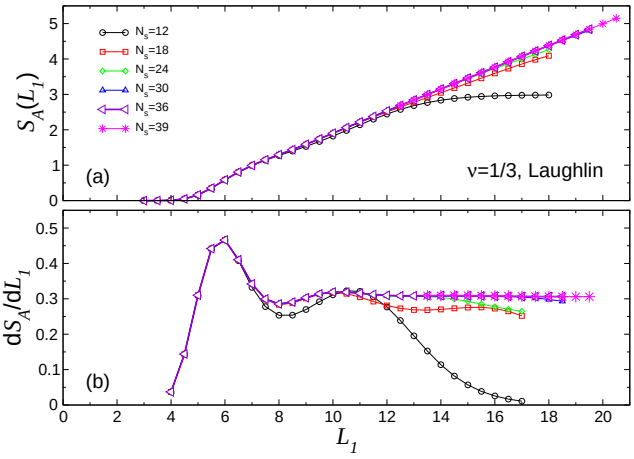

Figure 3: (a) Entanglement entropy S_A and (b) its derivative $\mathrm{d}S_A/\mathrm{d}L_1$ for the Laughlin state at $\nu = 1/3$ as a function of torus circumference L_1. Examining these continuous curves allows us to identify the region where the scaling regime has been reached, so that α and γ [Eq. 1] can be extracted.

Entanglement entropy scaling. In Fig. 3, we give an example of the utility of having the aspect ratio (or equivalently the torus width L_1) as a continuous variable, in studying the scaling of entanglement entropy. An analysis such as this shows that, with finite-size numerical data, there is a window of L_1 values which one can use to extract quantities in the scaling limit, such as the subleading topological term γ in Eq. 1.

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2.13 Quantum Spin Liquids in the Vicinity of Metal-Insulator Transitions

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The Hubbard model is one of the central paradigms in the field of strongly correlated systems for about five decades, and new aspects of its extremely rich phase diagram are still regularly unveiled. Even at half-filling, the popular wisdom according to which the model has only two phases, a metallic one at weak coupling and an insulating one at strong coupling separated by a first order transition [1], has been recently challenged. This goes back to the numerical work of Morita *et al.* [2] on the triangular lattice which revealed the presence of a non-magnetic insulating phase close to the metal-insulator transition. It is believed that this quantum spin liquid (QSL) has no spin gap and algebraically decaying correlations [3]. More recently, a different example of a quantum spin liquid phase on the insulating side of the metal-insulator transition has been identified on the honeycomb lattice using Quantum Monte Carlo simulations [4]. This spin liquid phase is reported to have a small spin gap and no appreciable correlations of any kind.

Given that there are now two different spin liquids on the insulating side of the Mott metal-insulator transition, we address here the conceptionally important question whether a *spin-only* description of the spin liquid is valid and if so, whether an accurate description of the physics is possible, despite the intermediate value of U/t and the vicinity of the Mott transition.

Triangular lattice The precise nature of the SL phase of the Hubbard model on the triangular lattice is also of direct experimental relevance for the 2D organic salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ [5]. As such, it has already attracted a lot of attention, but fundamental questions such as the appropriate low-energy effective theory remain unanswered. Since the phase is insulating, an effective model where charge fluctuations are treated as virtual excitations should be possible. However, whether a description in terms of a pure spin model is possible is far from obvious, in particular since there seems to be a jump in the double occupancy at the transition from the three-sublattice Néel phase to the QSL.

In Ref. [6] we have now showd that the correct low-energy theory of both insulating phases, and in particular of the QSL phase, is indeed a pure spin model. This has been achieved by deriving an effective spin model to high order (order 12) about the strong coupling limit using perturbative continuous unitary transformations (PCUTs) [7], and by showing that it gives a qualitative and quantitative account of the transition from the three-sublattice magnetic order to the SL state.

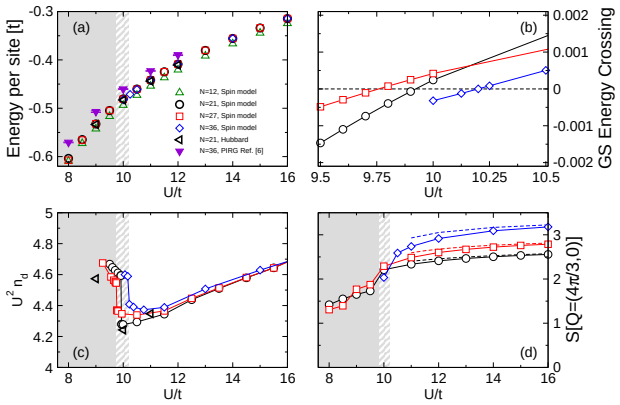

Figure 1: (a) Energy per site as a function of U/t for the Hubbard model and the effective spin model. The agreement between the two approaches is very good, despite the intermediate value of U/t. (b) Level crossings in the effective spin model signalled by the energy difference of the two lowest energies. This is an indicator for the first order phase transition from the three sublattice Néel state to the quantum spin liquid. (c) Double occupancy (times U^2) as a function of U/t. Note the small jump at the transition, which is faithfully reproduced in the spin model. (d) Magnetic structure factor at the 120° AFM ordering wave vector. In the Néel ordered phase the signal increases with system size, as expected. In the quantum spin liquid phase the structure factor saturates, indicating a magnetically disordered phase.

In Fig. 1 we display selected observables obtained by simulating the effective spin model including two-, four- and six-spin interactions using large scale exact diagonalizations (see caption of Fig. 1). We have also obtained detailed low energy spectra which exhibit a remarkable correspondence between the low-energy sector of the Hubbard model and the spin-model and which underline the first order nature of the transition from the magnetically ordered phase at large U/t and the quantum spin liquid at intermediate coupling. The quantum numbers of the low-energy spectrum also support the *spin-Bose-metal* description of the spin liquid phase put forward in Ref. [3].

This *spin-only* description thus gives deep insights into the nature of the QSL phase and clearly provides the appropriate framework for further studies, for example including the effect of hopping integral anisotropies and the long range nature of the Coulomb interaction in the spin liquid material κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ [8].

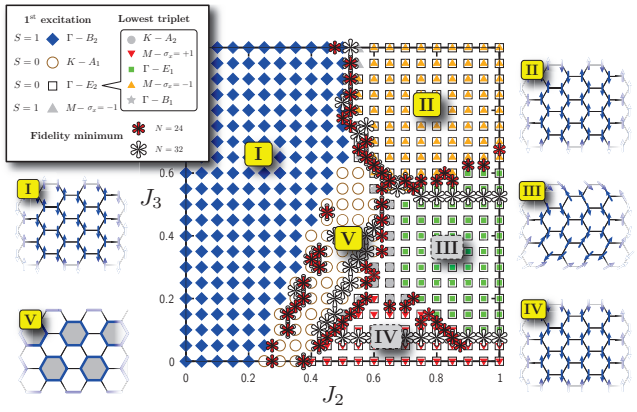

Figure 2: Phase diagram of the frustrated $S = 1/2$ Heisenberg model honeycomb lattice in the region $J_2, J_3 \in [0, 1]$, based on a combination of exact diagonalization results. The 5 regions identified here correspond to: **(I)** a Néel ordered phase with staggered magnetization, **(II)** a collinear magnetically ordered phase, **(III)** One or several phases corresponding to short or long range ordered non-collinear magnetic order, **(IV)** A different collinear magnetically ordered (or disordered) phase and **(V)** a magnetically disordered phase forming a *plaquette* valence bond crystal. The five phases are sketched in the panels around the phase diagram.

Honeycomb lattice The exciting finding of a novel quantum spin liquid in the half-filled Hubbard model on the honeycomb lattice [4] leads us again to the question of whether this spin liquid phase on the honeycomb lattice can be described within a pure $S = 1/2$ spin model, despite the vicinity of the insulator to semimetal transition. A high order derivation of the corresponding spin model is currently in progress, however the typical value of the expansion parameter $t/U \sim 0.25$ $(U/t \sim 4)$ relevant for the spin liquid phase renders this task much more challenging in comparison to the triangular lattice, where a typical value for the spin liquid regime is about $t/U \sim 0.11$ $(U/t \sim 9)$. In the absence of an accurate prediction for a relevant spin model, we start by exploring the effect of the next-to-leading order correction to the nearest neighbor Heisenberg model, which is a second neighbor Heisenberg coupling J_2 arising at fourth order in t/U. We thus consider in the following a frustrated $S = 1/2$ Heisenberg Hamiltonian on the honeycomb lattice, where we also include a third neighbor coupling J_3 for completeness.

The key finding of our numerical work [9] is the presence of a sizable magnetically disordered phase adjacent to the well studied Néel phase of the unfrustrated honeycomb Heisenberg model (c.f. Fig. 2). We identify this phase as a *plaquette* valence bond crystal (VBC). Interestingly we find evidence for a possibly continuous phase transition between the Néel phase and a *plaquette* valence bond crystal. In addition the energy and some of the key correlations of the frustrated spin model in the transition region are well captured by a simple Gutzwiller projected (GP) "Dirac sea" wave function (c.f. Fig. 3). These findings raise the possibility of a continuous quantum phase transition beyond the Ginzburg Landau paradigm in this honeycomb lattice spin model.

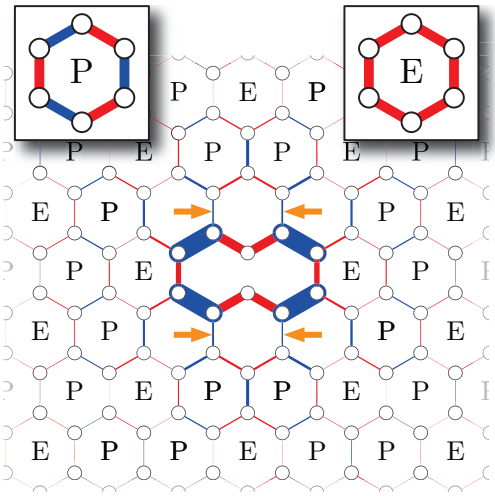

Figure 3: Structure of the dimer dimer correlations in the Gutzwiller projected Dirac sea wave function. This wave function has algebraic Néel and dimer-dimer correlations and can possibly describe a spin system at the Néel to spin liquid (here a valence bond crystal) transition. Surprisingly, these correlations are in qualitative agreement with the ones found in the spin liquid region of the Hubbard model in Ref. [4].

In subsequent work we will address the role of the six-spin terms which will enter the spin model at order six, and investigate whether these additional terms indeed reveal a gapped, featureless spin liquid as seen in the Hubbard model simulations [4], or whether even more extended spin interactions are required.

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2.14 Work Dissipation Along a Non Quasi-Static Process

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Many complex dynamical phenomena which have traditionally been interpreted in the framework of dynamical systems have more recently been considered from a statistical physics perspective. Most dynamical models, among them models for lasers, chemical reactions, or population dynamics, describe open systems, i.e., systems which are subject to some throughput of energy. In a more statistical setting, one would couple such models to one or more heat baths rather than relying on a perfectly deterministic description. Such systems are thermodynamic systems out of equilibrium, and their fluctuations, both of dynamical origin and due to the heat exchange with the baths, are non-equilibrium fluctuations. In the past two decades, much theoretical progress has been made towards a characterization of such fluctuations by *fluctuation theorems*. Even though these theorems do not yet cover the physically most relevant and interesting scenarios, they make important statements.

In classical thermodynamics, the *maximum work theorem* states that the maximum work $-W_\mathrm{r}$ [1] that can be extracted when driving a system between two given equilibrium states is obtained for a reversible process [1]. Such a process does not produce any entropy. If the system is in contact with a heat bath at constant temperature T, then a process is reversible if and only if it is quasi-static. In this case the *reversible work* W_r is the difference in free energy ΔF between the final and the initial state. If the system is quasi-statically driven from the final state back to the initial state, then the same amount of work $W_\mathrm{r} = \Delta F$ will be retrieved from the system. However, if the system is driven at a finite speed, then the work performed during the process is random and is generally greater than the reversible work. The excess work $W_\mathrm{d} = W - \Delta F$ is dissipated to the reservoir in the form of heat, leading to a total entropy production $\Delta_i S = W_\mathrm{d}/T$. Crooks' fluctuation relation is a statement about the asymmetry of the work distributions during a non quasi-static process and the corresponding reverse process. It links the probability $P(W)$ to perform a certain amount W of work when driving the system from the initial state to the final state to the probability $\bar{P}(-W)$ of performing the opposite amount when performing the reverse process [2]:

$$\frac{P(W)}{\bar{P}(-W)} = \exp\left(\frac{W-\Delta F}{k_\mathrm{B}T}\right). \tag{1}$$

The *fluctuating lattice-Boltzmann model* (FLBM) is a stochastic lattice model for a thermal ideal gas [3]. It provides a simple model for investigating the fluctuating dynamics of isothermal processes [4]. The FLBM simulates an ideal gas in contact with a heat bath and subjected to a force field per unit mass $\vec{f} = -\vec{\nabla}\phi_\lambda$, derived from a potential $\phi_\lambda(\vec{r})$. It consists of mass densities $\{n_i\}_{i=1}^b$ moving along the edges of a Bravais lattice $\{\vec{r}\}$ according to a finite set of b velocities $\{\vec{c}_i\}_{i=1}^b$. The dynamics takes place in discrete time. Each time step is divided into a collision and a propagation step. During the propagation step the post-collisional populations $\{n_i^*\}$ are simply propagated according to the set of velocities $\{\vec{c}_i\}$:

$$n_i(\vec{r}+\vec{c}_i, t+1) = n_i^*(\vec{r}, t). \tag{2}$$

During the collision step the populations at each node are randomly shuffled such that at each node $\vec{r}$ the mass $\rho(\vec{r},t) = \sum_i n_i(\vec{r},t)$ and momentum $\vec{j}(\vec{r},t) = \sum_i n_i(\vec{r},t)\vec{c}_i$ densities are exactly conserved and that the local stress $\sum_i n_i c_{i,\alpha} c_{i,\beta}$ relaxes to and fluctuates around the Euler stress $\rho k_\mathrm{B}T\delta_{\alpha,\beta} + \rho v_\alpha v_\beta$, where α and β are the Cartesian coordinates, $\delta_{\alpha,\beta} = 1$ if $\alpha = \beta$ and 0 otherwise, and $\vec{v} = \vec{j}/\rho$ is the local fluid velocity [2]. The effect of the body force $\vec{f}$ is to increase the momentum density by $\rho\vec{f}$ at each time step.

At thermal equilibrium, the density at point $\vec{r}$ fluctuates around its mean value given by the Boltzmann factor $\langle\rho(\vec{r})\rangle_\mathrm{eq} \propto \exp(-\phi_\lambda(\vec{r})/k_\mathrm{B}T)$. The potential energy $V[\rho,\phi_\lambda] = \sum_{\vec{r}}\rho(\vec{r})\phi_\lambda(\vec{r})$ of the system changes during one time step as λ changes to $\lambda+\delta\lambda$, with an amount of work δW performed on the system:

$$\delta W = V[\rho,\phi_{\lambda+\delta\lambda}] - V[\rho,\phi_\lambda] = \sum_{\vec{r}}\rho(\vec{r})\frac{\partial\phi_\lambda}{\partial\lambda}\delta\lambda \tag{3}$$

for small $\delta\lambda$. The total work W performed when switching λ from 0 to 1 in steps of $\delta\lambda$ is given by:

$$W = \int_0^1 \frac{\delta W}{\delta\lambda}\,\mathrm{d}\lambda. \tag{4}$$

The *time reversed* process is obtained by switching λ from 1 back to 0 in steps of $\delta\lambda$.

Fig. 1 shows examples of distributions of the work performed during a non quasi-static process (solid lines) and the work extracted during the corresponding reverse process (dashed lines). These distributions were obtained with the potential

$$\phi_\lambda(\vec{r}) = \lambda A\left[\cos\left(2\pi\frac{x}{l}\right)+1\right] \tag{5}$$

where $A = 0.01$ is the amplitude of the potential and $l = 100$ the length of the lattice.

[1] We consider the work *performed* on the system, which is the opposite of the work *extracted*.

[2] For a detailed description of the dynamics of the model, see [3]

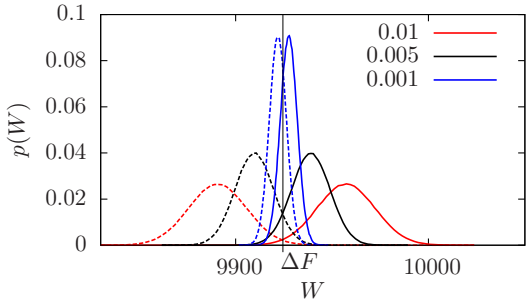

Figure 1: Distributions of the work performed during the direct process (solid lines) and extracted during the time-reversed process (dashed lines) for various values of the switching rate $\delta\lambda$.

The parameter $\delta\lambda$, *the switching rate*, controls how far from equilibrium the system is driven. With fast switching (red curve on fig. 1), the system is driven further away from equilibrium than with slow switching (blue curve). The mean dissipated work is greater, as are the fluctuations of the work. The maximum work theorem implies that in the quasi-static limit $\delta\lambda \to 0$, the distributions of the work for the direct and the time-reversed processes both tend towards a Dirac distribution centered on ΔF.

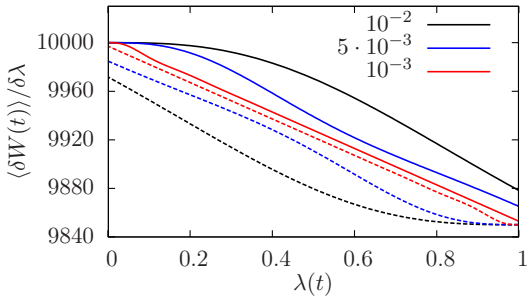

Figure 2: Evolution of the mean work performed (solid lines) and extracted (dashed lines) $\langle \frac{\delta W}{\delta\lambda} \rangle$ per time step along the direct and reverse processes for different switching rates $\delta\lambda$.

The evolution of the quantity $\frac{\delta W}{\delta\lambda}$ during switching helps to understand how the distributions in fig. 1 arise. Fig. 2 shows the evolution of its mean value $\langle \frac{\delta W}{\delta\lambda} \rangle$ along the process for different values of the switching rate $\delta\lambda$. Examples of the fluctuations of $\frac{\delta W}{\delta\lambda}$ around its mean value are shown on fig. 3. The mean value of $\frac{\delta W}{\delta\lambda}$ during the direct and the reverse process are very close to one another for a slow process and further apart for a fast one, implying an increase in the mean dissipated work as the switching rate increases. The amplitude of the fluctuations of $\frac{\delta W}{\delta\lambda}$ are not influenced by the switching rate. However, for slow switching (red curve on fig. 3), the system has more time to fluctuate and the fluctuations are partly averaged out when performing the integration (4).

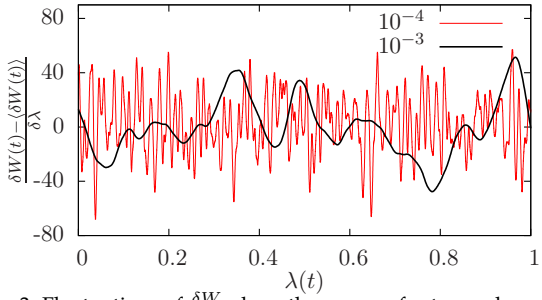

Figure 3: Fluctuations of $\frac{\delta W}{\delta\lambda}$ along the process for two values of $\delta\lambda$.

For Gaussian distributions of the dissipated work $W_{\rm d}$ one can easily verify that Crooks' relation (1) implies that the mean value $\overline{W}_{\rm d}$ and variance σ^2 of the dissipated work for the direct and the time-reversed processes coincide. Crooks' relation then reduces to a *generalized fluctuation-dissipation relation* [4]:

$$\sigma^2 = 2k_{\rm B}T\,\overline{W}_{\rm d} \tag{6}$$

Fig. 4 shows the distribution of the quantity $\widetilde{W}_{\rm d} = W_{\rm d}/\sigma - \sigma/2k_{\rm B}T$ for the direct and the time-reversed process for various values of the switching rate. This quantity has a Gaussian distribution with zero mean and unit variance for all values of the switching rate, implying that the dissipated work $W_{\rm d}$ has a Gaussian distribution and satisfies (6) and therefore Crooks' relation (1) as well.

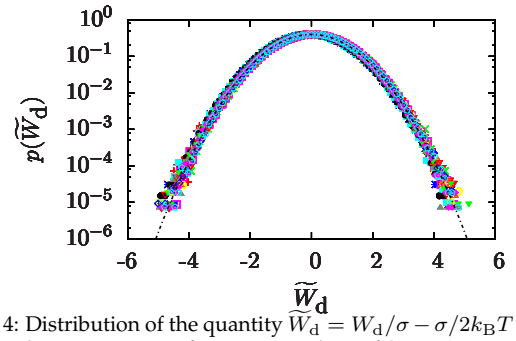

Figure 4: Distribution of the quantity $\widetilde{W}_{\rm d} = W_{\rm d}/\sigma - \sigma/2k_{\rm B}T$ for the direct and reverse process for various values of $\delta\lambda$.

A more careful analysis of the fluctuations suggests that these are equilibrium heat bath fluctuations in which only the mean value depends of the protocol and hence reflects the distance from equilibrium. It is evident that this cannot hold for arbitrary situations, in particular not in cases where the driving force creates dynamical instabilities. The details are still awaiting further investigation. This issue is relevant for macroscopic fluctuations in non-equilibrium systems that are close to the thermodynamic limit, for which pure heat bath fluctuations should become invisible.

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2.15 Probabilistic Forecasting

JOCHEN BRÖCKER, STEFAN SIEGERT, HOLGER KANTZ

A ubiquitous problem in our life (both as individuals as well as a society) is having to make decisions in the face of uncertainty. Forecasters are supposed to help in this process by making statements (i.e. forecasts) about the future course of events. In order to allow the forecast user to properly assess potential risks associated with various decisions, forecasters should, in addition, provide some information as to the uncertainty associated with their forecasts. Unequivocal or "deterministic" forecasts are often misleading as they give the false impression of high accuracy. Probabilities, in contrast, allow to quantify uncertainty in a well defined and consistent manner, if interpreted correctly.

Forecasts in terms of probabilities have a long and successful history in the atmospheric sciences. In the 1950's, several meteorological offices started issuing probability forecasts, then based on synoptic information as well as local station data. On a scientific (non–operational) level, probabilistic weather forecasts were discussed even much earlier.

Evaluation of probabilistic forecasts

Since the prediction in a probabilistic forecast is a probability (distribution) whereas the observation is a single value, quantifying the accuracy of such forecasts is a nontrivial issue. This is of interest not only for quality control of operational forecasting schemes, but also for a more fundamental understanding of predictability of dynamical systems; see for example [5]. Nowadays, probabilistic weather forecasts are often issued over a long period of time under (more or less) stationary conditions, allowing archives of forecast–observation pairs to be collected. Such archives permit to calculate observed frequencies and to compare them with forecast probabilities. The probability distribution of the observation y, conditioned on our probability forecast being p, ideally coincides with p; a forecast having this property is called *reliable* or *consistent*. If a large archive of forecast–observation pairs is available, reliability can be tested statistically. It is not difficult though to produce reliable probabilistic forecasts. The overall climatological frequency for example will always be a reliable forecast; this constant forecast is not very informative though. The forecast should delineate different observations from each other.

The question arises how virtuous forecast attributes (reliability and information content) can be quantified and evaluated. One therefore seeks for "scoring rules" which reward both reliable and informed forecasters. A *scoring rule* is a function $S(p, y)$ where p is a probability forecast and y a possible observation. Here, y is assumed to be one of a finite number of labels, say $\{1 \dots K\}$. A probability forecast would then consist of a vector $p = (p_1 \dots p_K)$ with $p_k \geq 0$ for all k, and $\sum_k p_k = 1$. The idea is that $S(p, y)$ quantifies how well p succeeded in forecasting y. The general quality of a forecasting system is ideally measured by the mathematical expectation $\mathbb{E}\,[S(p, y)]$, which can be estimated by the empirical mean

$$\mathbb{E}\,[S(p, y)] \cong \frac{1}{N} \sum_{n=1}^{N} S(p(n), y(n)) \tag{1}$$

over a sufficiently large data set $\{(p(n), y(n)); n = 1 \dots N\}$ of forecast–observation pairs.

Two important examples for scoring rules are the logarithmic score [8] (also called Ignorance)

$$S(p, y) = -\log(p_y), \tag{2}$$

and the Brier score [1]

$$S(p, y) = \sum_k (p_k - \delta_{y,k})^2. \tag{3}$$

The convention here is that a smaller score indicates a better forecast.

Although these two scoring rules seem ad hoc, they share an interesting property which arguably *any* scoring rule should possess in order to yield consistent results. Suppose that our forecast for some observation y is q, then the score of that forecast will be $S(q, y)$. If the correct distribution of y is p, then the expectation value of our score is

$$\mathbb{E}(S(q, y)) = \sum_k S(q, k) p_k. \tag{4}$$

The right hand side is referred to as the *scoring function* $s(q, p)$. Arguably, as p is the correct distribution of y, the expected score of q should be worse (i.e. larger in our convention) than the expected score of p. This is equivalent to requiring that the *divergence function*

$$d(q, p) := s(q, p) - s(p, p) \tag{5}$$

be non-negative and zero only if $p = q$. A scoring rule with this property (for all p, q) is called *strictly proper* [6,7]. The divergence function of the Brier score for example is $d(q, p) := \sum_k (q_k - p_k)^2$, demonstrating that this score is strictly proper. The Ignorance is proper as well, since (5) is then just the Kullback–Leibler–divergence, which is well known to be positive definite.

The expectation value $\mathbb{E}\,[S(p, y)]$ with strictly proper scoring rule S allows for the following decomposition [4]:

$$\mathbb{E}S(p, y) = s(\bar{\pi}, \bar{\pi}) + \mathbb{E}d(p, \pi) - \mathbb{E}d(\bar{\pi}, \pi), \tag{6}$$

where π and $\bar{\pi}$ are probability distributions with $\pi_k = \mathbb{P}(y = k|p)$, and $\bar{\pi}_k = \mathbb{P}(y = k)$, respectively. The first term is the inherent uncertainty of y—this quantity is not affected by the forecasts. The second term quantifies reliability; note that this term is always positive unless $p = \pi$, which is the mathematical definition of reliability. The third term quantifies the information content of π. It contributes negatively to (i.e. improves) the score, unless $\pi = \bar{\pi}$, in which case π is constant. Hence, this term penalises lack of variability of π; the larger the variability of π, the better the score. As a whole, the decomposition yields credence to the practice of assessing forecast quality through proper scoring rules.

Ensemble forecasts

Modern weather forecasts are generated using large dynamical atmospheric models, running on supercomputers. In order to initialise these simulations properly, the current state of the atmosphere has to be known at least approximately, and subsequently projected into the state space of the model; this process is known as data assimilation. The fact that the initial condition is not known with certainty (and also that the model is incorrect) is accounted for by generating not one but several simulations with minutely perturbed initial conditions, resulting in an *ensemble* of forecasts.

Although ensemble forecasts already provide vital information as to the inherent uncertainty, they need to be post-processed before they can be interpreted as probabilities. The interpretation of ensembles and how to generate useful forecast probabilities using ensembles is a very active area of research.

Several different interpretations exist, a very common one being the following *Monte–Carlo* interpretation: An *ensemble* is a collection $x_1, \ldots, x_K$ of random variables, drawn independently from a common distribution function p, the *forecast distribution*. The forecast distribution p can be considered as the distribution of the ensemble members conditioned on the internal state of the forecasting scheme. The forecast distribution p however is but a mental construct and not operationally available.

In this interpretation, the forecasting scheme is called *reliable* if the observation y along with the ensemble members $x_1 \ldots x_K$ are independent draws from the forecast distribution p. Less formally stated, the observation behaves like just another ensemble member. A necessary consequence of reliability is that the rank of y among all ensemble members assumes the values $1, \ldots, K+1$ with equal probability (namely $1/(K+1)$). This means that the histogram of rank(y) should be flat, which can be statistically tested, see for example [3].

In operational ensembles though, histograms are often found to be u–shaped, with the outermost ranks being too heavily populated (see Fig.1 for an example); in other words, outliers happen more often than they should in a reliable ensemble. This can have several reasons, such as insufficient spread or conditional bias. On the other hand, this means that we should be able to predict such outliers by looking at characteristic patterns in the ensemble. Indeed, as we could show, even for reliable ensemble forecasts, the spread of the actual specific ensemble is indicative of the probability that the future observation will be an outlier [10].

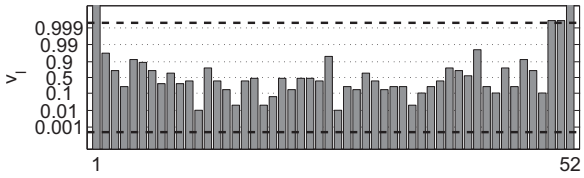

Figure 1: Rank diagram for temperature forecasts in Hannover: The verification falls much too often into the first and last bins, indicating that outliers are too frequent for reliability. This ensemble features 51 members. The y–axis shows Binomial probabilities, rather than actual counts.

Unfortunately, rank based reliability tests are restricted to scalar predictions. In [9], a rank analysis for vector valued predictions was suggested by measuring the length of a minimum spanning tree. Thereby, a new scalar ensemble is created which however ceases to be independent, that is, the Monte–Carlo interpretation no longer applies. This puts the assumptions behind the entire rank histogram analysis into question. However, as it could be shown in [2] the rank based reliability analysis can still be applied to such ensembles, due to some inherent symmetries called exchangeability. In particular, these investigations demonstrated that the minimum spanning tree approach is mathematically sound.

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2.16 Magnetically Driven Superconductivity in Heavy Fermion Systems

STEFAN KIRCHNER, OLIVER STOCKERT[3]

Unconventional superconductivity has attracted interest for more than thirty years. Unconventional here refers to superconducting phases where pairing is not phonon mediated and which therefore do not conform to classical BCS theory [1]. In strongly correlated electron systems unconventional superconductivity occurs predominantly in close vicinity to magnetism. This includes superconductivity occuring in the layered perovskite copper-oxides, the recently discovered iron-pnictides and the heavy fermions. Particularly the heavy fermions display a rich variety of superconducting behavior. In UPd_2Al_3 e.g. superconductivity occurs deep inside an antiferromagnetic phase [2]. $PuCoGa_5$ on the other hand enters a superconducting phase directly from a paramagnet with Curie behavior [3]. As a result, antiferromagnetic spin excitations have been discussed as a possible mechanism for superconducting pairing in heavy fermions [5] ever since the seminal discovery of superconductivity in $CeCu_2Si_2$ [4]. Until recently, however, no convincing verification had emerged that antiferromagnetic quantum critical fluctuations indeed underlie pairing. Based on an in-depth study of the magnetic excitation spectrum in momentum and energy space in the superconducting and normal states, we were able to conclusively demonstrate that magnetism drives superconductivity in the prototypical heavy-fermion compound $CeCu_2Si_2$ [6].

$CeCu_2Si_2$ crystallizes in a structure with body-centered tetragonal symmetry. The phase diagram is shown in Fig.1(a). So-called A-type crystals (see Fig.1(a)) display antiferromagnetism at sufficiently low temperatures. This antiferromagnetic order was found to be an incommensurate spin-density wave (SDW) with propagation vector $\mathbf{Q}_{AF} \approx (0.215\ 0.215\ 0.53)$, which can be ascribed to a nesting vector of the renormalized Fermi surface [7]. Approaching the antiferromagnetic quantum critical point (AF QCP), the thermodynamic and transport behavior [8] is in line with quantum critical fluctuations of a three-dimensional SDW; see also Fig.1(b). We here focus on a crystal located on the paramagnetic side of the quantum critical point (termed S-type $CeCu_2Si_2$, see Fig.1(a)) for which we are able to identify the magnetic excitations in the normal and superconducting state. In both cases, magnetic excitations are found only in close vicinity of the incommensurate wavevector $\mathbf{Q}_{AF}$. In the superconducting state, a clear spin excitation gap is observed, see Fig.2(a). The temperature dependence of the gap $\Delta(T)$ follows a rescaled BCS form ($\hbar\Delta(0) \approx 3.9 k_B T_c$) [6]. A linear dispersion of the spin excitation is visible in both the superconducting and normal state with a mode velocity $v \approx 4.4\,\mathrm{meV\AA}$. For the superconducting state this is shown in Fig.2(b). The value for v is substantially smaller than the Fermi velocity $v_F \approx 57\,\mathrm{meV\AA}$ [9] ($1\,\mathrm{meV\AA} = 153\,\mathrm{m/s}$), and indicates a retardation of the coupling between the quasiparticles and the quantum-critical spin excitations.

To address, if magnetism indeed drives superconductivity in $CeCu_2Si_2$, we study the energetics across the transition. The condensation energy ΔE_C characterizing the stability of the superconducting state (S) against a putative normal state (N) is

$$\Delta E_C = \lim_{T\to 0} \big(G_S(T, B=0) - G_N(T, B=0)\big) \quad (1)$$

where G_S/G_N is the Gibbs free energy of the superconducting/normal state. Eq.(1) implies that ΔE_C can be obtained from the heat capacity. We take the finite field ($B = 2\,\mathrm{T} > B_{c2}$) data as the putative normal state and find $\Delta E_C = -\eta\, 2.27 \cdot 10^{-4}\,\mathrm{meV/Ce}$. The factor $\eta > 1$ accounts for the fact that only the superconducting volume fraction contributes to ΔE_C.

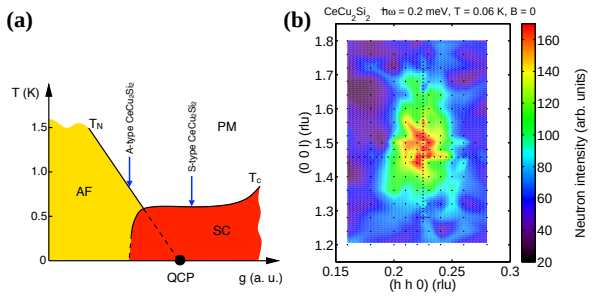

Figure 1: (a) Schematic $T-g$ phase diagram of $CeCu_2Si_2$ in the vicinity of the quantum critical point (QCP) where the antiferromagnetic phase vanishes as function of the effective coupling constant g. Superconductivity is observed around the QCP and extends far into the paramagnetic regime. Composition as well as hydrostatic pressure can be used to change the coupling constant g and to tune the system to the QCP. The positions of the A-type and the S-type single crystals in the phase diagram are marked. (b) Spin fluctuation spectrum at $T = 0.06$K, $B = 0$ and at an energy transfer $\hbar\omega = 0.2$meV. The anisotropy factor between the [110] and the [001] directions is roughly 1.5.

This has to be contrasted with the change in exchange energy across the superconducting transition, in order to ascertain whether the magnetic excitations contribute significantly to the condensation energy. We model the exchange interaction between the localized Ce-moments by including nearest neighbor and next-nearest neighbor terms appropriate for the tetragonal, body-centered unit cell: $I(\mathbf{q}) = I_1[\cos(q_x a) + \cos(q_y a)] + I_2 f_2(a, c, \mathbf{q})$ where $a = 4.1\,\mathrm{\AA}$ and $c = 9.9\,\mathrm{\AA}$ are the lattice constants for the a- and c-axis respectively, I_1

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and I_2 are the nearest and next-nearest neighbor exchange interactions, and the precise form of f_2 can be found in [6]. The ratio I_1/I_2 follows from the distance-dependence of the RKKY interaction: $I_2 \approx 0.35 I_1$. The magnitude of the exchange interaction I_1 can be estimated from the observed paramagnon velocity v, see inset of Fig. 4(a): $I_1 \approx 0.63$meV. The difference in exchange energy between superconducting and normal state follows as

$$\begin{aligned} \Delta E_x \;\equiv\; E_x^S - E_x^N \;=\; & \frac{A}{g^2\mu_B^2}\int_0^\infty \frac{d(\hbar\omega)}{\pi}\big[n(\hbar\omega)+1\big] \\ \times\; & \int_{-\pi/a}^{\pi/a} dq_x \int_{-\pi/a}^{\pi/a} dq_y \int_{-\pi/c}^{\pi/c} dq_z \; I(q_x,q_y,q_z) \\ \times\; & \mathrm{Im}\Big[\chi^S(q_x,q_y,q_z,\hbar\omega) - \chi^N(q_x,q_y,q_z,\hbar\omega)\Big]. \end{aligned}$$

Crystalline-electric-field effects split the $J = 5/2$ states of the Ce^{3+} ion up into a ground-state doublet and a quasi-quartet at high energies (> 30 meV) and result in g-factors $g_z \approx g_\perp \approx 2$, and an almost isotropic spin susceptibility. The constant A is given by $A = \eta \cdot 8 \cdot 3/(2V_B)$ with V_B being the volume of the Brillouin zone. The volume fraction η enters again, since the magnetically ordered regions in S and N yield (essentially) identical responses for $B = 0$ and $B = 2$ T. We finally obtain $\Delta E_x/\Delta E_C = 21.1$, so that the gain in exchange energy is more than an order of magnitude larger than the condensation energy, thus identifying the build up of magnetic correlations near the AF QCP as the major driving force for superconductivity in $CeCu_2Si_2$. It is important to note that the gain in ΔE_x comes from the opening of the spin gap and not the "resonance"-like feature above the spin gap, which tends to reduce the energy gain (see Fig. 2(c)). This follows from the fact that $\mathrm{Im}\chi^{N/S}(\mathbf{q},\hbar\omega)$ is peaked around the incommensurate wave vector at which $I(\mathbf{q})$ is positive, i.e. $I(\mathbf{Q}_{\rm AF}) > \mathbf{0}$. Note that a spin resonance as it occurs e.g. in the cuprate superconductors is not expected for three-dimensional superconductors [11].

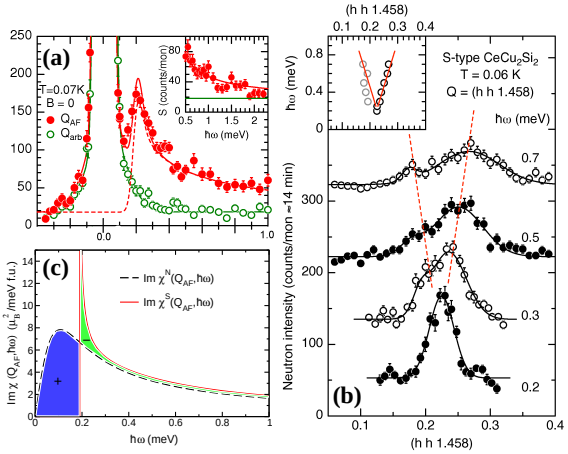

Figure 2: (a) Neutron intensity versus energy transfer $\hbar\omega$ in S-type $CeCu_2Si_2$ at $\mathbf{Q}_{\rm AF}$. The inset in (a) shows the magnetic response at $\mathbf{Q}_{\rm AF}$ extending beyond $\hbar\omega = 2$meV. (b) Wave vector $\mathbf{Q}$ dependence of the magnetic response around $\mathbf{Q}_{\rm AF}$ in S-type $CeCu_2Si_2$ in the superconducting state at $T = 0.06$ K for different energy transfers $\hbar\omega$. Inset: Dispersion of the magnetic excitation around $\mathbf{Q}_{\rm AF}$ at T=0.06 K. The solid line indicates a fit to the data with a linear dispersion relation yielding a paramagnon velocity $v = (4.44 \pm 0.86)$ meVÅ (c) Schematic plot of the imaginay part of the dynamic spin susceptibility $\mathrm{Im}\chi(\mathbf{Q}_{\rm AF},\omega)$ in the normal (N) and superconducting (S) states. The blue area marked with a '+' contributes to the gain in ΔE_x whereas the green area (marked with a '-') leads to a reduction in the overall gain in ΔE_x.

These are striking differences between $CeCu_2Si_2$ on the one hand, and $CeCoIn_5$ [10] and high-T_c cuprate superconductors on the other. For $CeCu_2Si_2$, we can unequivocally conclude that the build-up of magnetic correlations near the AF QCP energetically drives the superconductivity.

Evidently, there is a sizeable kinetic energy loss. Superconductivity in $CeCu_2Si_2$ occurs in the spin-singlet channel. As a result of the opening of the superconducting gap, the Kondo-singlet formation is weakened and the spectral weight of the Kondo resonance is reduced. Since the kinetic energy of the quasiparticles appears through the Kondo-interaction term in a Kondo-lattice Hamiltonian, this naturally yields a large loss to the f-electron kinetic energy.

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2.17 Quantum Criticality out of Equilibrium: Steady States and Effective Temperatures

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Quantum phase transitions are of extensive current interest in a variety of strongly correlated electronic and atomic systems [1]. A quantum critical point occurs when such transitions are second order. As a consequence, there is no intrinsic energy scale in the excitation spectrum of a quantum critical state. Out-of-equilibrium states near quantum phase transitions have so far received only limited theoretical attention despite a long-standing interest in their classical counterparts. Experimentally, on the other hand, it seems unavoidable to generate out-of-equilibrium states during a measurement in the quantum critical regime as this regime is characterized by the absence of any intrinsic scale. Any measurement may therefore potentially perturb the system beyond the linear response regime where the fluctuation-dissipation theorem (FDT) no longer holds. To make progress theoretically, approaches are needed that can capture the scaling properties of a quantum critical point in equilibrium and that can be extended to out of equilibrium settings. This is impeded by the lack of a general understanding of how to generalize the free energy functional to stationary nonequilibrium states from which scaling relations could be obtained.

We have identified a system in which quantum criticality out of equilibrium can be systematically studied [2,3]. It was shown earlier that single-electron transistors (SET) attached to ferromagnetic leads can undergo a continuous quantum phase transition as their gate voltage is tuned [4]. The corresponding quantum critical point separates a Fermi liquid phase from a non-Fermi liquid one. The key physics is the critical destruction of the Kondo effect, which underlies a new class of quantum criticality that has been argued to apply to heavy fermion metals [5].

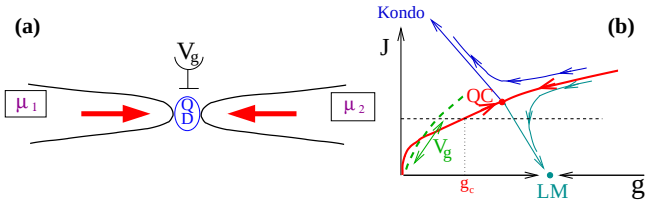

Figure 1: (a) Schematic setup of the magnetic SET. The arrows in the left and right leads indicate the direction of the magnetization in the leads. For antiparallel alignment, the local magnetic field generated by the leads vanishes. (b) Phase diagram: the Fermi liquid phase ("Kondo") and the critical local moment ("LM") phase are separated by a QCP. The voltage V_g allows to tune the system through a quantum phase transition.

The couplings of the local degrees of freedom to the conduction electrons and to the magnons in the leads allow for a dynamical competition between the Kondo singlet formation and the magnon drag. As a result, the low-energy properties are governed by a Bose-Fermi Kondo model (BFKM) [4,6].

$$\begin{aligned}\mathcal{H}_{\rm bfk} &= \sum_{k,k',\sigma,\sigma'}^{i,j} J_{i,j}\mathbf{S}\cdot c^\dagger_{k,\sigma,i}\frac{\sigma}{2}c_{\sigma',j} \\ &+ \sum_{\mathbf{k},i,\sigma}\tilde{\epsilon}_{\mathbf{k}\sigma i}\, c^\dagger_{\mathbf{k}\sigma i}c_{\mathbf{k}\sigma i} + h_{\rm loc}S_z \\ &+ g\sum_{\beta,\mathbf{q},i} S_\beta(\phi_{\beta,\mathbf{q},i}+\phi^\dagger_{\beta,\mathbf{q},i}) + \sum_{\beta,\mathbf{q},i}\omega_{\mathbf{q}}\,\phi^\dagger_{\beta,\mathbf{q},i}\phi_{\beta,\mathbf{q},i}.\end{aligned}$$

where $i,j\varepsilon\{L,R\}$ and $h_{\rm loc}=g\sum_i m_i$, is a local magnetic field with m_L/m_R being the ordered moment of the left/right leads. For antiparallel alignment and equal couplings one finds $m_L=-m_R$. $\tilde{\epsilon}_{\mathbf{k}\sigma i}$ is the Zeeman-shifted conduction electron dispersion, and $\phi_{\beta,i}$, with $\beta=x,y$, describes the magnon excitations. The spectrum of the bosonic modes is determined by the density of states of the magnons, $\sum_q[\delta(\omega-\omega_q)-\delta(\omega+\omega_q)]\sim|\omega|^{1/2}sgn(\omega)$ up to some cutoff Λ. A sketch of the magnetic SET is shown in Fig. 1(a). The resulting equilibrium phase diagram of the system is displayed in Fig. 1(b). Nonequilibrium states can be created by keeping left and right lead at different chemical potentials but the same temperature T, ($eV=\mu_L-\mu_R$). For such a finite bias voltage, we work on the Keldysh contour. The current-carrying steady state at arbitrary bias voltage V has been explicitly studied by an extension of the dynamical large-N limit onto the Keldysh contour [2]. The dynamical large-N limit in equilibrium has been shown to correctly capture the dynamical scaling properties (including, in particular, the finite-temperature relaxational properties) of the $N=2$ case [4,7]. For a finite bias voltage, we work on the Keldysh contour. Since we are interested in the steady state limit, we specify the state of the system at the infinite past $t_0=-\infty$, so that at finite time all initial correlations will have washed out.

In this model system, we have shown that the universal scaling is obeyed by the steady state current, the pertinent spectral densities, and the associated fluctuation-dissipation ratios. We have been able to calculate the entire scaling function for each of these non-equilibrium quantities. This allows us to elucidate the concept of effective temperatures. Our theoretical approach can even be extended to study the transient behavior and other non-equilibrium probes of quantum

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criticality. The current in the steady state limit is

$$I(V,T) = \frac{e}{2\hbar}\int d\omega\,\rho(\omega)\,[f_L(\omega)-f_R(\omega)] \times \mathrm{Im}\big[\mathcal{T}^a_{LL}(\omega,T,V)+\mathcal{T}^a_{RR}(\omega,T,V)\big].$$

Here, $\mathcal{T}_{\alpha,\beta}$, $(\alpha,\beta = L/R)$, is the T-matrix of the Bose-Fermi Kondo model. In the linear response regime of the quantum critical LM phase, the conductance is proportional to $T^{1/2}$ [4]. In the non-linear regime, $V \to 0$ at $T = 0$, the conductance goes as $V^{1/2}$. Fig. 2(a) shows a scaling collapse of $I/T^{3/2}$ vs. V/T. Fig. 2(b) demonstrates scaling of the dynamical spin susceptibiltity in terms of ω/T and V/T.

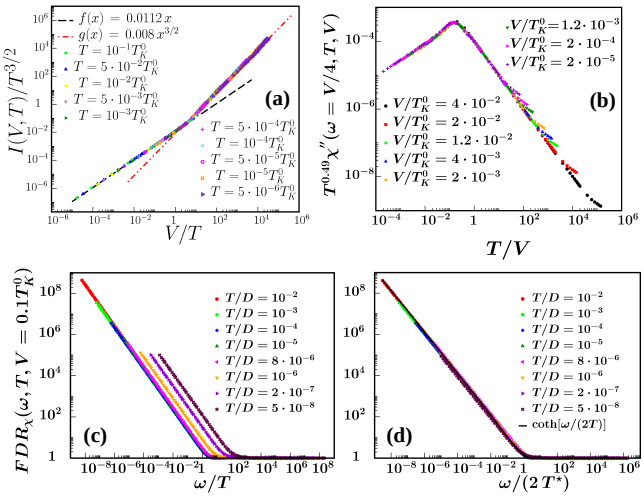

Figure 2: (a) Scaling of the current-voltage characteristics in the critical local moment phase and (b) scaling of the imaginary part of the local dynamical spin susceptibility. (c) The fluctuation-dissipation ratio for the spin susceptibility in the critical local moment phase $(g = 4\cdot g_c)$ for $V/D = 5.0\cdot 10^{-3} = 0.1T_K^0$, where T_K^0 is the Kondo temperature in the absence of magnons $(g = 0)$. (d) An effective temperature T^*_χ can be defined such that the $FDR_\chi(\omega,T,V)$ of (c) collapses on $\coth(\omega/2T)$, the equilibrium FDR of a bosonic field.

The ω/T and V/T scaling occurs only in the scaling regime of the quantum critical LM phase and at the quantum critical point. As in the equilibrium relaxational regime ($V = 0$, $\omega \ll k_BT/\hbar$) where an ω/T scaling implies a linear-in-T spin relaxation rate, in the non-equilibrium relaxational regime here ($T = 0$, $\omega \ll eV/\hbar$), the ω/V scaling implies a linear-in-V dependence of the decoherence rate, $\Gamma_V \equiv [-i\partial \ln \chi^a(\omega,T=0,V)/\partial\omega]^{-1}_{\omega=0} = c(e/\hbar)V$. It is worth stressing that, in contrast to its counterpart in the high-voltage ($V \gg k_BT_K^0/e$) perturbative regime, the decoherence rate here is universal: c is a number characterizing the fixed point.

We now turn to the concept of effective temperature in the non-linear regime. The notion of an effective temperature for extending the FDT to non-equilibrium states was first introduced in the context of steady states in chaotic systems [8], and was later used for non-stationary states in glassy systems [9] and in the context of coupled noisy oscillators [10]. Fig. 2(c) displays the $FDR_\chi(\omega,T,V)$ for $V = 5\cdot 10^{-3}D = 0.1T_K^0$, with T_K^0 being the Kondo temperature in the absence of magnons $(g = 0)$. The scaling regime extends up to energies of the order of T_K^0, so that bias voltages larger than $V = 0.1T_K^0$ might be affected by sub-leading contributions. Three important observations underly the results displayed in Fig. 2(a): (1) for $\omega >> T$, $FDR_\chi(\omega,T,V)$ approaches the value predicted by the FDT, $(\coth(\omega/2T) \to 1)$, (2) for $T >\approx 10^{-3}V$, the deviations from the linear response behavior are hardly discernible, (3) for $T <\approx 10^{-3}V$,it appears as if a simple scaling factor could collapse $FDR_\chi(\omega,T,V)$ on the high-temperature curve, where (for $T \gg V$) the FDT applies. (1)-(3) suggest, that an effective temperature of the form

$$T^*_\chi(T,V) = \frac{T}{\tanh\left(\alpha\frac{2T}{V}\right)}$$

could restore the FDT for all frequencies ω.
As Fig. 2(d) demonstrates, this is indeed the case! It is worth noting that the same $T^*_\chi(T,V)$ applies to other V in the scaling regime (with the same α). The scaling factor α is determined by some dimensionless combination of the 'non-universal' parameters D, g_c, T_K^0 and Λ. Whether the concept of effective temperatures, applied here to the spin-spin correlator, can be extended to more general cases, will be explored in forthcoming work.

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2.18 High-Quality Ion Beams from Nanometric Double-Layer Targets Using Petawatt Lasers

M. GRECH, S. SKUPIN, R. NUTER, L. GREMILLET, E. LEFEBVRE

Generating high-energy ion beams by irradiating a solid target with an ultra-intense laser pulse has many potential applications from medicine to controlled nuclear fusion. In this paper, we revisit ion acceleration from a double-layer target and propose a new laser-based acceleration scheme which allows for an excellent control of the ion beam properties. Using two-dimensional (2D) particle-in-cell (PIC) simulations and an analytical model, we demonstrate that high-energy (> 100 MeV/nucleon) ion beams can be generated over a few laser periods only. These beams are characterized by small and adjustable energy ($\lesssim 10\,\%$) and angular ($\lesssim 5^\circ$) dispersions, which makes them suitable for applications such as hadron-therapy.

To illustrate this new acceleration mechanism, we present numerical simulations performed using the PIC code CALDER [1]. We consider a double-layer target whose first layer is made of heavy ions with mass $m_h \gg m_p$ ($m_p = 1836$ is the proton mass) and charge Z_h. The second target layer (or a small dot placed at the rear-side of the first layer) consists of ions with a larger charge-over-mass ratio. We denote by n_h, d_h and w_h the atomic density, thickness and transverse size of the first layer, respectively. Similarly, n_l, d_l and w_l denote the corresponding parameters for the second layer. In what follows, all quantities are normalized to laser and electron related units (see Refs. [2,3] for more details). A laser pulse with field amplitude $a_L = 100$ is focused at normal incidence on the ultra-thin ($d_h + d_l \ll 1$) target. A circularly polarized pulse with flat-top temporal intensity profile is used so that electron sweeping by the laser radiation pressure is more efficient [4]. The pulse duration is $\tau_p \sim 62.8$ [10 optical cycles (τ_L)] only. Along the transverse $y-$direction, the laser intensity follows a 6-th order super-Gaussian profile. Two values for the laser focal-spot full-width at half-maximum are considered: $w_L = 62.8$ and 125.6 [10 and 20 laser wavelengths (λ_L), respectively]. The first target layer is made of fully ionized carbon ($Z_h = 6, m_h = 12\,m_p$) with atomic density $n_h = 58$ and thickness $d_h = 0.08$. Its transverse size is $w_h \sim 200$ ($\sim 30\ \lambda_L$). A fully ionized hydrogen dot ($Z_l = 1$, $m_l = m_p$) with transverse size $w_l = \lambda_L = 6.28$ and thickness $d_l = 0.16$ is placed at the rear-side of the first layer. Two hydrogen densities, $n_l = 6$ and $n_l = 12$, are considered.

The simulation results are summarized in Fig. 1. Four laser-periods after the beginning of the interaction, all electrons in a region with diameter $w_\perp \sim 70 \sim w_L$ irradiated by the laser pulse have been removed from the target (Fig. 1a). In contrast to previous works [5, 6] where electrons are strongly heated and generate an accelerating sheath at the target rear-side, they form here a compact bunch that propagates with the front of the laser pulse. This occurs if the laser radiation pressure $\sim a_L^2$ is sufficient to overcome both the electron thermal pressure (kept to a small level by using circular polarization [4]), and the maximum electrostatic pressure $a_{tot}^2/2$ resulting from complete electron-ion separation. Here $a_{tot} = a_h + a_l$, where $a_h = Z_h\, n_h\, d_h$ and $a_l = Z_l\, n_l\, d_l$, is the maximum electrostatic field between the bare ion layers and the electron cloud. This defines a simple threshold condition on the laser field amplitude for complete electron removal $a_L > a_{tot}/\sqrt{2}$.

As electrons are separated from the ions, the target exhibits a capacitor-like structure and a quasi-homogeneous electrostatic field is built up between the bare heavy ion layer and the electron bunch. Ions in the second layer are accelerated by this field which amplitude linearly increases from a_h to $a_h + a_l$ so that they see a quasi-constant accelerating field. Equations of motion can then be solved analytically. We obtain for the time evolutions of the light ion mean energy ϵ and energy dispersion $\Delta\epsilon$ (in units of $m_e\, c^2$) [2]:

$$\epsilon_{linPA} = m_l \left[\sqrt{1 + t^2/t_r^2} - 1\right], \quad (1)$$

$$\Delta\epsilon_{linPA} = m_l \left[\sqrt{1 + \left(1 + a_l/a_h\right)^2 t^2/t_r^2} - \sqrt{1 + t^2/t_r^2}\right], \quad (2)$$

where linPA stands for linear plasma acceleration (by analogy to conventional acceleration techniques), and $t_r = m_l/(Z_l\, a_h)$ denotes the time over which light ions gain relativistic energies. For $t \ll t_r$, ions behave classically and one has $\epsilon^{(c)} \sim m_l\, t^2/(2\, t_r^2)$ and $(\Delta\epsilon/\epsilon)^{(c)} \sim 2\, a_l/a_h$, respectively. If light ions experience the field $\sim a_h$ over a time $t \gg t_r$, they gain ultra-relativistic energies $\epsilon^{(ur)} \sim m_l\, t/t_r$ and $(\Delta\epsilon/\epsilon)^{(ur)} \sim a_l/a_h$.

These analytical estimates are in good agreement with PIC simulations (see Fig. 1b,c). Ions gain high energies in a few optical cycles only. Four optical cycles after the beginning of the interaction, Fig. 1e shows that protons have already reached $\epsilon \sim 70\,\mathrm{MeV}$ (blue line, square). Moreover, controlling the target parameters so that $a_h \gg a_l$ ensures that both the relative energy dispersion and aperture angle remain small (Figs. 1e and 1f). Especially, both dispersions are, at this stage of the acceleration process, sensitive only to the charge density in the proton dot: electrostatic repulsion between the protons themselves is the main source of energy and angular dispersion.

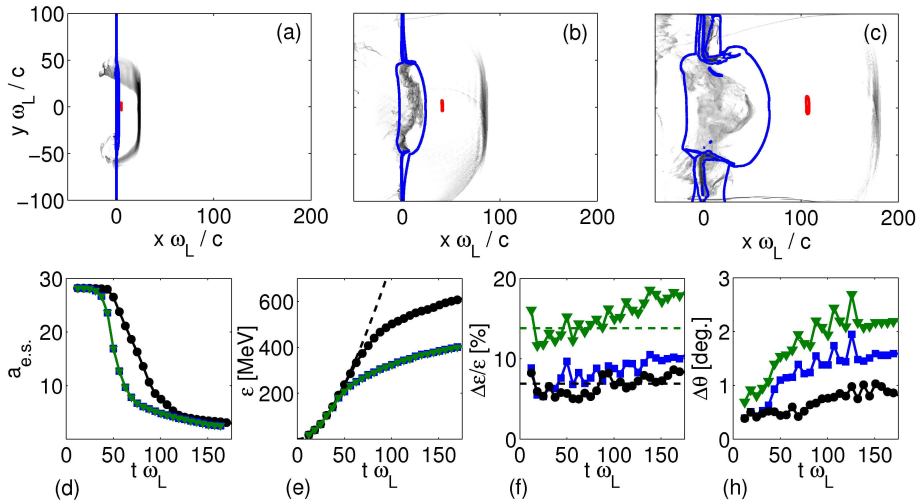

Figure 1: (a,b,c) Snapshots of the electron density (gray scale), carbon contour plot (blue) and proton contour plot (red) at: $t = 4\,\tau_L$ (a); $t = 14\,\tau_L$ (b) and $t = 30\,\tau_L$ (c). In this simulation, $w_L = 62.8$ and $n_l = 6$. (d-g) Temporal evolution of: (a) the accelerating electrostatic field see by the protons; (b) the proton mean energy; (c) the proton energy dispersion and (d) the proton angular aperture. For $n_l = 6$, $w_L = 10\,\lambda_L$ (blue, square), $n_l = 12$, $w_L = 10\,\lambda_L$ (green, triangle) and $n_l = 6$, $w_L = 20\,\lambda_L$ (black, circle). Dashed curves account for analytical predictions.

This early stage of proton acceleration ends once the distance between the electron cloud and the bare heavy ion layer becomes similar to their transverse size $w_\perp$, at $t \sim 8\,\tau_L$ for $w_L \sim 10\,\lambda_L$ and $t \sim 13\,\tau_L$ for $w_L \sim 20\,\lambda_L$. The electrostatic field seen by the protons then strongly decreases due to geometrical effects (Fig. 1d) and the acceleration process slows down (Fig. 1e). Ion acceleration in this later stage occurs in the heavy ion field in a way similar to directed Coulomb explosion (DCE) [5,6]. Assuming $Z_h/m_h \ll Z_l/m_l$, the ion energy gain is simply the remaining proton potential energy:

$$\epsilon_{DCE} \sim Z_l\, a_h\, w_\perp/4 - \epsilon_{linPA}/2\,. \qquad (3)$$

Energy and angular dispersions also slightly increase (Figs. 1f,g) but do not exceed $10\,\%$ (for $n_l = 6$) and $3°$, respectively. Figure 1g also shows that angular dispersion now depends on both w_L and n_l thus suggesting that both the transverse inhomogeneity of the accelerating field and Coulomb repulsion in the proton bunch are responsible for it. Energy dispersion on the contrary remains mainly sensitive to n_l: it follows primarily from Coulomb repulsion between protons. This effect can be estimated by approximating the second ion layer by a uniformly charged sphere with radius $R \sim w_l/2$ expanding due to its own charge Q_l (in units of $e\,n_c/k_L^3$). The final energy dispersion can then be derived as a function of the final ion energy ϵ:

$$\Delta\epsilon_{DCE} \sim 4\,\sqrt{\epsilon\,\epsilon_p}\,, \qquad (4)$$

where $\epsilon_p = Z_l\,Q_l/(2\pi\,w_l)$ is the initial potential energy of a light ion on the outer shell of the sphere. As a result, small energy dispersions can be obtained only by limiting the total proton charge.

Now, comparing Eqs. 1 and 3 allows one to infer which of the two stages is dominant in the acceleration process. One obtains that ions with the final energy $\epsilon \lesssim m_l/8$ gain most of their energy during the later (DCE) stage. For these ions, the final energy is $\epsilon \sim Z_l\,a_h\,w_\perp/4$ and $\Delta\epsilon/\epsilon \sim 4\,\sqrt{\epsilon_p/\epsilon}$. Moreover, since $w_\perp \sim w_L$, the condition for electron removal, $a_L > a_h$, defines a threshold for the laser power $P_L \sim w_L^2\,a_L^2$ and the light ion energy scales as $\epsilon \propto Z_l\,\sqrt{P_L}/4$. On the contrary, energetic ions (in particular relativistic ions) quickly separate from the heavy ion layer. They gain most of their energy during the early (linPA) stage. Writing $t_{linPA} \sim w_\perp \sim w_L$ the duration of this stage and considering $a_L > a_h$, Eq. (1) can be rewritten as a function of P_L. One then obtains a threshold power, $P_L > m_l^2/Z_l^2$, above which relativistic ions with energy $\epsilon \propto Z_l\,\sqrt{P_L}$ are expected.

In summary, this new mechanism of ion acceleration allows for the generation of high-quality ion beams which properties can be controlled by a careful target design. This makes it an interesting candidate for applications such as hadron-therapy. Scaling laws presented here suggest that this particular application might be considered on petawatt laser systems [3].

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2.19 Terahertz Generation by Ionizing Two-Color Femtosecond Pulses in Gases

C. KÖHLER, S. SKUPIN, I. BABUSHKIN, W. KUEHN, L. BERGÉ, K. REIMANN, M. WOERNER, J. HERRMANN, T. ELSAESSER

Far-infrared radiation in the THz range has developed into a sensitive probe of low-frequency excitations of condensed matter and into an analytical and imaging tool for a broad range of applications. Recently, intense THz pulses have been applied for inducing nonlinear light-matter interactions and for studying quantum-coherent charge transport phenomena in solids. In this new area of research, the generation of well-defined THz field transients with a high amplitude represents a key issue. Conventional laser-driven THz sources are based on semiconductor photoconductive switches and nonlinear frequency conversion in crystals, providing a comparably small THz field strength in a spectral range limited by the absorption of the crystals. In an alternative approach [1], a short pump pulse at 800 nm and its second harmonic at 400 nm are focused into a gas to generate a plasma. Intense THz pulses with field amplitudes as high as 400 kV/cm and remarkably broad spectra have been reported with this method [1–3]. Here we present a combined theoretical and experimental study of THz generation by ionizing two-color femtosecond pulses in a gas [6]. Extensive numerical simulations were performed using for the first time a (3+1)-dimensional code based on a unidirectional pulse propagation equation, which includes the plasma dynamics responsible for THz generation. This approach allows a comprehensive description of the propagation of all fields taking into account their spatio-temporal reshaping induced by the plasma effects and by the optical Kerr nonlinearity. In both experiment and simulation we observe a remarkable broadening of the THz spectrum with increasing gas pressure. We show that such broadening is a result of a sensitive dependence of the THz spectrum on small phase and frequency shifts induced by nonlinear propagation of pump pulses.

Our THz plasma source (inset of Fig. 1) is driven by 40 fs pulses (800 nm) with pulse energies of $\sim$ 300 μJ, focused by an achromatic lens (L) of 40 mm focal length. A 0.1 mm thin β-barium borate (BBO) crystal (C) cut for type I second-harmonic generation is additionally inserted into the beam 7 mm before the focus. The setup is placed in a closed chamber filled with argon at various pressures between 1 and 1000 mbar. THz radiation emitted from the plasma volume in the focal spot is collected by a parabolic mirror (M). Intensity interferograms were recorded with a HgCdTe detector by varying the path difference between the two arms of a Michelson interferometer. THz spectra were derived by Fourier transformation.

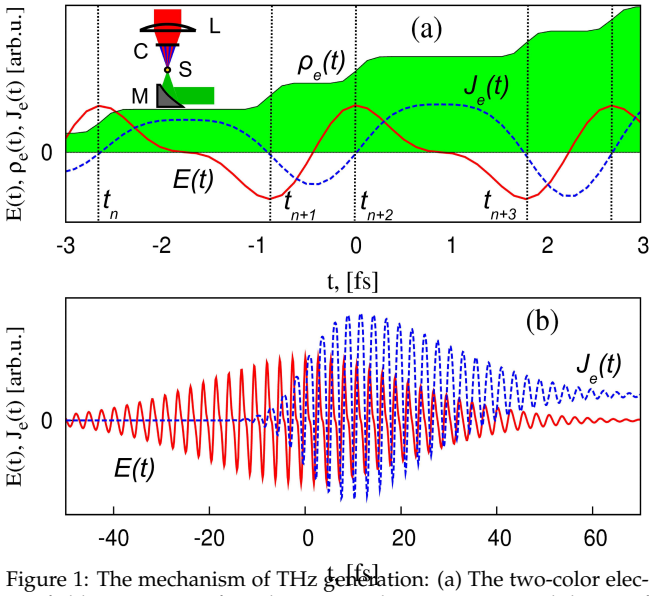

Figure 1: The mechanism of THz generation: (a) The two-color electric field E generates free electrons with a step-wise modulation of the electron density ρ_e via tunneling photoionization. The ionization occurs mostly near the maxima of electric field at times t_n. This leads to a slow component of the current J_e (b) which acts as a source for THz emission. Inset in (a): scheme of the experimental setup.

For the description of the nonlinear propagation of electromagnetic fields valid in the full range from THz down to UV/VUV wavelengths beyond paraxial and slowly-varying envelope approximations we use the following unidirectional pulse propagation equation [4] for linearly polarized pulses,

$$\partial_z \hat{E} = i\sqrt{k(\omega)^2 - k_x^2 - k_y^2}\,\hat{E} + i\frac{\mu_0\omega^2}{2k(\omega)}\hat{\mathcal{P}}_{\rm NL}. \qquad (1)$$

Here, $\hat{E}(k_x, k_y, z, \omega)$ is the Fourier transform (indicated by $\hat{}$) of the electric field with respect to x, y, and t, $k(\omega) = \omega n(\omega)/c$ is the wavenumber, $\nu = \omega/2\pi$ the frequency, c is the speed of light and $n(\omega)$ is the refractive index of the gas, in our case argon [5]. The nonlinear polarization $\hat{\mathcal{P}}_{\rm NL} = \hat{P}_{\rm Kerr} + i\hat{J}_e/\omega + i\hat{J}_{\rm loss}/\omega$ originates from the optical Kerr effect $P_{\rm Kerr}$, the electron current J_e and a loss term $J_{\rm loss}$ due to photon absorption during ionization. In Eq. (1) , radiation in backward direction is neglected, as it does neither influence the propagation of the forward fields, nor is it detected in our experiment. In $\hat{P}_{\rm Kerr}$ we take into account different nonlinear susceptibilities for neutral atoms and ions. The plasma dynamics is described by the electron density $\rho_e(t)$, obeying $\dot{\rho}_e(t) = W_{\rm ST}(E)[\rho_{at} - \rho_e(t)]$, where ρ_{at} denotes the neutral atomic density and dot the time-derivative. We use a quasi-static tunneling ionization rate $W_{\rm ST}$ for hydrogen-like atoms given in [3]. The macroscopic plasma current $J_e(t)$ is determined by the

microscopic velocity distribution $v(t,t_0)$ of electrons born at the time t_0 [2,3],

$$J_e(t) = q \int_{-\infty}^{t} v(t,t_0)\dot{\rho}_e(t_0)dt_0. \qquad (2)$$

Assuming zero velocity for new-born electrons and neglecting the influence of the magnetic field and electron-electron interaction, the electron velocity reads $v(t,t_0) = \frac{q}{m_e}\int_{t_0}^{t} E(\tau)\exp[-\nu_e(t-\tau)]d\tau$, where ν_e is the electron-ion collision rate. With Eq. (2) we obtain

$$\dot{J}_e(t) + \nu_e J_e(t) = \frac{q^2}{m_e} E(t)\rho_e(t). \qquad (3)$$

Let us now investigate the dependence of THz generation on the gas pressure. Measured spectra over the complete pressure range between 1 mbar and 1000 mbar are shown as a contour plot in Fig. 2(a). Our HgCdTe detector is sensitive in a frequency range from 20 THz to 170 THz. For a comparison of theory and experiment, this high-frequency part of the spectra is most relevant. Fig. 2(c) shows a low-frequency spectrum with the characteristic maximum below 5 THz, in agreement with the simulated spectra.

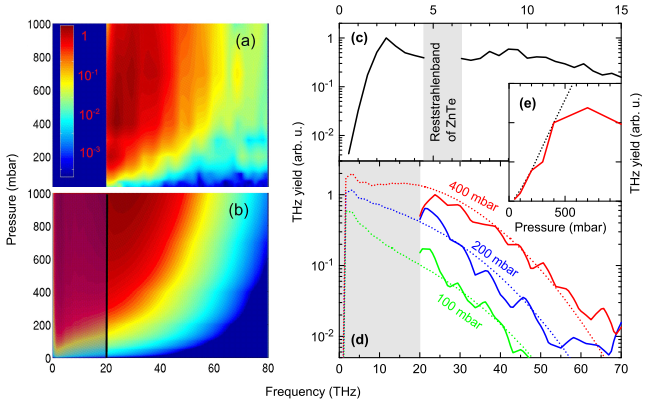

Figure 2: Measured THz spectra (a) and simulation results (b) for pressures between 1 and 1000 mbar. In (d), experimental (solid lines) and theoretical (dashed lines) spectra are compared for various pressures. In (e), the overall THz yield versus pressure is shown (simulation: dashed line, experiment: solid line). (c) Low frequency spectrum for 1000 mbar measured by electro-optic sampling in ZnTe, corrected for the frequency-dependent detector response. Shading signifies frequency ranges where no experimental data are available.

The observed dependence of the spectral width on the pressure can not be explained by the local plasma current, in which the variation of pressure only results in an amplitude scaling of the current. Instead, it originates from pressure dependent nonlinear propagation effects. We observe small blue-shifts $\delta\nu$ of the central frequencies caused by the nonlinear plasma-induced change of the refraction index. These shifts are 1 THz in the fundamental and ~ 0.4 THz in the second harmonic at $z = 0.2$ mm for 400 mbar, and depend strongly on the gas pressure. Surprisingly, these very small frequency shifts have a dramatic influence on the generated THz spectrum. To explain the physical origin of this very sensitive dependence, let us first illustrate the mechanism behind THz generation. In Fig. 1(a) we present the electron density, which shows a stepwise increase near the tunnel ionization events at the field maxima. In a simplified model, we can assume rectangular steps in the electron density [$\dot{\rho}_e(t) = \Sigma_n \rho_n \delta(t - t_n)$] and $\nu_e = 0$, and thereby obtain a discrete version of Eq. (2):

$$J_e(t) \sim \sum_n \rho_n H(t - t_n)[v_f(t) - v_f(t_n)], \qquad (4)$$

where $H(t)$ is the Heaviside step function, $v_f(t) = \frac{q}{m_e}\int_{-\infty}^{t} E(\tau)d\tau$ is the free electron velocity such that $v(t,t_n) = [v_f(t) - v_f(t_n)]$, and ρ_n is the electron density created in the nth ionization event. For a monochromatic electric field $v_f(t_n) = 0$. The Fourier transformation of the step function $H(t)$ exhibits a low-frequency spectrum $\propto 1/\omega$. Therefore THz radiation is generated by the second term in Eq. (4) proportional to $v_f(t_n)$, while the first term contributes in the spectral range of the pump fields. For a two-color optical field, $E = A_1\cos[(\omega_0 + \delta\omega)t] + A_2\cos(2\omega_0 t + \theta)$, the field maxima in every half-cycle are given by $\omega_0 t_n \approx n\pi - n\pi\delta\omega/\omega_0 - (-1)^n 2r\sin\theta$, provided that $A_2/A_1 = r \ll 1$ and $n\delta\omega \ll \omega_0$. Hence, the points in time t_n and therefore the free velocities $v_f(t_n)$ alter significantly when $\delta\omega$ (and θ) change upon the propagation. As seen above, the low-frequency spectrum is determined by a sum over contributions $\sim v_f(t_n)$, and this sum finally determines the THz spectral shape. In the full (3+1)-dimensional geometry, the spectral shapes generated at different spatial points are added and averaged, leading to the observed strong spectral broadening, which is thus explained by propagation effects of the pump.

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2.20 Many-body effects in mesoscopic systems: Beyond the Anderson power law

MARTINA HENTSCHEL, SWARNALI BANDOPADHYAY

Introduction. Many-body phenomena such as the Kondo effect, Fermi-edge singularities, or Anderson orthogonality catastrophe (AOC), have attracted a lot of interest in condensed matter physics for many decades. Here we will focus on AOC, an universal many-body response of a system to a sudden perturbation, for example the appearance of a localized hole potential after the excitation of a core electron into the conduction band. Many-body effects have always been an inspiration to deepen and widen our physical understanding. We shall see here that this remains true when shrinking the system sizes to the mesoscopic scale (determined by the phase coherence length of the system and typically in the micrometer range), i.e. when we consider quantum dots, metallic nanoparticles or graphene rather than bulk metals. Instead of energy bands and Bloch waves, the electrons occupy now discrete energy levels. Their wave functions depend, among others, also on the system geometry (we confine ourselves to the ballistic case in the following). Moreover, the treasure box of mesoscopic systems allows to customize systems with properties that are not known from the macroscopic, metallic case: the possibility to have degenerate levels such as in circular or parabolic quantum dots, for example. Will these new, mesoscopic features – discrete energy levels, finite number of particles (as compared to 10^{23}), role of system geometry, degeneracies – leave their traces in many-body signatures?

The answer is a clear Yes. We have seen the importance of mesoscopic properties in a number of cases, for example in Fermi-edge singularities determining the photoabsorption response of quantum dots [1, 6] and graphene, the mesoscopic Kondo box [2], in AOC of chaotic [3], integrable [4], and parabolic [5] quantum dots. We have found a broad distribution of photoabsorption rates at threshold, as well as of Kondo temperatures and Anderson overlaps, that directly reflect the importance of the well-known mesoscopic fluctuations. Besides this sample-specific properties, we also made predictions about the behaviour of the averages, e.g., of the photoabsorption cross section. These data can be compared to the metallic case, and we found considerably deviating behaviour between a metallic sample and a quantum dot. Surprisingly, in addition to the above-mentioned mesoscopic features, the mere existence of a system boundary turns out to be mainly responsible for a peaked photoabsorption at the Fermi threshold [6], that has to be contrasted to a rounded Fermi edge singularity in the metallic case (the so-called K-edge is considered in both cases).

Anderson orthogonality catastrophe in parabolic quantum dots. In this report we will focus on AOC in parabolic quantum dots (PQDs). The shell structure characteristic for such typically few electron quantum dots was confirmed in experiments [7]. As in the harmonic oscillator, the lowest shell contains just one level, the next shell hosts two levels and so on. This introduces two energy scales, see Fig. 1: The inter-shell spacing ω_0 and the intra-shell spacing ω_c that is (very close to) zero in the (quasi-) degenerate case (that we consider for practical reasons) and increases as an external magnetic field lifts the degeneracies. The strength V_c of a sudden and localized perturbation that induces the AOC response has to be compared to these two energy scales. We shall see that this, together with the intrinic size dependence of the harmonic oscillator energy scales, is the origin of the very different bahaviour of PQDs and general ballistic quantum dots (e.g., chaotic dots), respectively; in the latter the energy levels are characterized by only one scale, namely the mean level spacing d.

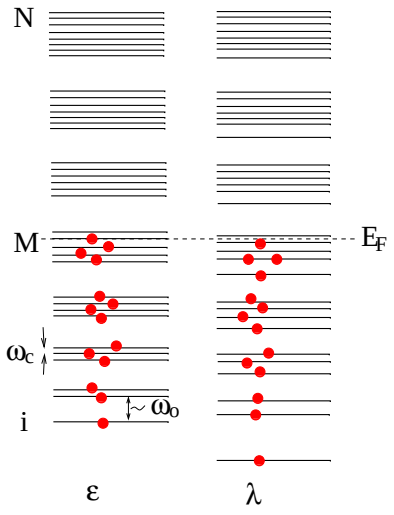

Figure 1: Energy levels in a parabolic quantum dot, before (left) and after (right) a sudden perturbation leading to AOC is applied. E_F denotes the Fermi energy, M the number of electrons on the PQD, and N the total number of levels.

This results in a rich behaviour of AOC in PQDs and we have to distinguish three regimes (we assume half filling as usual):

For (i) very small perturbation strengths (V_c/ω_c small), the physics is governed by the Fermi shell, i.e., the shell containing the Fermi energy level - and interestingly, the other shells do not play a role. Consequently, the

power law for the Anderson overlap,

$$|\Delta|^2 \; M_{\rm eff}^{-\delta^2/\pi^2} \; , \qquad (1)$$

where $M_{\rm eff}$ is the number of participating electrons and δ is the phase shift induced by the perturbation, at the Fermi energy, still holds with $M_{\rm eff}$ now being the number of electrons *on the Fermi shell*. Since this number is of the order $\sqrt{N}$, N being the total number of dot levels, the effective AOC response is characterized by $|\Delta|^2 \; N^{-0.5\,\delta^2/\pi^2}$, i.e. by an additional factor of 1/2 in the exponent. This behaviour is denoted by the solid line in the topmost curve of Fig. 2.

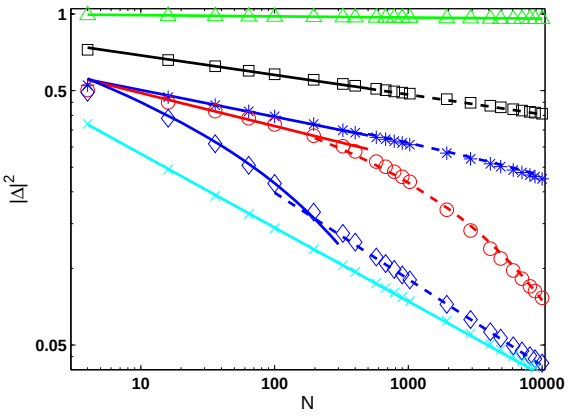

Figure 2: Modified Anderson power law in parabolic quantum dots.V_c/ω_c increases from top to bottom and takes the value 0.1, 1, 10, 100 and 10^5. The solid and dashed curves represent analyitcal forms of the Anderson overlap. See text for details. Note that the spatial dependence of the wave functions is omitted here for clarity.

When (ii) very strong perturbations strengths (V_c/ω_0 large) are considered, the whole system participates, and we find the usual Anderson power law, Eq. (1), for the AOC response, see the lowermost curve in Fig. 2.

The transition regime of (iii) intermediate perturbation strengths is the most interesting, as here the size of the quantum dot (i.e., the number of electrons on it) also plays a role, simply because the inter- and intra-shell energy scales depend on N. This is illustrated by the central curves of Fig. 2 that clearly show a transition in the power law. For small N, the shell seperation remains relatively large, and one is back to case (i). The opposite holds for (very) large N, where the small shell spacing results in a response of the whole, or at least of a large part of the system as in (ii), of the large N-part (dashed) of the last but one curve. For the transition regime of intermediate N we have analytically computed the Anderson overlap assuming that the shells right below and above the Fermi shell participate [5]. Taking these three shells into account, we were able to analytically describe the transition regime, see Fig. 2, that is characterized by an exponential correction term in the Anderson power law that enhances the effect of AOC compared to the case-(i) behaviour. It is denoted by the dashed lines in the 2nd, 3rd and 4th curve from to as well as the solid line in the last but one curve and cleanly illustrates the deviation from the Anderson power law.

Eventually, we briefly mention the importance of shell effects as the number of electrons on the parabolic dot is varied. Most remarkably, AOC is enhanced especially for small perturbations, where the Anderson overlap drops to a value 1/degeneracy, rather than being close to one, whenever a new shell is opened. This is understood by a phase-space argument: The sudden perturbation "shakes up" the electrons on the dot, and a single electron on an otherwise empty shell can rechoose its level, resulting in a correction factor 1/degeneracy [5]. We have studied this behaviour also in detail for circular quantum dots [4] where the characteristic two-fold level degeneracies leaves its traces also in the photoabsorption cross section [6]. We point out that the effects persist if the degeneracy is slightly perturbed.

Another direction of our research on the group's many-body topic is graphene. Here, the special properties of the density of states – no states at the Dirac point and the possibility of having edge states – provide new features not available or known in bulk metals that turn into specific properties of the many-body responses. For example, an additional singularity develops in the photoabsorption cross section at the Dirac point.

In summary, we have found that the variety of mesoscpopic systems considerably enriches the field of many-body physics and contributes to its deeper understanding. The availability of high quality samples raises the hope for experimental confirmation of our predicitions in the near future.

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2.21 Remodeling Bone Remodeling

THILO GROSS, MARTIN ZUMSANDE

Bone is a complex tissue that is being repaired and rebuilt continuously throughout an individual's life. The process of bone remodeling consists of two subprocesses: the resorption of old bone and the formation of new bone. In the past decades it has become clear that, at the cellular level, bone remodeling depends on the interplay between two different types of cells, osteoclasts and osteoblasts. The former resorb bone, whereas the latter fill the gaps left by osteoclasts with newly formed bone tissue [1].

In humans, the process of bone remodeling is regulated by several factors. In particular, it has been discovered that a signaling pathway involving the Receptor Activator of NF-κB (RANK), its ligand RANKL, and osteoprotegerin (OPG) play an important role in the regulation of bone remodeling [2].

For osteoclasts to mature, it is necessary that RANKL, expressed by cells of osteoblastic lineage, attaches to RANK, expressed on cells of osteoclastic lineage. This process is regulated by the decoy receptor OPG, which is expressed by osteoblastic cells and inhibits the differentiation of osteoclasts by binding to RANKL and thus sequestering it. Another important regulator, TGFβ, is known to influence both osteoclasts and osteoblasts [2]. Over- or underexpression of TGFβ and the protagonists of the RANKL pathway has been implicated in several diseases of bone, such as osteoporosis and Paget's disease of bone [3].

From a theoretical perspective, bone remodeling is interesting because biological requirements seem to pose contradictory demands. On the one hand, the system must be robust against respect to naturally occurring fluctuations. On the other hand, the system must be adaptive allowing relevant changes in the external conditions that require an increased or decreased rate of bone remodeling.

Several authors have pointed out that under physiological conditions and in absence of external stimuli, the system should reside in a steady state, where the numbers of osteoclasts and osteoblasts remain approximately constant in time. For the system to remain close to the steady state, the state has to be dynamically stable, so that the system is driven back to the steady state after small perturbations. At the same time it is desirable that the stationary densities of osteoblasts and osteoclasts react sensitively to external influences, communicated through the signaling molecules. Mathematically speaking, this means that the system should be robust against fluctuations of the variables, but sensitive to changes in the parameters. In dynamical systems, the strongest response of steady states to parameter change is often found close to bifurcations. Therefore, it is intuitive that there should be some trade-off between dynamical stability and responsiveness. It is thus possible that the physiological state of the bone remodeling system is characterized by parameter values close to a bifurcation point.

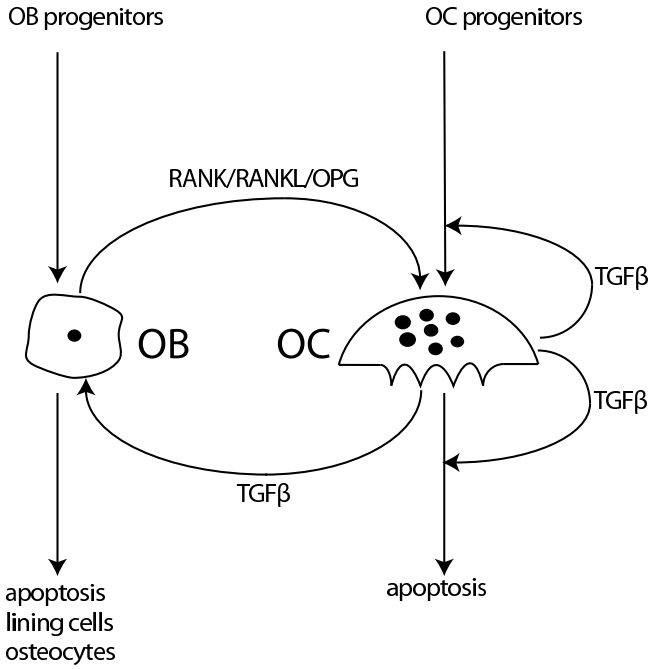

Figure 1: Schematic sketch of the two-variable model. Osteoblasts (OB) influence osteoclasts (OC) via the RANKL/RANK/OPG pathway, while the TGF-β pathway exerts a positive feedback from osteoclasts to both osteoclasts and osteoblasts.

In a recent publication [4], we used the approach of generalized modeling [5] for analyzing two different types of models for bone remodeling, which differed in the number of variables that were taken into account. In a generalized model it is not necessary to restrict the processes in the system to specific functional forms. Therefore, a single generalized model can comprise a class of different conventional models. Despite this generality, the local stability and dynamics in generalized models can be analyzed efficiently by the tools of dynamical systems theory. This analysis reveals the stability of the system depending on a number of parameters that have a straight forward interpretation in the context of the model.

In our analysis of bone remodeling we focused first on two-variable models in which only the abundance of active osteoblasts and osteoclasts are represented by state variables. In these models stability requires that the effect of OPG dominates over that of RANKL. However, this requirement is currently not supported by experimental evidence indicating that these types of

models miss an important factor.

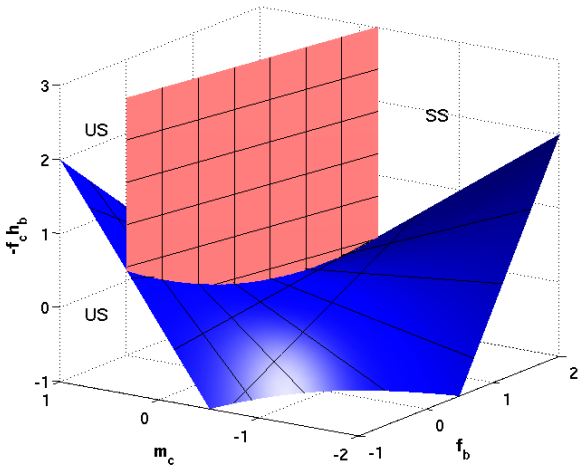

Figure 2: Bifurcation diagram for the 2-variable model, depending on three parameters. Each combination of the parameters in the three-dimensional volume corresponds to the steady state in a particular model. There are two distinct bifurcation surfaces that divide the regions where steady states are stable (SS) from regions where steady state unstable (US). The red surface is formed by Hopf bifurcation points, whereas the blue surface is formed by saddle-node bifurcation points.

A potentially important player in bone remodeling are responding osteoblasts, i.e. cells that have not yet matured into fully functional active osteoblasts, but are already commited to the osteoblastic lineage. We therefore studied a three-dimensional generalized model, in which responding osteoblasts were represented by a state variable. The model incorporated experimental findings, suggesting that RANKL is expressed preferentially on responding osteoblasts, while its antagonist OPG is mainly expressed on matured active osteoblasts.

Current experimental data, places the system into an area of the bifurcation diagram where a stable steady state is close to both saddle-node and Hopf bifurcation points. The stability analysis therefore shows that in the dynamical system of bone remodeling, various bifurcations not only exist but are located in a parameter space supported by experimental findings. The main benefit of operating close to a region of instability is probably that a stronger adaptive response to external changes of the model parameters is possible. Although our modeling approach was not designed to study the response of the model to perturbations directly, it has been shown before by direct simulations that conventional models in this parameter range respond strongly to perturbations, thus allowing a better functional control of bone remodeling [6].

Despite the benefits, operating close to a bifurcation also poses risks to the system. A change in the parameters by an external process can shift the system over the bifurcation, so that the stable steady state becomes unstable or ceases to exist. It is therefore reasonable to ask whether certain diseases of bone can be related to bifurcations. It is known that several diseases of bone are related to dysfunctions in the regulation of bone remodeling, among them postmenopausal osteoporosis, Pagets disease, osteopetrosis and osteopenia. There is some evidence that diseases may lead to qualitatively different dynamical behavior. In particular, periodic activity of osteoclasts has been observed in Pagets disease of bone [3]. It is conceivable that these dynamics are evoked by the transition of a steady state to instability in a Hopf bifurcation. In the three-dimensional model stability is lost in a Hopf bifurcation when the RANKL/OPG ratio is increased. This is consistent with previous findings implicating dysfunction of RANKL pathway as a cause of Pagets disease.

It is still unclear if known diseases of bone can be connected to bifurcation phenomena. However, the analysis, described above, suggests that Hopf and saddle-node bifurcations exist close to the physiological steady state. Although we cannot show that specific diseases can be related to these bifurcations, a bifurcation occurring in vivo should certainly lead to a pathological condition. Therefore, it seems very plausible that a connection for instance between the crossing of a Hopf bifurcation and the onset of Pagets disease may exist. If this is indeed confirmed it would imply that powerful tools of bifurcation theory and related data analysis techniques, can be applied to explore the dynamics of the disease.

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2.22 Evolution of Fragile Cooperation

THILO GROSS, GERD ZSCHALER

Cooperation is a central phenomenon in biology. The functioning of biological cells depends crucially on the cooperation between different genes. On higher levels, cells cooperate to form tissues, organs, and organisms and organisms cooperate to form social groups. Cooperation is not restricted to humans, but can be observed in almost every major family of species. Yet, only humans have succeeded in scaling cooperation beyond the level of relatives and direct acquaintances to form companies, nations and supernational structures. In modern society the stability of these higher forms of cooperation is a major concern.

Understanding the evolution of cooperation between selfish players is of importance not only because of the central role of cooperation in biology but also to address the emergence and failure of cooperation in human societies. The central challenge in this field is to understand how costly cooperative behavior can emerge from a process of natural selection that acts on the level of the individual.

Previous work has identified several key mechanisms leading to the evolution and fixation of cooperation [1]. Among others, it was found that cooperation is promoted if the interactions between agents are confined to a certain topology such as a lattice or a complex network. A recent development is the investigation of games on adaptive networks [2,3], in which the agents' behavior feeds back on the network topology. Cooperation is promoted if cooperating players can secure an advantageous topological position, directly due to avoidance of defectors, or indirectly due to the continuous arrival of new players or other ongoing changes of the topology. Furthermore, cooperation in adaptive networks can profit from the emergence of a self-organized leadership structure and the formation of strongly heterogeneous topologies, which are known to promote cooperation.

In a recent publication [4], we studied a model of the evolution of cooperation in an adaptive network. In this model a state can be reached in which every agent cooperates, although this state is dynamically unstable against certain perturbations. The model thereby reveals a powerful mechanism by which asymptotically full cooperation can be achieved, but also points to a possible mode of failure of this *fragile cooperation*.

We consider an undirected network of nodes, representing agents, and links, representing interactions. Each agent can either cooperate or defect, i.e. refuse to cooperate. The outcome of interactions is modeled by a snowdrift game, a paradigmatic model of cooperation. If two agents cooperate then they share the benefit and cost of the cooperation. If one of the agents defects while the other cooperates, the defecting agent (the defector) reaps the whole benefit without contributing to the cost. However if both agents defect, neither cost nor benefit is generated, which is considered the worst outcome in this type of game.

The proposed model describes the fundamental processes of social adaptation, i.e. adoption of social traits from other agents, and social distancing, i.e., the avoidance of certain other agents. Starting from a random graph and randomly assigned equiprobable strategies, we evolve the network as follows: In every time step, one link is selected at random. With probability p, this link is rewired. Otherwise, i.e., with probability $q = 1 - p$, one of the linked players adopts the other player's strategy. For large p, players thus tend to change their interaction partners, whereas for small p they tend to revise their behavior.

Finally, we have to specify which agent copies the other's strategy in a strategy adoption event and which agent keeps the link in a rewiring event. Concerning strategy adoption, it is reasonable to assume that the less successful agent is more likely to adopt the more successful agents strategy than vice versa. Concerning rewiring, we assume that the more successful agent is more likely to keep the link. This implies that the agents following the more successful strategy will on average have a higher number of links than agents following the less successful strategy.

But how do agents estimate the success of their neighbors? Most previous models assume that the agents' access to information is governed by the same network as the underlying games, forcing the agents to base their decisions on information from direct interactions. The same network topology thus determines three different aspects of the system: the interaction partners of an agent, against whom the game is played, the potential role models, whose strategies can be adopted, and the agents from which information can be obtained. However, for intelligent agents, and especially humans, there is no reason to assume that these three network roles are all fulfilled by coinciding topologies. We therefore assume that information transfer in the population is not governed exclusively by the interaction network. As a first approximation, we consider the simplest case in which the information transmission network is replaced by an effective global coupling, as information can be rapidly transmitted and in the human population is also transported by the mass media. In the main part of this work, we assume that the agents rely on their perception of a strategy's *general* performance, i.e. the average payoff received by all

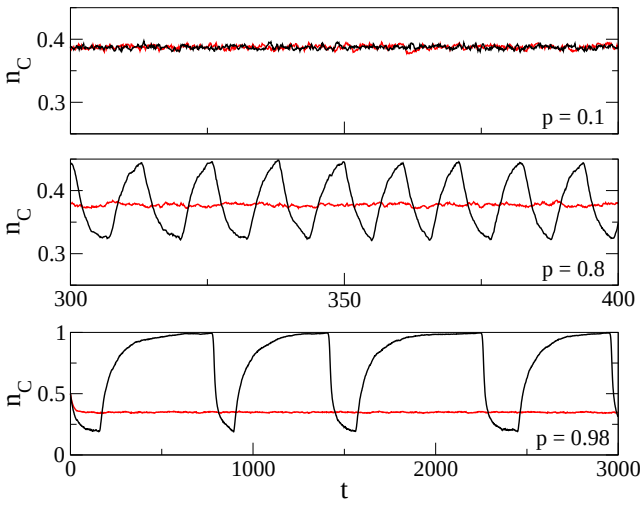

Figure 1: Time series of the fraction of cooperators in an adaptive network for different rewiring rates p. When rewiring occurs almost at random (red) the fraction of cooperators approaches a steady state that is almost independent of the rewiring rate p. However, if rewiring favors more successful individuals, there is a critical rewiring rate at which the steady state becomes unstable and oscillatory dynamics start. When the rewiring rate is increased the amplitude of the oscillations grows until finally a homoclinic orbit connecting to the fully cooperative state is formed. Moving along this orbit the system can reach a highly cooperative state and remain there for long periods of time. However, in a network of finite size, fluctuations eventually drive the system over to the unstable manifold of the saddle, corresponding to a sudden collapse of cooperation in the population.

The model proposed above, was analyzed in large agent-based simulations and by deriving a low-dimensional moment-closure approximation [5] that was investigated analytically. Typical time series for different rewiring rates p are shown in Fig. 1. If rewiring is approximately random, the system approaches a stable steady state where both strategies coexist. In this regime the stationary proportion of cooperators depends only weakly on p. Also, if rewiring favors agents following the more successful strategy the dependence of the steady state on p is weak. However, as p is increased, the system undergoes a Hopf bifurcation, in which the steady state loses its stability and a stable limit cycle emerges. As p is increased further, the amplitude and period of the limit cycle grows. Eventually the limit cycle hits the state of full cooperation.

In the low-dimensional model the state of full cooperation is an unstable saddle. Upon connecting to this saddle the limit cycle undergoes a homoclinic bifurcation and becomes a homoclinic loop. Due to a symmetry in the system this homoclinic loop remains in existence even when p is increased beyond the homoclinic bifurcation point.

On the homoclinic loop, the system asymptotically approaches full cooperation. In the infinite system described by the analytical approximation, this approach takes infinitely long so that, with probability 1, the system is found to be arbitrarily close to the fully cooperative state if observed at a random time.

In finite systems, the state of full cooperation is an absorbing state of the strategy dynamics because there is no defector left from which defective behavior could be adopted. If this state is reached in a simulation the system will remain their indefinitely. This behavior is indeed observed in very small systems. Therefore both very small and extremely large systems are likely to exhibit full cooperation, albeit for different reasons.

Also in systems of large size, the system asymptotically approaches the neighborhood of the fully cooperative state and can remain there for a long time. However, large systems will typically not reach the absorbing state before some fluctuation drives them from the stable to the unstable manifold of the saddle. Once on this manifold the number of cooperators declines rapidly as the system moves along the homoclinic orbit before approaching the fully cooperative state again.

The main message of the model proposed here is perhaps that, at least in adaptive network models, dynamical mechanisms can have a strong impact on the evolution of cooperation.

For systems of reasonable size the dynamics described above imply that long periods of high levels of cooperation are interrupted by sudden episodes of predominant defection. This effect of fragile cooperation is reminiscent of the Chinese dynastic cycle where periods of corruption, crime, and civil war led to pronounced oscillations in the population density.

More work is certainly necessary to explore the role of the homoclinic mechanism in nature. This work will, offer the intriguing possibility to identify not only a mechanism that strongly enhances cooperation but also a potential cause of the sudden collapses of cooperative behavior.

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2.23 Measuring the Complete Force Field of an Optical Trap

MARCUS JAHNEL, MARTIN BEHRNDT, ANITA JANNASCH, ERIK SCHÄFFER, STEPHAN W. GRILL

Optical traps are widely used to investigate forces and displacements encountered on the molecular level, for example in the movement of molecular motors. To measure or apply forces in such studies requires the precise knowledge of the trapping force field, which is typically approximated as linear in the displacement of the trapped microsphere. Close to the trap center this linear assumption is valid and successfully used to set the scale of the measured forces and displacements when performing a thermal calibration. Here, thermal fluctuations of the microsphere around the center of the optical trap are measured and compared with theories of Brownian fluctuations in a confining harmonic potential [1, 2]. However, as this assumed linear force-displacement relation breaks down at larger microsphere displacements, applications demanding high forces at low laser intensities can probe the light-microsphere interaction beyond the linear regime. Thus, an exact mapping of the complete optical force field is not only necessary to determine the validity of the linear approximation, but enables the use of the full force range of an optical trap.

Here, we measured the full non-linear force and displacement response of an optical trap in two dimensions [3]. We used a dual-beam optical trap setup with back-focal-plane photodetection [4] that allowed for independent adjustment of the positions and intensities of two optical traps [5]. A strong, thermally-calibrated trap [1], $\mathrm{T_C}$, in its linear operating regime acted as a precise sensor of force (and position) for analyzing a weaker, uncalibrated trap of interest, $\mathrm{T_A}$. While keeping $\mathrm{T_C}$ stationary, we scanned $\mathrm{T_A}$ in $10\,\mathrm{nm}$ steps over the whole microsphere-interaction regime. At each step—with stationary traps and measurement times long enough to average over thermal fluctuations—the balance of the optical forces yields $\langle \boldsymbol{F}_\mathrm{C}(\boldsymbol{r})\rangle_{t_{av}} = -\langle \boldsymbol{F}_\mathrm{A}(\boldsymbol{r})\rangle_{t_{av}}$. To ensure the validity of the linear force-displacement approximation for the calibration trap to within 5 % (see below), we adjusted the relative intensities in both traps such that $\mathrm{T_C}$ had at least a five times higher trap stiffness than $\mathrm{T_A}$. This then allows for measuring the full force-displacement relation of $\mathrm{T_A}$. Under the above conditions, we have

$$\hat{\boldsymbol{\kappa}}_\mathrm{C}\langle \boldsymbol{r} - \boldsymbol{d}\rangle_{t_{av}} = \langle \boldsymbol{F}_\mathrm{A}(\boldsymbol{r})\rangle_{t_{av}}, \qquad (1)$$

where the diagonal matrix $\hat{\boldsymbol{\kappa}}_\mathrm{C}$ contains the trap stiffness of $\mathrm{T_C}$ in the x- and y-direction. The distance vector between the two traps is denoted by $\boldsymbol{d}$ and is changed by scanning $\mathrm{T_A}$. Allowing the microsphere to relax to its new equilibrium position, we sampled the complete optical force profile for arbitrary displacement $\boldsymbol{r}$ relative to the center of $\mathrm{T_A}$. We determined a two-dimensional map of the optical forces exerted by $\mathrm{T_A}$ on a polystyrene microsphere of diameter $1.26\,\mu\mathrm{m}$ [Fig. 1(a)]. The net force, obtained by combining the parallel (F_x) and perpendicular (F_y) force components relative to the trap polarization, demonstrates that for this microsphere size the optical forces are nearly radially symmetric [Fig. 1(b)]. We therefore restrict our remaining discussion to cross-sections of the force map in x [dashed line in Fig. 1(c)]. Fitting the experimental data using numerical calculations based on the T-matrix method [6] showed excellent agreement of our measurements with Mie scattering theory [Fig. 1(c)].

Close to the origin, a constant trap stiffness—assuming Hooke's law—is expected. However, numerical differentiation of the measured force curve shows that the trap stiffness continuously deviated from its value at the origin, $\kappa_0 = 72 \pm 3\,\mathrm{pN}/\mu\mathrm{m}$ [Fig. 1(d)]. Displacing the microsphere from the center, the trap stiffness increased moderately within the first 300 nm towards a maximum, before it fell off, and eventually became negative. In this region, the analogy between optical traps and mechanical springs fails; the trap stiffness is negative for a decreasing, yet, still restoring force.

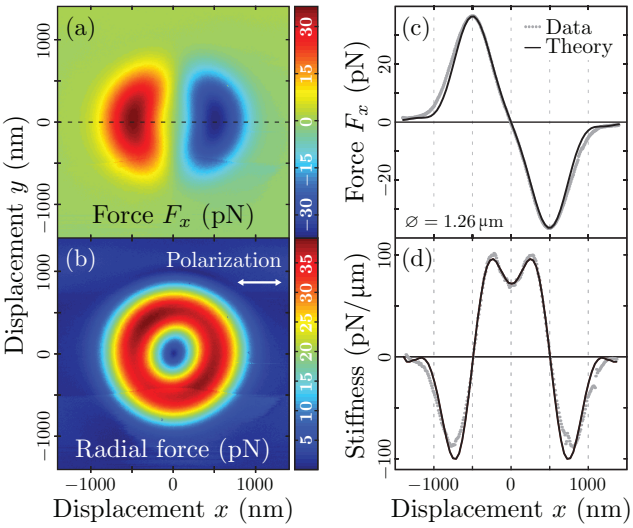

Figure 1: 2D maps of (a) optical forces on a $1.26\,\mu\mathrm{m}$ microsphere in the direction of polarization and of (b) the magnitude of the radial force $|\boldsymbol{F}| = \sqrt{F_x^2 + F_y^2}$. Force magnitudes are color-coded by corresponding heat maps. (c) Complete force response along the polarization axis [dashed line in (a)]. (d) Numerical differentiation, $\kappa(x) = -\partial_x F(\boldsymbol{r})$, yielded the trap stiffness with respect to the microsphere displacement.

Note that the stiffening effect was substantial even for small displacements. A displacement from the trap center of 250 nm already lead to a deviation of the trap stiffness of more than 30 % as compared with its value at the origin, which would be probed by thermal calibration. Thus, without any preliminary assumptions about the trap of interest (T_A), we measured its full force field and analyzed the validity of the linear force-displacement approximation.

A distinct second linear regime of higher constant trap stiffness was recently reported for $2.01\,\mu$m microspheres [7]. To study the microsphere size dependence of the observed stiffening effect in more detail, we use our setup to compare the $1.26\,\mu$m microspheres with larger ones of diameters $2.01\,\mu$m and $2.40\,\mu$m in Fig. 2(a) and (b). Indeed, the stiffening was more pronounced for larger microspheres and depended sensitively on their exact size. Figure 2(b) shows that the measured stiffness landscapes are complex, displaying ripples, yet no extended linear regime. Importantly, these non-linear effects are well described by Mie theory calculations [6]. Therefore, our approach allows for a detailed investigation of these optical phenomena.

Next, we used our assay to evaluate the accuracy of the back-focal-plane detection method [4]. This sensitive detection method infers both the displacement and force from a single differential voltage signal on a position-sensitive photodetector. For small displacements, both measures are well approximated as linear functions of the differential voltage signal. For larger displacements, we found that the linear force-displacement relation breaks down [Figs. 1(c) and 2(a)].

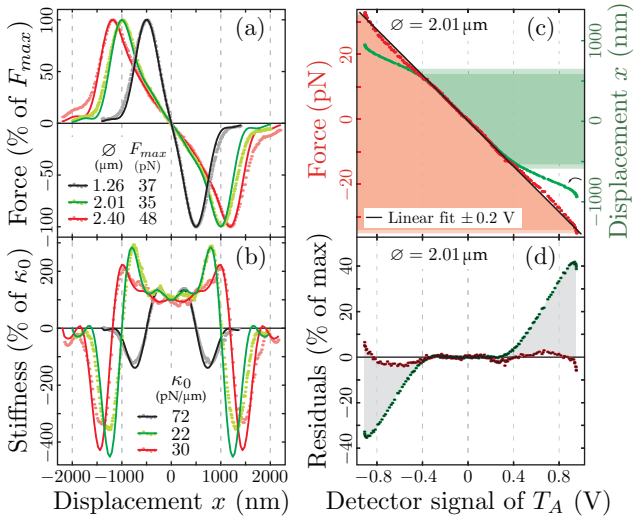

Figure 2: (a) Normalized force-extension curves and (b) thereof derived trap stiffnesses for indicated microsphere sizes. (c) Comparing forces (red) and displacements (green) to the detector signal of T_A for a $2.01\,\mu$m microsphere. Shaded areas indicate where residuals [see (d)] of the linear fit are less than 5 % (dark) or less than 10 % (bright). (d) Force (red) and displacement (green) residuals of the fit in (c) normalized to $F(V_{max}) = 33$ pN and $x(V_{max}) = 950$ nm, respectively.

However, it remains elusive to what extend each single quantity (force or displacement) can still be accurately described by a linear dependence of the detector signal. To address this, we correlated the calibrated force and displacement signals of the strong trap with the detector signal of the weak trap. As depicted in Fig. 2(c) and (d) for microspheres of diameter $2.01\,\mu$m, assuming a linear relationship between force and voltage signal is correct to within ± 5 %, even for very large displacements close to the force maximum. On the other hand, inferring microsphere position from the same voltage signal—again assuming linearity—lead to significantly larger errors of up to 40 % [Fig. 2(d)].

To conclude, an optical trap with back-focal-plane detection is foremost a sensor of force and not of position [4]. Positional information is inferred from a linear approximation of the optical force field, which does not hold for large microsphere displacements [Figs. 1(c) and 2(a)]. These findings have implications for detection methods that infer force from microsphere position, such as high-speed video microscopy [8]. Without a full characterization of the force field, accurate force measurements are in this case limited to the range where the linear force-displacement relation holds.

In summary, we have shown how to measure the complete 2D force field of an optical trap with a dual-beam optical trap setup. A strong calibration trap in its linear regime acts as an accurate force sensor. Our calibration strategy directly addresses the difficulties associated with inferring physical quantities from optical tweezers measurements that are based on the assumption of a linear trapping force field. The treatment of optical tweezers as springs is an approximation, valid only close to the trap center, and its validity depends sensitively on the size of the trapped object. By reporting a simple calibration scheme for absolute forces and displacements in an optical trap we provide a robust means for the study of the complete light-microsphere-interactions; for accurate tweezers measurements beyond the linear regime.

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2.24 Pattern Formation in Active Fluids

JUSTIN S. BOIS, FRANK JÜLICHER, STEPHAN W. GRILL

Active stresses are exerted in cells and tissues by motor protein-driven contraction of the cytoskeleton. Concurrently, chemical species are reacting and diffusing within the material. Reaction-diffusion mechanisms have long been implicated in biological pattern formation of chemical species, but mechanical stresses are also crucial for developmental processes [1]. The active stress and distribution of chemical species associated with pattern formation are coupled in two ways. First, the active stress is under control of biochemical regulators affecting motor activity and actin polymerization, which may themselves diffuse and undergo chemical reactions. Secondly, the flow of contractile material transports chemical species by advection. In this work [2], we developed a new framework for biological pattern formation considering these two forms of coupling.

In this first simplified treatment, we treat a contracting cytoskeleton or tissue as a thin film of an active viscous fluid and consider only movements in the x-direction. The equation of motion is then [3,4]

$$\partial_x \, \zeta \Delta\mu(\mathbf{c}) = -\eta \partial_x^2 \, v + \gamma \, v,$$

where v is the fluid flow velocity, η is the viscosity, γ is a friction coefficient that takes into account boundary stresses, and $\zeta\Delta\mu$ is the active stress, dependent on the concentrations of chemical species, $\mathbf{c} \equiv (c_1, \ldots, c_n)$. The equation of motion reveals a physical length scale of the system, $\ell \equiv \sqrt{\eta/\gamma}$, which is the decay length of fluid velocity in response to a local active stress gradient [4]. In addition, mass conservation gives

$$\partial_t \, c_i = D_i \, \partial_x^2 \, c_i + R_i(\mathbf{c}) - \partial_x (c_i \, v) \; \forall i \in [1, n],$$

where D_i is the diffusivity of species i and $R_i(\mathbf{c})$ is the rate of production of species i by chemical reaction. The last term accounts for advective transport of species i that occurs by virtue of bulk fluid motion. The relevant dimensionless parameters are the ratio of diffusivities, D_i/D_1, and the Péclet number $\mathrm{Pe} \equiv (\zeta\Delta\mu)_0 \, /\gamma D_1$, where $(\zeta\Delta\mu)_0$ is the maximal possible active stress. The Péclet number is the ratio of diffusive to advective times scales and is therefore a measure of the relative importance of advection in the system dynamics. Additionally, the functional forms of $R_i(\mathbf{c})$ and $\zeta\Delta\mu(\mathbf{c})$, as well as the dimensionless length of the system L/ℓ (the ratio of the total system extent to the hydrodynamic length), are important for the dynamics.

Case study 1: active stress-driven instabilities. As a first case study, we consider a single biochemical species with concentration c that regulates active stress and undergoes no chemical reactions ($R(c) = 0$). This is the simplest nontrivial case of this general theory.

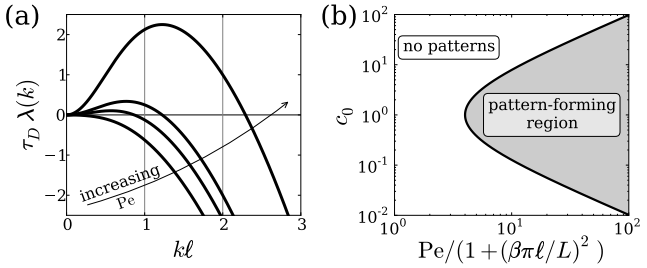

Figure 1: (a) Dispersion relation for $\zeta\Delta\mu = (\zeta\Delta\mu)_0 \, c/(1+c)$ and $c_0 = 1$ for $\mathrm{Pe} = 3$, 7, 10, and 25. The eigenvalue for the linearized system, $\lambda(k)$, is nondimensionalized by the diffusive time scale, $\tau_D = \ell^2/D$. For $L/\ell = 2\pi$ with periodic boundary conditions, as in Fig. 2, $k\ell$ may take only integer values (vertical gray lines). (b) Linear stability diagram for the same active stress function.

When will spontaneous patterns form in this system? Assuming no-flux boundary conditions, the system has a unique homogeneous steady state $c = c_0$. Small perturbations to this steady state can spontaneously give patterns if $\mathrm{Pe}\, c_0 \, \zeta_c > 1 + (\beta\pi\ell/L)^2$, where $\zeta_c \equiv \partial_c \, \zeta\Delta\mu(c_0)$ and $\beta = 1, 2$ for no-flux and periodic boundary conditions, respectively, as can be seen from the dispersion relation, plotted in Fig. 1a. The shaded region in Fig. 1b depicts the region in parameter space where this inequality holds and patterns, accompanied by fluid flow, may spontaneously form. The physical implication is that the active stress must be strong enough to promote advective flux into regions of high concentrations to counteract frictional resistance and diffusive counter-flux.

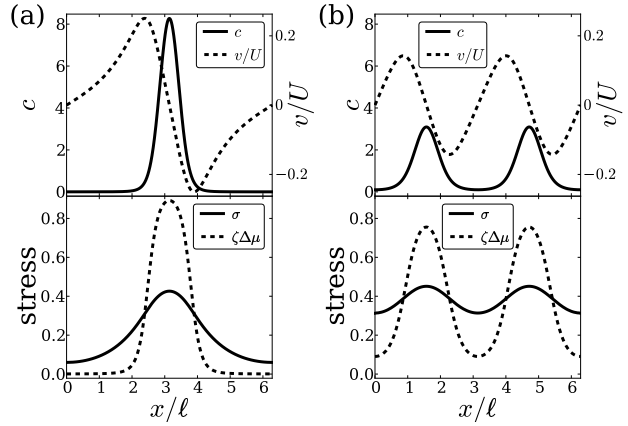

Figure 2: The nonhomogeneous steady states with (a) one maximum and (b) two maxima for $\zeta\Delta\mu(c) = (\zeta\Delta\mu)_0 \, c/(1+c)$, $\mathrm{Pe} = 25$, $L/\ell = 2\pi$, and $c_0 = 1$, with periodic boundary conditions. The total stress σ and active stress $\zeta\Delta\mu$ are given in units of $(\zeta\Delta\mu)_0$.

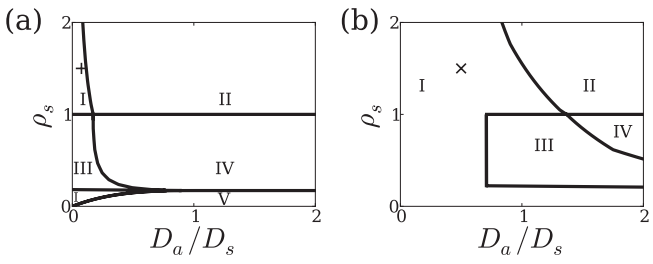

Figure 3: (a) Linear stability diagram in the absence of flow ($\mathrm{Pe} = 0$) for $\rho_a = 1$, assuming $L \gg 1$. Here, $d \equiv D_s/D_a$. Region I: This is the pattern-forming region. Region II: Stable homogeneous steady state. Region III: Patterns may form in this region, depending on initial conditions. Region IV: A homogeneous concentration profile oscillates in time. Region V: Unphysical region. (b) Linear stability diagram for $\mathrm{Pe} = 7$, $\rho_a = 1$, and $\zeta\Delta\mu = a/(1+a)$.

Interestingly, Pe, L, and ζ_c are material properties of the contractile fluid (e.g., an actomyosin cortex or a tissue), while c_0 may be regulated by gene expression. Thus, increasing (or decreasing) c_0 may shift a system from a homogeneous state to one with steady flow.

The resulting nonhomogeneous steady concentration profile consists of evenly-spaced symmetric extrema. The velocity profile, given by $v(x) = \mathrm{Pe}^{-1}\,\partial_x \ln c$, crosses zero at the peaks and valleys such that fluid flows into the peaks and out of the valleys. This provides a mechanism for chemical pattern maintenance in which a peak in concentration gives an active stress gradient which drives fluid flow, resulting in advective flux into a peak balancing diffusive flux out of it. In this way, active stress-driven fluid flow provides both the local activation and lateral inhibition that are the general requirements for spontaneous chemical pattern formation by at once delivering regulator into a peak and depleting it from a valley.

Case study 2: ASDM with active stress regulation. The activator substrate depletion model (ASDM) is a classic model for biochemical pattern formation first proposed by Gierer and Meinhardt in 1972 [5]. The ASDM consists of an activator (with concentration a) and a substrate (with concentration s) that undergo chemical reactions with the following properties: 1) The activator is auto catalytic, consuming substrate in the process. 2) The activator has a constant degradation rate. 3) The substrate has a constant production rate. The simplest form of the chemical kinetics is $R_a = \rho_a(a^2 s - a)$ and $R_s = \rho_s(1 - a^2 s)$, where ρ_a and ρ_s are chemical rate constants. The unique homogeneous steady state is $a_0 = s_0 = 1$. When $\mathrm{Pe} = 0$, or in the absence of active stress, we recover the classic ASDM, whose linear stability diagram is depicted in Fig. 3a. In region I of parameter space, the substrate acts as a fast-diffusing "inhibitor" (since its depletion slows the production of the activator), the hallmark of a Turing instability. In the presence of advection due to active stress up-regulation by the activator, the region of parameter space in which patterns form grows, as depicted in Fig. 3b. The steady concentration profile features peaks in activator concentration that contract fluid into them, providing an influx of activator, as shown in Fig. 4. This stabilizes the peaks against diffusion in a manner similar to the previous example, even in regimes where the activator diffuses faster than the inhibitor. Thus, active stress-driven flow serves to broaden the pattern-forming region of parameter space, giving patterns not only in concentration of chemical species but also in mechanical stress and fluid motion.

Summary We have developed a general hydrodynamic theory of chemically-regulated active stress in viscous fluids and identified general principles of pattern formation in such systems. This approach can be extended to higher dimensions and to include polar and nematic order, viscoelasticity, and other reaction systems. In the two scenarios presented here, peaks in concentration of stress activator are amplified by advective influx due to active flows. This simultaneously depletes activator from areas around a concentration maximum. Thus, active stress-driven flow provides both the local activation and lateral inhibition required to form stable patterns. This mechanism leads to pattern formation even in the absence of chemical reactions. We conclude that integration of active hydrodynamics with molecular signaling processes is an important theme for future studies of biological processes.

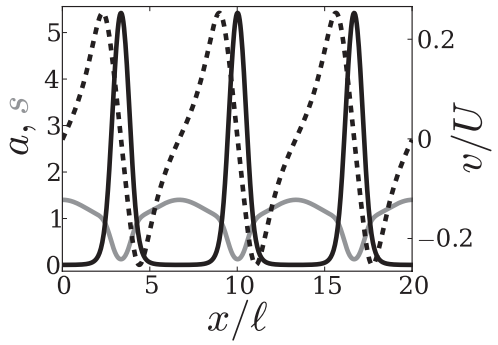

Figure 4: Nonhomogeneous steady state for $\mathrm{Pe} = 7$ and parameters given by the "×" in Fig. 3b with no-flux boundary conditions. The activator and substrate concentrations are given by the gray and dashed lines, respectively. The velocity is the solid black curve.

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2.25 Magnon Pairing in a Quantum Spin Nematic

MIKE ZHITOMIRSKY, HIROKAZU TSUNETSUGU

Introduction. Strong quantum fluctuations can destroy conventional long-range magnetic order. A spin system remains, then, in a disordered liquid-like state down to zero temperature. Many theoretical studies in the field of magnetism in the past two decades have been devoted to the investigation of possible types of quantum spin liquids. The enhanced fluctuations may also stabilize magnetic analogues of liquid crystals—states with partially broken rotational symmetry characterized by the tensor order parameter:

$$Q_{ij}^{\alpha\beta} = \frac{1}{2}\left\langle S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right\rangle - \frac{1}{3}\delta_{\alpha\beta}\left\langle \mathbf{S}_i \cdot \mathbf{S}_j \right\rangle , \qquad (1)$$

where i, j belong to a nearest-neighbor bond. So far such exotic spin-nematic states were considered either phenomenologically [1] or by introducing an *ad hoc* biquadratic exchange [2]. Identification of the relevant microscopic mechanism for the spin-nematic order remains, therefore, a challenging theoretical problem.

Recently, we have explored [3] a novel mechanism for the spin-nematic ordering based on competition between ferro- and antiferromagnetic interactions in quantum magnets. The mechanism operates in strong magnetic field and is based on the formation of bound magnon pairs in the fully polarized state, see illustration in Fig. 1. The high-field magnetization study of the frustrated chain material $LiCuVO_4$ [4] has indeed observed a new phase in the predicted range of magnetic fields. Note, that the phenomenon of magnon pair condensation, discussed in more detail in the following, has a close relationship to the old problem of particle versus pair-superfluidity in an attractive Bose gas [5], which again attracts significant interest in relation to experiments in ultra-cold atomic gases.

Two-magnon bound states. We consider a quantum Heisenberg antiferromagnet in an external magnetic field:

$$\hat{\mathcal{H}} = \frac{1}{2}\sum_{i,\mathbf{r}} J(\mathbf{r})\, \mathbf{S}_i \cdot \mathbf{S}_{i+\mathbf{r}} - H\sum_i S_i^z , \qquad (2)$$

In strong fields the Zeeman energy dominates over the exchange interactions and stabilizes the fully polarized state $|0\rangle$. This state is the vacuum for single spin-flips or magnons with the excitation energy $\varepsilon_{\mathbf{q}} = H + S(J_{\mathbf{q}} - J_0)$, where $J_{\mathbf{q}}$ is the Fourier transform of $J(\mathbf{r})$. In ordinary antiferromagnets spin-flips repel each other. Then, once the band gap in $\varepsilon_{\mathbf{q}}$ vanishes at a certain momentum $\mathbf{Q}$, an antiferromagnet undergoes a phase transition at the critical field $H_{s1} = S(J_0 - J_{\mathbf{Q}})$.

The conventional scenario for a high-field transition may change if some of the exchange bonds are ferromagnetic. In this case two spin-flips sitting on the same bond with $J(\mathbf{r}) < 0$ can lower the Ising part of their interaction energy and may form a bound pair [6–8]. Note, that any gain in the potential energy competes with a kinetic energy loss upon creation of the bound state. Bound states are, therefore, typical for frustrated models, where the single-magnon hopping is significantly suppressed due to the competing exchange interactions.

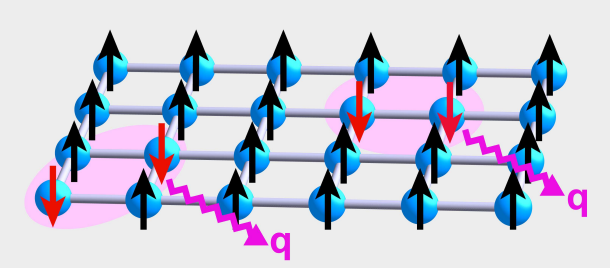

Figure 1: Bound magnon pairs formed in the fully polarized state of a quantum antiferromagnet in strong magnetic fields.

To treat exactly the problem of bound magnon pairs we introduce a general two-magnon state

$$|2\rangle = \frac{1}{2}\sum_{i,j} f_{ij}\, S_i^- S_j^- |0\rangle , \qquad (3)$$

with f_{ij} being the magnon pair wave-function, see also Fig. 1. Separating the center of mass motion $f_{ij} = e^{i\mathbf{k}(\mathbf{r}_i+\mathbf{r}_j)/2} f_{\mathbf{k}}(\mathbf{r})$ we obtain the Bethe-Salpeter equation for bound magnon states:

$$\left(E_B - \varepsilon_{\mathbf{k}/2+\mathbf{q}} - \varepsilon_{\mathbf{k}/2-\mathbf{q}}\right) f_{\mathbf{k}}(\mathbf{q}) = \qquad (4)$$
$$= \frac{1}{2N}\sum_{\mathbf{p}} \left(J_{\mathbf{p}+\mathbf{q}} + J_{\mathbf{p}-\mathbf{q}} - J_{\mathbf{k}/2+\mathbf{q}} - J_{\mathbf{k}/2-\mathbf{q}}\right) f_{\mathbf{k}}(\mathbf{p}),$$

where E_B is the total energy of the pair. If bound states are present ($E_B < 0$), they start to condense at $H_{s2} = H_{s1} + \frac{1}{2}|E_B|$ prior to the onset of the conventional one-magnon condensation, see Fig. 2. Eq. (4) provides a *rigorous condition* for the appearance of the exotic spin-nematic state in the high-field region of a quantum antiferromagnet.

Condensate of magnon pairs. Below H_{s2} the bound magnon pairs form a coherent condensate. Using the Holstein-Primakoff bosons a_i and $a_i^\dagger$ instead of spin operators, the many-body state with a macroscopic number of the lowest-energy pairs below H_{s2} can be expressed as a coherent boson state of the pair creation operator:

$$|\Delta\rangle = e^{-N|\Delta|^2/2} \exp\Big[\frac{1}{2}\,\Delta \sum_{i,j} f_{ij} a_i^\dagger a_j^\dagger\Big]|0\rangle . \qquad (5)$$

Here $f_{ij} = e^{i\mathbf{K}(\mathbf{r}_i+\mathbf{r}_j)/2} f_{\mathbf{K}}(\mathbf{r})$ is the wave-function of the lowest energy pairs and Δ is the complex amplitude of the condensate. The state (5) is a bosonic equivalent of the BCS pairing wave-function for fermions and represents a variational ansatz for the exact ground-state wave-function.

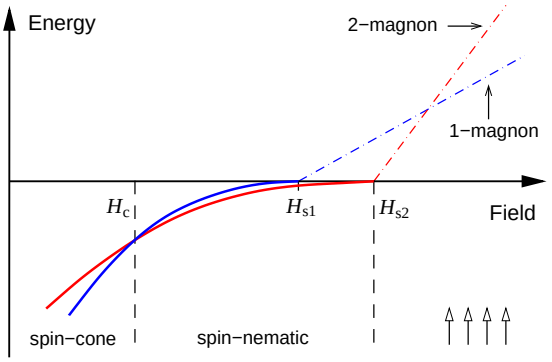

Figure 2: Energy-field diagram for a frustrated quantum magnet close to the saturation field. Dot-dashed lines represent lowest one- and two-magnon states. Solid lines illustrate the field dependence of the ground state energy for the one-magnon and the two-magnon condensate.

In the bosonic language the wave-function (5) has no single-particle condensate, $\langle a_{\mathbf{q}} \rangle = 0$, while superfluidity is present in the two-particle channel:

$$\langle a_{\mathbf{K}/2+\mathbf{q}} a_{\mathbf{K}/2-\mathbf{q}} \rangle = \frac{\Delta f_{\mathbf{K}}(\mathbf{q})}{1 - |\Delta|^2 f^2_{\mathbf{K}}(\mathbf{q})} \,. \qquad (6)$$

The anomalous average (6) is reminiscent of that for a superconductor in the FFLO state. The phase of the order parameter Δ determines the orientation of the nematic-director in the plane perpendicular to the applied magnetic field.

Knowledge of various bosonic correlators allows to compute spin-spin correlators and the ground-state energy. In particular, the transverse spin correlations are expressed as

$$\langle S^-_i S^+_j \rangle \approx |\Delta|^2 \sum_l f^*_{il} f_{lj} \qquad (7)$$

and exhibit an exponential decay with distance. With decreasing magnetic field, the bound magnon pairs overlap more and more appreciably and at a certain point give way to a conventional one-particle condensate, as illustrated in Fig. 2. The corresponding transition field can be calculated explicitly for a given set of exchange parameters. Breaking of a bound pair corresponds to an energy loss $\sim E_B$. Hence, the excitation spectrum observed in the inelastic neutron-scattering experiments remains gapped in the nematic phase. The gapless collective branch related to motion of the nematic director can be observed only in higher-order spin correlators.

Frustrated chain material $\mathbf{LiCuVO_4}$ Let us briefly discuss the probable experimental realization of the spin nematic state in $\mathrm{LiCuVO_4}$. This material consists of planar arrays of spin-1/2 copper chains with a ferromagnetic nearest-neighbor exchange $J_1 = -1.6$ meV and an antiferromagnetic second-neighbor coupling $J_{=}3.8$ meV [9]. The chains are coupled by a weaker exchange $J_3 = -0.4$ meV. For the above set of coupling constants our theory predicts the following values for critical fields: $H_{s1} = 46.2$ T and $H_{s2} = 47$ T. The spin-nematic phases remain stable down to $H_c \approx 44$ T.

The pulsed magnetic field magnetization experiments performed in response to our prediction has indeed observed a new phase in $\mathrm{LiCuVO_4}$ in the field range 40–44 T [4], which is in quite good correspondence with the predicted theoretical values. In addition, there is good quantitative agreement between the slope of the magnetization curve in the nematic phase and the measured value of dM/dH. Thus, $\mathrm{LiCuVO_4}$ provides the first experimental observation of the exotic spin-nematic order in magnetism.

In summary, competing ferro- and antiferromagnetic interactions may lead to formation of bound magnon pairs in quantum magnets. Condensation of magnon pairs leads to formation of a spin nematic state in high magnetic fields. The spin-nematic state is predicted to exist in the chain compound $\mathrm{LiCuVO_4}$ at high fields. Another promising candidate is a frustrated planar material $\mathrm{BaCdVO(PO_4)_2}$, which was recently studied at MPI-CPfS [10].

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2.26 Shortcuts to Adiabaticity in Quantum Systems

J. GONZALO MUGA, E. TORRONTEGUI, A. RUSCHHAUPT, D. GUÉRY-ODELIN

Introduction. An "adiabatic process" in quantum mechanics is a slow change of Hamiltonian parameters that keeps the populations of the instantaneous eigenstates constant. These processes are frequently used to drive or prepare states in a robust and controllable way, and have also been proposed to solve complicated computational problems, but they are, by definition, slow. Our objective is to find "shortcuts to adiabaticity", cutting down the time to arrive at the same final state. We have proposed different ways to achieve this goal for general or specific cases based on Lewis-Riesenfeld invariants and inverse engineering [1].

A different approach to shortcuts to adiabaticity is due to Berry [2]. He has proposed a Hamiltonian $\mathcal{H}(t)$ for which the adiabatic approximation of the state evolution under a time-dependent reference Hamiltonian $H_0(t)$ becomes the exact dynamics with $\mathcal{H}(t)$. This has been applied at least formally to spins in magnetic fields, harmonic oscillators, or to speed up adiabatic state-preparation methods such as Rapid Adiabatic Passage (RAP), Stimulated Rapid Adiabatic Passage (STIRAP) and its variants [3].

Basic theory. A one-dimensional Hamiltonian with an invariant which is quadratic in momentum must have the form $H = p^2/2m + V(q,t)$, with the potential (see [4] for details)

$$V(q,t) = -F(t)q + \frac{m}{2}\omega^2(t)q^2 + \frac{1}{\rho(t)^2}U\left[\frac{q-\alpha(t)}{\rho(t)}\right]. \quad (1)$$

ρ, α, ω, and F are arbitrary functions of time that satisfy two auxiliary equations

$$\ddot{\rho} + \omega^2(t)\rho = \frac{\omega_0^2}{\rho^3}, \quad \ddot{\alpha} + \omega^2(t)\alpha = F(t)/m, \quad (2)$$

with ω_0 constant. The quadratic dynamical invariants, up to a constant factor, are given by

$$\begin{aligned} I &= \frac{1}{2m}[\rho(p - m\dot{\alpha}) - m\dot{\rho}(q-\alpha)]^2 \\ &+ \frac{1}{2}m\omega_0^2\left(\frac{q-\alpha}{\rho}\right)^2 + U\left(\frac{q-\alpha}{\rho}\right). \end{aligned} \quad (3)$$

We may expand any wavefunction $\psi(t)$ in terms of constant coefficients c_n and eigenvectors ψ_n ($n = 0, 1, 2...$) of I multiplied by Lewis-Riesenfeld phase factors $e^{i\alpha_n}$. The basic strategy of invariant-based inverse engineering methods is to design ρ and α first to achieve desired objectives, and deduce the Hamiltonian afterwards. In most applications so far the key point is to control the boundary conditions of the auxiliary functions and their time derivatives at initial and final times. In particular, they may be set so that the eigenvectors of H and I coincide at initial and final times, and the process produces no final excitation. It is however not adiabatic, as excitations are allowed at intermediate times.

Fast expansions. Performing fast expansions of trapped atoms without losses or vibrational excitation is important, for example to reduce velocity dispersion and collisional shifts in spectroscopy and atomic clocks, to reach extremely low temperatures unaccessible by standard cooling techniques or, in experiments with optical lattices, to broaden the atomic cloud before turning on the lattice. Trap contractions are also common to prepare the state. For a harmonic oscillator trap we may consider these expansion or contraction processes by setting $\alpha = U = F = 0$. Once $\rho(t)$ is designed to make $H(t)$ and $I(t)$ commute at the boundary times, with frequencies ω_0 and ω_f, we get $\omega(t)$ from (2). This has been implemented experimentally to decompress ^{87}Rb cold atoms in a harmonic magnetic trap [5]. The extension to Bose-Einstein condensates may be carried out with a variational ansatz and has been realized experimentally too [5]. This poses in principle no fundamental lower limit to the final time t_f, which could be arbitrarily small, but for short enough t_f, $\omega(t)$ may become purely imaginary at some t [1], which corresponds to a parabolic repeller configuration. Also, the energy required may be too high, as analyzed next.

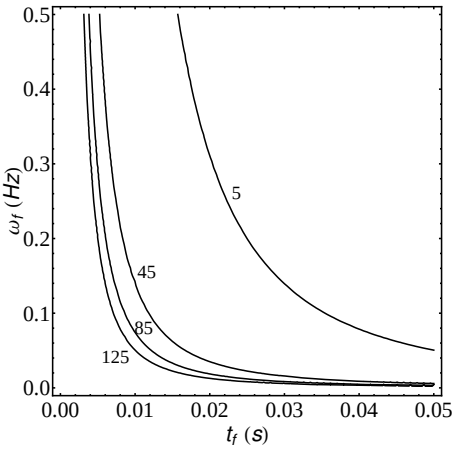

Figure 1: Contour plot of the lower bound for time-averaged energy (in units of $\hbar\omega_0/2$) as a function of t_f and ω_f. $\omega_0 = 2\pi \times 250$ Hz.

Energy cost. One may expect the transient system energy and the time of the process to be "conjugate". Clearly, the energy excitation will set practical limits to the possible speed-up. The transient excitation energy is also important to quantify the principle of unattainability of zero temperature, first enunciated by Nernst. It is usually formulated as the impossibility to reduce the temperature to the absolute zero in a finite number of operations, and identified with the third law of

thermodynamics. Kosloff and coworkers [6] have restated the unattainability principle as the vanishing of the cooling rate in quantum refrigerators when the temperature of the cold bath approaches zero, and quantify it by the scaling law relating cooling rate and cold bath temperature. We have examined the consequences of the transient energy excitation on the unattainability principle for a single, isolated expansion, and considering the expansion as one of the branches of a quantum refrigerator cycle.

A lower bound for the time-averaged energy of the n-th expanding mode $\overline{E_n}$ is found by calculus of variations [7]. When the final frequency ω_f is small enough to satisfy $t_f \ll 1/\sqrt{\omega_0\omega_f}$, and $\omega_0/\omega_f \gg 1$, the lower bound has the asymptotic form $\mathcal{B}_n \approx \frac{(2n+1)\hbar}{2\omega_f t_f^2}$, see Fig. 1. A consequence is $t_f \geq \sqrt{\frac{(2n+1)\hbar}{2\omega_f \overline{E_n}}}$. If $\overline{E_n}$ is limited by some maximal value, because of anharmonicities or a finite trap depth, the scaling is fundamentally the same as for bang-bang methods and leads to a cooling rate $R \propto T_c^{3/2}$ in an inverse quantum Otto cycle (T_c is the temperature of the cold bath), although an opportunity is offered to improve the proportionality factor by increasing the allowed $\overline{E_n}$. This dependence had been previously conjectured to be a universal dependence characterizing the unattainability principle for any cooling cycle by Kosloff and coworkers [6].

For a single expansion, let us assume that the initial and final states are canonical density operators characterized by temperatures T_0 and T_f related by $T_f = (\omega_f/\omega_0)T_0$ for a population-preserving process. For a parabolic potential expansion, we may reformulate the unattainability of a zero temperature as follows: The transient excitation energy becomes infinite for any population-preserving and finite-time process if the final temperature is zero (which requires $\omega_f = 0$). This excitation energy has to be provided by an external device, so there remains a fundamental obstruction to reach $T_f = 0$ in a finite time, in the form of the need for a source of infinite power.

The standard deviation can also be studied [7]. The dominant dependences of the time averages found numerically scale on ω_f and t_f in the same way as the average energy. These dependences differ from the ones in the Anandan-Aharonov (AA) relation [8]. The AA bound, although correct, is not tight.

Fast transport. A key element for controlling the states and dynamics of cold neutral atoms and ions is their efficient transport by moving the confining trap. In spite of the broad span of conditions, heating mechanisms, transport distances (from microns to tens of centimeters), transport times, and accelerations that can be found, there are common elements that allow for a rather generic theoretical treatment as the one presented in [4]. Transport should ideally be fast, lossless, and lead to a final state as close as possible ("faithful") to the initial one, up to global phase factors, in the transporting trap frame.

As done for expansions, we may use the dynamical invariants associated with the Hamiltonian of an atom in a one dimensional moving trap to inverse engineer the trap motion and perform fast atomic transport without final vibrational heating. The atom is driven nonadiabatically through a shortcut to the result of adiabatic, slow trap motion. For harmonic potentials this only requires designing appropriate trap trajectories, whereas perfect transport in anharmonic traps may be achieved by applying an extra field to compensate the forces in the rest frame of the trap. The results can be extended to atom stopping or launching. The limitations due to geometrical constraints, energies and accelerations involved are analyzed in [4], as well as the relation to previous approaches (based on classical trajectories or "fast-forward" and "bang-bang" methods) which can be integrated in the invariant-based framework.

Discussion. Extensions and applications of the above results to treat noise and BECs are in preparation. We also intend to apply these techniques to accelerate Fock state preparation [9], atom diodes (one-way barriers) [10], decay [11], and detection of time-of-flight observables [12, 13].

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2.27 Itinerant Magnetism in Iron Based Superconductors

JOHANNES KNOLLE, ILYA EREMIN, RODERICH MOESSNER

Introduction. The ferropnictide (FP) superconductors have captured the imagination of the condensed matter physics community, not least because of their remarkably high critical temperature of up to $T_c \approx 56$K. Like their brethren, the cuprate high-T_c materials, they are quasi two-dimensional layered materials, and their parent compounds are antiferromagnetically ordered below 150K. Also, upon doping of either electrons or holes into the FeAs layers, magnetism is supressed and superconductivity emerges. It has by now become clear that superconductivity is not mediated by phonons [2].

However, there are important differences to the cuprates. The FPs are always metallic, even in the magnetically ordered phase. Moreover, the order parameter has an unusual extended s-wave ($s^{\pm}$) symmetry.

These facts immediately pose a broader set of questions, beyond "Why is T_c so high?". Firstly and foremostly, what is the minimal model which can account for the magnetic properties, such as nature of the ordering and excitations? Secondly, how can one probe the special features arising from the multiband nature and the unusual order parameter in the FPs? This latter question is in part motivated by measurements of spectroscopic imaging-scanning tunneling microscopy (SI-STM), which claimed the presence of "nematic ordering" in the FPs [3].

Indeed, one of the central attractions of FP physics is the rapid availability of many types of experimental data, and here we therefore focus on two of these: firstly, neutron scattering and secondly, SI-STM.

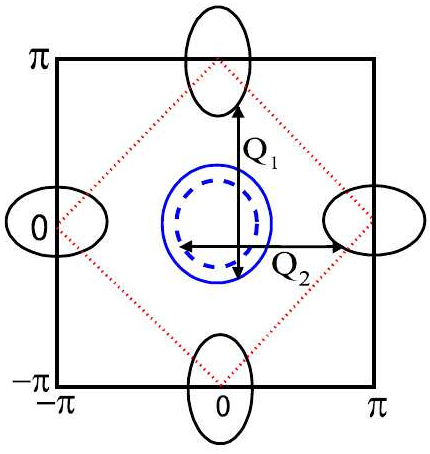

Figure 1: The Fermi surface topology of iron based superconductors for the BZ based on one iron per unit cell. The two nesting vectors $\mathbf{Q_1}$ and $\mathbf{Q_2}$ are shown.

The magnetic structure of FPs is of the $\mathbf{Q_{AF}} = (\pi, 0)$ type with ferromagnetic chains in one direction and antiferromagnetic chains in the other one. The Fermi surface (FS), shown in Fig.1, consists of two hole-like pockets at the center of the Brillouin zone (BZ) and electron-like elliptical pockets at the $(\pm\pi, 0)$ and $(0, \pm\pi)$ points. By looking at the Fermi surface topology we observe that the special nesting wave vector $\mathbf{Q_2}$ corresponds to the magnetic wave vector $\mathbf{Q_{AF}}$. At first sight, both nesting vectors $\mathbf{Q_1}$ and $\mathbf{Q_2}$ are similar under a 90 degree rotation and the following natural question arises: How does the system choose the magnetic odering $\mathbf{Q_{AF}} = \mathbf{Q_2}$ over the other vector $\mathbf{Q_1}$? We have constructed a minimal four band model with input parameters from experiments [4], and in a general Ginzburg-Landau mean-field treatment of the inter- and intraband interactions we showed that the free energy of the system is minimized if only one of the vectors is chosen [5]. Having understood the selection of the magnetic order from our itinerant starting point we have computed different observables to make a connection with available experiments.

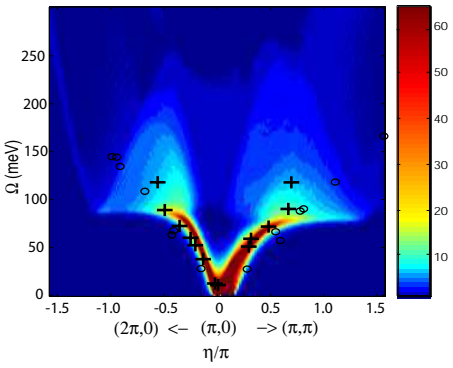

Figure 2: Spin wave dispersion in energy-momentum space together with experimental data. Starting at the ordering wave vector $(\pi, 0)$ the imaginary part of the spin susceptibility is plotted for two perpendicular directions. This shows the anisotropy of the spin wave velocities.

Spin Waves. Due to the broken spin rotational symmetry in the antiferromagnetic phase, Goldstone modes, namely spin waves, appear as low-energy fluctuations transverse to the magnetic ordering. They can be directly probed via inelastic neutron scattering (INS). For FPs, the INS experiments had only been analyzed by models of local moments, which however are not obviously well suited for metallic systems. Therefore, by computing the spin waves via a self-consistent mean-field plus random phase approximation, we provided an alternative explanation of the measurements

from an itinerant perspective [4]. The results are shown in Fig.2 together with experimental data. Beginning at the ordering vector $(\pi, 0)$, the momentum versus energy dispersion of the imaginary part of the spin susceptibility in two perpendicular directions is plotted. The spin wave velocities differ strongly in $\mathbf{q_x}$ and $\mathbf{q_y}$ directions - an experimental fact that had been quite puzzling in the beginning. In our itinerant description, the anisotropy is nicely reproduced and a consequence of the ellipticity of the electron pockets.

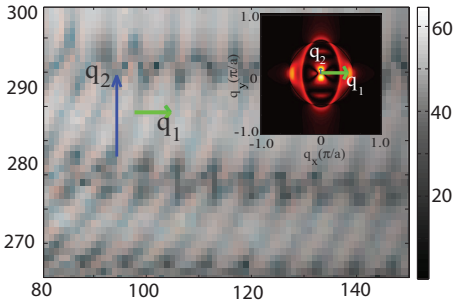

Figure 3: Real space image of our calculated QPI maps with a Fourier transform in the inset. Our T-matrix calculation reproduces the quasi-one-dimensional features observed in SI-STM experiments [3].

Quasiparticle Interference. In recent years SI-STM has become a powerful experimental tool for elucidating the nature of the many-body states in novel superconductors. In the presence of perturbations internal to the sample, such as nonmagnetic or magnetic impurities, elastic scattering mixes two quasiparticle eigenstates with momenta $\mathbf{k_1}$ and $\mathbf{k_2}$ on a contour of constant energy. The resulting quasiparticle interference (QPI) at wavevector $\mathbf{q} = \mathbf{k_2} - \mathbf{k_1}$ reveals a modulation of the local density of states. The phase-sensitive interference pattern in momentum space is what is visualized by means of the SI-STM.

Experiments performed in the magnetic state of FPs revealed quasi one-dimensional features in the tunneling spectra [3] with strongly broken rotational symmetry. Since the magnetic $(\pi, 0)$ state breaks the rotational symmetry, we expected that our itinerant model should be able to account for the SI-STM measurements. Therefore, we introduced an impurity term in our four band hamiltonian,

$$H_{imp} = \sum_{\mathbf{k}\mathbf{k}' ii' \sigma\sigma'} \left(V^{ii'}_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} + J^{ii'}_{\sigma\sigma'} \mathbf{S} \cdot \sigma_{\sigma\sigma'} \right) c^{\dagger}_{i\mathbf{k}\sigma} c_{i'\mathbf{k}'\sigma'}. \tag{1}$$

and performed a T-matrix calculation of the local density of states [6]. The result is displayed in Fig.3. A real space map of the QPI from the impurity is shown together with the Fourier transformed quantity as an inset. Our itinerant model reproduces the quasi one-dimensional features which are visible as stripe like patterns in real space.

Probing the symmetry of the superconducting order parameter requires phase sensitive measurements such as QPI. The conjectured $s^{\pm}$ symmetry of FPs is especially difficult because it does not have nodes and only changes sign between the FS pockets at the BZ center and the pockets at the boundaries. Recent experiments [7] have reported the results of SI-STM measurements in the superconducting phase. They interpreted the different scattering behaviour of various wave vectors for magnetic and non-magnetc impurities as a proof of the $s^{\pm}$ symmetry. In an additional study [8] we extended our QPI calculations to the superconducting phase and confirmed their interpretation. Furthermore, we looked at the effect of possible gap minima and studied the QPI signatures of a coexistence phase in which the itinerant electrons are antiferromagnetically ordered and simultaneously superconducting.

In summary we have developed an itinerant description of the newly discovered iron based superconductors. Within our model we have calculated spin waves as measured in inelastic neutron scattering experiments, as well as quasiparticle interference signatures that are believed to appear in SI-STM measurements. The agreement of our theoretical treatment and the available experiments leads to the conclusion that basic physical properties of these new high-T_c materials can be understood from an itinerant point of view. In the future we like to investigate to what extent stronger correlation effects and orbital degrees of freedom become important.

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2.28 Kinetochores are Captured by Microtubules Performing Random Angular Movement

IANA KALININA, AMITABHA NANDI, ALEXANDER KRULL, BENJAMIN LINDNER, NENAD PAVIN, IVA M.TOLIĆ-NØRRELYKKE

In living cells, proper segregation of genetic material between the two daughter cells requires all chromosomes to be connected to the spindle microtubules (MTs). Linkers between chromosomes and MTs are kinetochores (KCs), protein complexes on the chromosome. In fission yeast, KCs are at the spindle pole body (SPB), which facilitates their interaction with MTs that grow from the SPB. If the spindle is disassembled, it is able to recover including capturing KCs that have been lost in the nucleoplasm. It is, however, unknown how MTs find lost KCs. We found that lost KCs can be captured by MTs performing random angular movement. By using live cell imaging, we observed that astral MTs pivot around the SPB, in cell with and without lost KCs. By studying the relationship between the MT angular movement and MT length, we found that this movement is most likely driven by thermal fluctuations. In addition, we found that KCs and astral MTs by performing random movement explore a comparable fraction of space. Finally, by introducing a theoretical model, we show that the process of KC capture can be explained by the observed random movement of astral MTs and of the KC.

A pioneering idea that could explain how MTs find KCs is based on MT dynamics [1]. In this search-and-capture scenario, the MTs are assumed to grow in random directions from the centrosomes. If a MT does not interact with a KC, it will undergo catastrophe and shrink back to the centrosome. New MTs are nucleated, each of them having a chance to reach a KC. At some point, a lucky MT will capture a KC and became stabilized by this interaction. Eventually, all KCs will get captured. This mechanism, however, relies on a large number of MTs and their high dynamicity. We hypothesize that a so-far unknown mechanism may exist to increase the efficiency of KC capture.

To study how MTs search for KCs we use fission yeast, where we can follow the dynamics of each astral MT during its lifetime, due to a small number of MTs. At the onset of mitosis in fission yeast, KCs are close to the duplicated spindle pole body (SPB). The SPBs nucleate MTs that form a spindle and attach to KCs (Fig. 1). To detach KCs from MTs, we use the lost kinetochore assay, where MTs are disassembled by exposing the cells in early mitosis to cold stress [2]. This type of stress most likely also occurs in nature. After MT disassembly, a large fraction of KCs are lost in the nucleoplasm, while the remaining KCs are at the SPB. Once the stress is relieved, MTs regrow from the SPB. The MTs that grow in the direction of the other SPB contact the MTs growing from that SPB, thereby reassembling the spindle (spindle MTs), while several other MTs grow in other directions (astral MTs). Astral MTs capture lost KCs, retrieve it to the SPB, and mitosis progresses regularly [2] (Fig. 1).

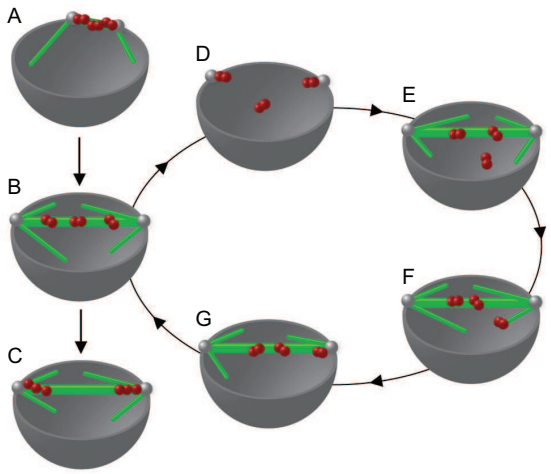

Figure 1: Mitosis in fission yeast. (A) At the onset of mitosis, the spindle pole bodies (small grey spheres) nucleate microtubules (green) that form a spindle and attach to kinetochores (red). (B) In metaphase, kinetochores oscillate on the spindle. (C) In anaphase A, sister kinetochores separate from each other and move to opposite spindle poles. (D) If microtubules depolymerize during prometaphase, kinetochores may get lost in the nucleoplasm. (E) When microtubules re-polymerize, spindle re-forms. (F) An astral microtubule captures the lost kinetochore. (G) The captured kinetochore is retrieved to the spindle pole body, and (B) subsequently moves on the spindle. Thus, a normal metaphase is established again.

We imaged cells with KCs labeled in red and MTs in green and found that after 1 hour of cold treatment (4°C), MTs were absent and 60% of cells in metaphase had one or more lost KCs. When the cells were rewarmed to 25°C, the number of cells with lost KCs was halved within 4 minutes. Live cell imaging revealed that astral MTs, which are straight, change their orientation with respect to the cell and to the spindle, where one end of the MT is attached to the SPB and the other end moves in the nucleoplasm (Fig. 2). This pivoting of the MTs around the SPB changes the distance between the MTs and the lost KC. The distance between one of the MTs and the lost KC eventually diminishes and this MT captures the lost KC (Fig. 2). The attachment of the KC is typically close to the MT tip but attachment away from the tip was also observed. These findings suggest that pivoting of astral MTs may play a crucial role in finding lost KCs.

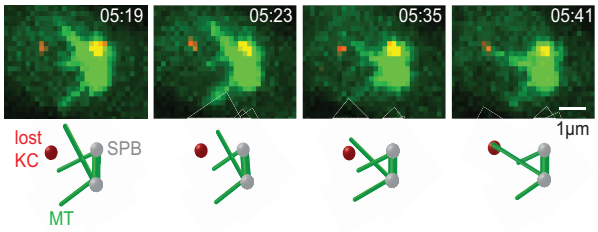

Figure 2: Astral microtubules pivot around the spindle pole body. Time-lapse images of a cell in mitosis, in which kinetochores were labeled in red (Ndc80-tdTomato) and microtubules in green (α-tubulin-GFP). The cell was kept at 4°C to depolymerize microtubules. Subsequently, the temperature was increased to 25°C, in order to allow for microtubule re-polymerization. The time after the temperature increase is shown in minutes and seconds. The schemes below the images show the position of the kinetochore (red), microtubules (green), and spindle pole bodies (grey). Kinetochore capture occurs at the last frame. Note that the microtubule that captured the kinetochore changed its angle with respect to the spindle.

To reveal the mechanism of KC capture, we first quantified the pivoting of astral MTs as a time series of the angle between the astral MT and the horizontal axis of the image. To distinguish whether this movement is directed or random, we calculated the mean squared angular displacement, and found that it scales with time to the power of ~0.8. The exponent smaller than one suggests that the angular movement is random, and in particular subdiffusive. In addition to the movement of astral MTs, we observed movement of lost KCs, which was also subdiffusive [3]. Taken together, our results indicate that the movement of the lost KC, as well as of the astral MTs, plays an important role for KC capture.

In order to test whether the process of KC capture could be driven by the observed random movement of astral MTs and the KC, we introduce a simple three-dimensional model consisting of an SPB, a MT, and a KC. We use a spherical coordinate system, by placing the origin at the SPB, which is assumed to be stationary. The orientation of the coordinate system is fixed with respect to the cell. One end of the MT is at the origin, while the orientation of the MT is described by the inclination angle θ and the azimuth angle φ. The KC is placed at an arbitrary position (θ_k, φ_k), and its size is described by the parameter δ. Therefore, KC capture occurs when the MT and the KC overlap in the angular space, i.e., $|\theta - \theta_k| < \delta/2$ and $|\varphi - \varphi_k| < \delta/(2sin\theta_k)$. This description implies that the distance between the KC and the SPB is smaller than the length of the MT, as well as that the KC can bind along the length of the MT. The angular diffusion of the MT is described by the following stochastic differential equations

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = D\frac{cos\theta}{sin\theta} + \sqrt{2D}\xi_\theta \quad (1)$$

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \frac{\sqrt{2D}}{sin\theta}\xi_\varphi \quad (2)$$

Here, D is the angular diffusion coefficient of the MT of a length L, and ξ_θ, ξ_φ is a Gaussian white noise obeying $\langle \xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t'),\ i,j = \theta,\varphi$. In the model, we use the reflecting boundary conditions $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq \pi$. We keep the KC fixed, while its diffusion is described by including it in the diffusion coefficient D of the MT.

We numerically solved Eqs. (1) and (2) for a set of random initial positions of the MT and calculated the time it takes a MT to reach the KC for the first time. The number of lost KCs decreases exponentially with time, and for a typical values of free parameters $\delta = 0.2\ rad$ and $D = 0.005\ rad^2/s$, half of the lost KCs are captured in 5 minutes (Fig. 3). The agreement between the capture time obtained by the model and by the experiment shows that the kinetics of KC capture can be explained by random movement of astral MTs and of the KC.

We found that thermal fluctuations drive angular movement of MTs, as well as the movement of the KC. We propose this movement of MTs as a search strategy by which MTs explore space in order to find a KC. This mechanism allows for KC capture with only a few astral MTs.

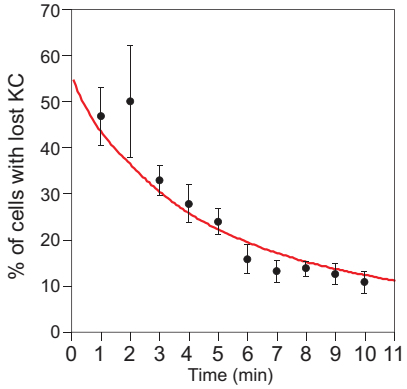

Figure 3: Results from the model: The kinetics of kinetochore capture can be explained by random movement of astral microtubules and of the kinetochore. The fraction of cells with lost kinetochores is shown as a function of time elapsed since the temperature was increased from 4°C to 25°C. Circles represent the experimental data and the line shows the result from the model.

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Chapter 3

Details and Data

3.1 PhD Program

The training of PhD students is one of the central educative tasks of the mpi**pks**. It is realized through a large institute PhD program, our leading role in the IMPRS *Dynamical Processes in Atoms, Molecules and Solids* (see next section) and our participation in the IMPRS *Molecular Cell Biology and Bioengineering* which is coordinated by the Max Planck Institute for Cell Biology and Genetics.

Prospective PhD students have several options of contacting scientific advisors at mpi**pks**. PhD positions funded through external grants are advertised in scientific journals and on the internet pages of the institute. Additionally there is a permanent advertisement of PhD positions funded through the Visitors Program on the internet pages of the institute and in several information booklets. Finally, a significant part of PhD students is recruited through personal contacts with potential scientific advisors at mpi**pks**. Since the start of operation of the International Max Planck Research School the number of PhD students substantially increased.

The recruitment strategy is well documented in previous scientific reports of mpi**pks**. In 2009 we had a total of 78 PhD students at mpi**pks**, including 51 students from abroad (these numbers count all students, also those who finished their PhD studies or started their studies during that year). The respective numbers for 2010 were a total of 97 PhD students at mpi**pks**, including 66 students from abroad. We counted 6 successful final PhD exams for the year 2009 and 9 exams for the year 2010.

Besides their scientific work at mpi**pks** our PhD students use several further types of activities to strengthen their academic and communicative skills. In addition to lecture courses offered at the TU Dresden the mpi**pks** provides lecture courses on modern topics of theoretical physics on a regular basis. PhD students can join workshop talks and seminar lectures of the Workshop and Seminar Program of mpi**pks**. Many of them participate actively in these events by presenting short talks or posters. Our institute organizes annual PhD Student Days (1-2 days). All students of mpi**pks** participate in this meeting and present short talks on their current research results. A PhD student exchange program with East European countries such as Poland or the Czech Republic, supported by the Max Planck Society, allows our students to visit cooperating research groups and to present talks, as well as to coach visiting PhD students from those groups at mpi**pks**. The mpi**pks** offers financial and logistic support for joining German language courses for our PhD students from abroad in order to help with integration into the German speaking community.

A growing number of PhD students passes the final PhD exams at the TU Dresden. Still, some students obtain the PhD degree from various universities throughout Germany. After the PhD degree most of our students continue their research work by accepting postdoc positions at research institutions in various countries. A significant part is also successfully applying for positions in companies in such areas as applied research, computer science, finance and consulting. The mpi**pks** organizes regular alumni meetings of former PhD students with discussion rounds to provide a transfer of experience for our present PhD students.

3.2 International Max Planck Research School

The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* (hereafter referred to as IMPRS) has completed its first full funding period of six years from January 2005 to December 2010. In 2008 it was evaluated by an evaluation committee appointed by the Max Planck Society. Based on the very positive report from the committee we have applied for a second funding period, which was approved by the Max Planck Society in January 2011. Starting with the second funding period the research focus will be shifted to maintain a pioneering role in the changing scientific landscape of Dresden, for details see page 100.

The IMPRS is a collaboration of the following institutions

- Technische Universität Dresden — TUD
- Forschungszentrum Dresden-Rossendorf — FZD
- Leibniz Institute for Solid State and Materials Research — IFW
- Max Planck Institute for Chemical Physics of Solids — MPI-CPfS
- Max Planck Institute for the Physics of Complex Systems
- Institute of Low Temperature and Structure Research — ILTSR (Polish Academy of Science Wrocław/Poland)
- Institute of Organic Chemistry and Biochemistry — IOCB (Prague/Czech Republic)
- Institute of Chemical Technology — ICT (Prague/Czech Republic)

PhD students

The IMPRS has admitted so far 94 PhD students, 38 of which have obtained their doctoral degree by the end of 2010. While about 40 % of the students are Germans, the other 60 % come from all over the world. The predominant countries of origin are China (7 students), Czech Republic (7), Poland (6), Ukraine (4), and India (4). The affiliation to the participating partners is as follows, TUD: 19, FZD: 1, IFW: 6, MPI-CPfS: 3, mpi**pks**: 14, ILTSR: 2, IOCB & ICT: 6. The Polish students are enrolled in Wrocław universities and are financed by grants of the Klaus-Tschira foundation. The Czech are members of Czech Academy of Sciences and are financially supported by the IMPRS.

Scientific events

After the official opening ceremony in September 2005 we started a series of annual IMPRS retreats held in autumn at different locations in the Sächsiche Schweiz (see picture). In these meetings the PhD students present their work in extended talks to provoke discussions among all students including those working in different fields. Furthermore, contact with new students of the IMPRS is initiated.

In order to closely integrate our Polish and Czech branches we organized joint block seminars. These were devoted to special scientific subjects presented by our Polish and Czech partners. The first one of this series was organized by our Polish partners in May 2006 in Wrocław and dealt with Modern Aspects of Superconductivity. The second one took place in the Czech Academy of Sciences in Prague in November 2008 and focused on Biomolecules: Physical Principles and Mechanisms. Both seminars were open to local students.

Seminar and lecture program

One of the regular meeting points for all students is the monthly IMPRS seminar. Each seminar starts with a talk given by an IMPRS student, followed by an invited talk given by an external speaker. The external speakers are proposed by supervisors and students from the participating research groups and thus cover the broad scientific spectrum of the IMPRS.

The lecture program follows the schedule of the Technische Universität Dresden with winter (October – February) and summer (April – July) terms. The lectures are given by professors from the university and

IMPRS meeting in Bad Schandau (Sächsiche Schweiz) in April 2009.

young researchers from the various partner institutions including the mpi**pks**. We offer approximately four lectures per term. They are open to students from the Technische Universität Dresden. Participation of the IMPRS students in the lectures is monitored by a credit-point system.

Organization and administrative matters

The school is operated by the IMPRS board with the following members:

Prof. Jan-Michael Rost (chairman, mpi**pks**)
Prof. Roland Ketzmerick (TUD)
Prof. Gotthard Seifert (TUD)
Prof. Yuri Grin (MPI-CPfS)
Prof. Bernd Büchner (IFW)
Prof. Pavel Jungwirth (IOCB Prague)
Prof. Jozef Sznajd (ILTSR Wrocław)
Dr. Ulf Saalmann (coordinator, mpi**pks**)

There are two board meetings a year, in which the board discusses and decides all matters regarding the operation of the IMPRS. This includes the admission of new students, the distribution of the IMPRS resources (in particular grants), the seminar and lecture program, organization of summer/winter schools or other IMPRS meetings.

The executive board, consisting of Prof. Rost, Prof. Büchner and Dr. Saalmann, meets upon demand. In particular it pre-screens the numerous applications. The daily coordination, i. e. contact to students, application and admission procedure, advertisements, organization of the lectures and seminar program and maintenance of the web-page is handled at the mpi**pks**.

Application for second funding period and future development

Over the last 5 years the scientific landscape in Dresden has undergone significant development, not the least thanks to the IMPRS regarding PhD training. In fact, we have had numerous requests from colleagues to join our IMPRS. Partially, we have accommodated these requests but refrained from a major extension of our IMPRS, since we strongly believe that in order to maintain the benefit of an IMPRS, its students should have a chance to know each other which limits in our experience the size of the school to about 50–70 PhD student members.

These developments allow us to focus the research of the IMPRS on "Modelling in the natural sciences — from algorithms to applications" by including new colleagues who have recently been appointed in Dresden. At the same time we increase significantly the number of participating departments from the TU Dresden, by engineering, math and computer science. The concentration on theoretical research has been planned in coordination with our experimental colleagues from IFW who will apply for a mainly

experimental PhD school. This new PhD school and our IMPRS will closely collaborate with a harmonized lectures program in the areas of common interest and by mutual recognition of lectures to collect credit points.

The unifying scheme is theoretical treatment and in most cases modelling processes in nature. For this reason the emphasis of the IMPRS on modelling is not only very suitable for the Dresden research area as detailed before, but also for mpi**pks**. Moreover, the international character of the IMPRS (with about half the students from abroad and half from Germany) finds its ideal counterpart at mpi**pks** with its larger visitors program (exchange of people, workshop program).

Dresden is close to the Polish and Czech borders. Therefore, it was one of the hopes of the founding committee of the mpi**pks** that it would establish close ties in particular to the universities of Wrocław and Prague. With the IMPRS these ties have been established, put on a formal basis and filled with scientific life, in the mean time tremendously facilitated through the EC membership of Poland and the Czech Republic

3.3 Workshop and Visitors Program

The Visitors Program of mpi**pks** hosts guest scientists for a period of usually up to two years. Excellent working conditions are offered to qualified, mostly young, scientists. This also includes logistic help, e.g., for finding suitable accommodation, solving visa problems, etc. The close collaboration with administrative units responsible for example for the computational and technical equipment of the offices, allows the guest scientists to fully concentrate their efforts on research. Informal Tea Seminars, a weekly *Young Scientists Jam Session* and financial support for joining German language courses help to integrate guest scientists fast and easily into the local community. Many guest scientists participate actively in the Workshop and Seminar Program of mpi**pks**.

International Workshop "Exploring Complex Dynamics in High-Dimensional Chaotic Systems: From Weather Forecasting to Oceanic Flows", January 25 - 29, 2010

During 2009 the mpi**pks** hosted 201 guest scientists with contracts for at least three months, and 212 during the year 2010, including predocs. We enjoyed a large number of senior scientists who used their sabbatical time for long-term research stays at mpi**pks**. This led to an enhancement of transfer of experience to young scientists at the institute.

In 2007 the institute launched its first *Advanced Study Group*. These groups consist of 3-5 experienced researchers, who join forces for up to one year to do cutting-edge research on a topic from the field of

the physics of complex systems. In 2009 we hosted one *Advanced Study Group*, and in 2010 we enjoyed large scale activities of two *Advanced Study Groups*.

The guest scientists are usually linked to the research groups at mpi**pks**. In some cases they conduct more independent research, which leads to synergetic effects, including recent temporary collaborations at the institute on *ultracold atoms*. Synergetic effects are further enhanced due to the opportunity to listen to talks and lectures within the Seminar and Workshop Program of mpi**pks** (see p. 112).

In addition to the regular positions of the Visitors Program the institute annually offers a Distinguished PKS Postdoctoral Position for experienced postdoctoral scientists for up to three years. PKS Fellows do research in areas related to but not directly covered by the work done in the mpi**pks** research groups. Three PKS Fellows are currently working at mpi**pks**: *Dr. Emil Bergholtz* on *Correlated quantum matter*, *Dr. Achilleas Lazarides* on *Collective phenomena*, and *Dr. Chiu Fan Lee* on *Physical properties and pathogenesis of protein aggregation*, see report on p. 102. Two PKS fellows have left the institute: *Dr. Vitali Averbukh* (*Interatomic Decay Processes*) took a faculty position at the Imperial College in London, and *Dr. Balasz Dora* (*Magnetic Impurities in d-Density Waves*) moved to a staff position at the University of Technology in Budapest. Another former PKS fellow *Dr. Masudul Haque* (*Quantum Many-Body Phenomena in Condensed Matter*) moved to a staff position with the *Condensed Matter Department* at mpi**pks**.

Together with the TU Braunschweig the institute supported a junior professorship (*Prof. Ilya Eremin*, see report on p. 107). *Prof. Eremin* was teaching at the TU Braunschweig, and conducting research at mpi**pks**. In the meantime he has accepted and moved to a faculty position with the Ruhr-Universität Bochum.

To strengthen the transfer of knowledge and experience at mpi**pks**, the institute annually awards the Martin Gutzwiller Fellowship to a senior scientist who made exceptional contributions in the area of the physics of complex systems. Gutzwiller Fellows spend up to one year at mpi**pks** and can nominate a young guest scientist for the Visitors Program. The 2009 and 2010 fellows were *Prof. S. Aubry* and *Prof. Y. Kevrekidis* (see report on p. 108).

A considerable number of guest scientists leave the institute for permanent positions in the academic sector, besides many others who continue with postdoctoral positions at other institutions in Germany or abroad. Several guest scientists leave for positions in the non-academic sector, such as applied research, informatics, finance, or consulting.

In addition to the long-term guest scientist positions the Visitors Program also hosts many short-term visits (for up to three months). These visits are usually due to collaborations of the research groups at mpi**pks** with other institutes. Their number reached higher levels again, 314 during the year 2009 and 328 during the year 2010.

3.3.1 PKS-Fellowship

Inner-shell ionization of polyatomic systems
(Dr. Vitali Averbukh)

Based on accurate quantum chemical methods we study the effect of a (multiply) charged environment on the decay of inner-shell vacancies in polyatomic systems [1–3]. This kind of dynamics takes place under illumination of matter with short intense X-ray pulses as available from Free Electron Laser Sources, such as FLASH and LCLS in Hamburg and Stanford, respectively. Electronic decay is a major doorway for radiation damage which needs to be quantified and understood for advanced use of FEL-radiation.

The advent of powerful free-electron lasers (FELs) operating in the UV and X-ray domains [4] takes the study of radiation-matter interaction to a new dynamical regime of both, high photon energies and high photon fluxes. When incident on atoms, molecules or clusters, the strong fluxes of high-energy FEL photons lead to multiple inner-shell ionization (see, e.g. Ref. [5]). The ensuing electronic decay of the formed inner-shell vacancies is a major contributor to radiation damage occurring through positive charge accumulation and eventually to disintegration of the target systems by Coulomb explosion. We describe first our quantum based approach to characterize such phenomena and present results for three different scenarios.

The Fano-ADC formulation for doubly ionized states Using the algebraic diagrammatic construction (ADC) ab initio technique of the group around L. Cederbaum (Heidelberg), we have generalized our Fano-ADC computational method [6] to decay of doubly ionized states [9] in collaboration with P. Kolorenč (Prague) and the Heidelberg group. The new method has been applied to a cascade Auger-ICD process [7, 8] in heteronuclear diatoms (NeAr, MgNe). Knowledge of the decay widths of the doubly ionized states resulting from Ne $1s$ Auger decay in these systems is essential for the quantitative prediction of the kinetic energy spectra of the ICD electrons emitted on the second stage of the cascade [9].

The Fano-ADC approach as formulated in [6] is not applicable to systems in which the decaying excitation is delocalized due to inversion (or higher-order) symmetry as is the case for the physical situation considered below. For these situations we have formulated an extension of the Fano-ADC scheme [1], for a review of the recent advances in the development of Fano-ADC, see the review [10].

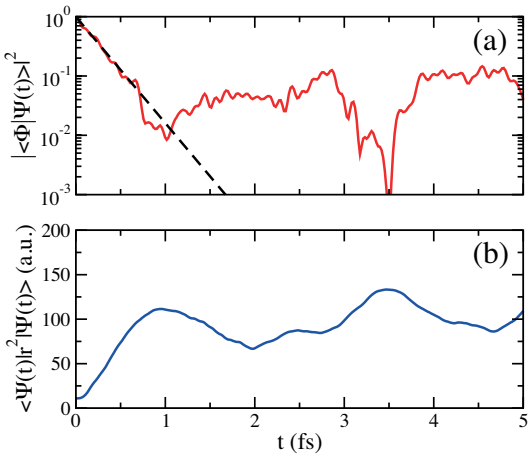

Figure 1: (a) Survival probability of the $2s$ vacancy in $Ar^+(H^+)_{12}$ (solid) and in an isolated Ar^+ (dashed). (b) Time dependence of the r^2 expectation value measuring the spatial extension of the $Ar^+(H^+)_{12}$ electronic wave function.

As mentioned above, the availability of the high-power FEL sources calls for a thorough investigation of electronic decay in multiply charged systems. Indeed, any given inner-shell vacancy created by the FEL radiation can interact with the neighboring vacancies which are abundant due to the high photon fluxes. These neighboring vacancies can participate in a collective electronic transition or, probably more frequently, are spectators that affect the decay process without undergoing a transition themselves. These scenarios are discussed below.

Collective inter-atomic decay of inner-shell vacancies in doubly charged clusters we have identified as a new inter-atomic decay process, cICD [2]. Two inner-shell vacancies in two different atoms or molecules can be filled simultaneously, while a neighboring neutral species is ionized. cICD can be regarded as a transfer of two or more virtual photons from the ionized cluster units to a neutral one. Using our Fano-ADC theory for doubly ionized states, we have determined the decay rate of two Kr $4s$ vacancies in Kr_2Ar for a variety of cluster geometries as an example. The virtual two-photon transition is orders of magnitude faster than the radiative decay of $(4s^{-1})$ Kr^+ and the collective decay can compete successfully with the dissociative nuclear dynamics of the doubly ionized system [2].

Atomic Auger decay in the field of a positive charge The simplest possible model for the study of the effect of a neighboring charge on an Auger transition is that of the atom (or molecule) bearing a core vacancy in the field of a point charge. We have studied the decay widths of a series of atomic Auger transitions as functions of atom-proton distance, namely $(2s^{-1})$ Mg^+ Coster-Kronig decay as well as $(2p^{-1})$ Mg^+ and $(2p^{-1})$ Ar^+ Auger decay. In all cases, we have found an appreciable effect of the proton on the decay width, ranging from about 20% in the cases of $(2s^{-1})$ Mg^+ and $(2p^{-1})$ Ar^+ to more than an order of magnitude in the case of $(2p^{-1})$ Mg^+ [11]. We interprete this effect in terms of the distortion of a valence orbital by the strong electric field of the point charge. When a single decay channel dominates the Auger transition, a more detailed understanding can be gained via multipole expansion analysis of the corresponding Auger matrix element. Calculations of the sizes and the dipole moments of the valence orbitals as functions of the atom-proton distance have shown that, just as the appreciable changes in the decay widths, such distortions occur at the "chemical" distances of about $1-2$Å, while at distances typical of van der Waals clusters (~ 3Å), the neighboring charge effect can be neglected. These findings are relevant for the simulation of cluster and molecular disintegration in an XFEL beam. Such simulations usually approximate the rates of Auger transitions in multiply ionized polyatomic systems by the Auger rates of isolated atoms. Our work shows that this assumption is justified for rare gas clusters but very questionable for molecules which has consequences for the validity of results on radiation damage of molecules in the XFEL field [12].

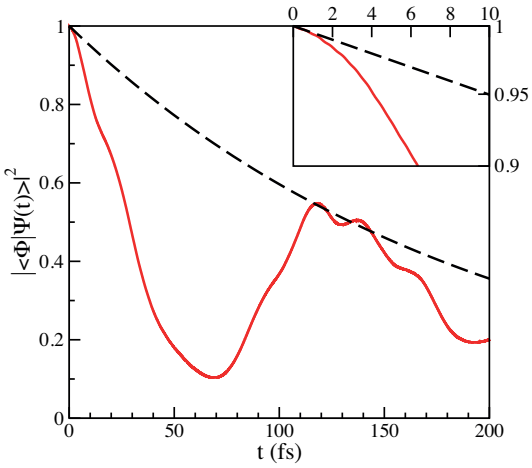

Figure 2: Survival probability of a $2s$ vacancy in Ne_5H^+ (solid line) - the exponential decay is shown with a dashed line. The inset (logarithmic scale) shows the deviation from the exponential decay at short times. Note, that for times beyond that of the inset the beginning motion of the nuclei will change the present results which is based on static nuclei.

Electronic decay in charged environment While the presence of a single charge can modify the rate of the exponential decay of a core-ionized state, a multiple positive environment can dramatically change the decay and even lead to an oscillatory behavior [3].

This is due to the fact that the Auger electron is not ejected into a true continuum, but rather into a manifold of shake-up bound states. As a consequence, the outgoing electron wave is eventually reflected from the effective potential boundary. A similar problem was encountered by Bixon and Jortner in the context of non-radiative decay [13] and solved there for a model problem. We have developed an ADC-based time-dependent first-principles approach that is able to predict the true dynamics of electronic decay in a given highly ionized system. For Coster-Kronig decay of $(2s^{-1})$ Ar^+ Ar in multiply ionized Ar_{13} cluster, we find a roughly exponential decay in the beginning which is eventually suppressed by the oscillatory wave-packet dynamics at later times, see Fig. 1. For the much slower exponential ICD in a doubly ionized Ne_6 cluster, we find a sub-exponential decay in the charged environment (Fig. 2).

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The physics of protein aggregation phenomena

(Dr. Chiu Fan Lee)

The physics of protein aggregation phenomena My current main research interests concern the phenomena of protein aggregation, and their relations to human pathology and developmental biology. Specifically, I am investigating the aggregation phenomena of (i) protein amyloids, which are linear self-assembled structure of proteins that are intimately related to a great variety of human diseases such as the Alzheimer's disease and type II diabetes, and (ii) P granules, which are germ cell granules in the one-cell embryo of the round worm *C. elegans*. These granules are instrumental to the proper development of the gametes of the organism.

Collaborations at the mpipks With professor Frank Jülicher and his graduate student Jöbin Gharakhani, I am employing the theory of phase separation in physics to understand how P granules are assembled upon the fertilization of the embryo. Specifically, we recently found that by combining a simple mean-field free-energy based model and the classic Lifshitz-Slyozov droplet growth model, we are capable of explaining all of the salient aspects observed in the protein aggregation process. With a range of experimental techniques that include fluorescence correlation spectroscopy, confocal imaging and three-dimensional particle tracking, we are now attempting to quantitatively verify the model. To achieve this task, a number of outstanding theoretical issues have to be addressed. For instance, to describe the dynamics of the aggregation phenomenon, one will need to generalize the Lifshitz-Slyozov model substantially to allow for simultaneous dissolution and condensation events in different parts of the cell. These challenges are of interest to physicists as well as biologists. Our research is also relevant to other self-assembled structures observed in cells such as the P bodies, Cajal bodies, and stress granules. It is therefore our ultimate goal to establish a quantitative theory that can explain collectively these diverse intracellular assembly processes.

Besides my main focus on protein aggregation phenomena, I am also interested in applying far from equilibrium techniques in physics to study biological systems. This approach is important because most biological processes happen in the far from equilibrium regime. Various methods are available to investigate these nonequilibrium processes. For instance, Kramers escape theory is suitable for the analysis of the rate of a certain rare event in a fluctuating system. Using this theory, I have investigated the rate of uncontrolled cell proliferation in relation to skin cancer [1]. Another approach to study nonequilibrium systems is with the use of the Fokker-Planck equation. Based on this formalism, I have employed both naive [2] and renormalization group improved [5] perturbative methods to study the phenomenon of collective motion in self-propelled particles. Furthermore, with Dr. Fernando Peruani, I have recently initiated a study of collective motion in self-propelled particles on a lattice from a field-theoretic perspective.

External collaborations For the project on the investigation of P granules formation, my external collaborators include

- The Hyman group at the Max Planck Institute of Molecular Cell Biology and Genetics.
- Professor Clifford Brangwynne at the Department of Chemical and Biological Engineering, Princeton University.
- Dr. Zdenek Petrášek at the Biotechnology Center (BIOTEC) of the Technische Universität Dresden.

For the protein amyloid project, I am collaborating with the Vaux group at the Dunn School of Pathology, University of Oxford.

External presentations

Invited talks:

- C.F. Lee. "The physics of protein amyloid formation." Department of Physics and Astronomy, University of Edinburgh, August 2010.
- C.F. Lee. "Protein aggregation phenomena." Department of Physiology, McGill University, November 2010.

Contributed talks:

- C.F. Lee. "Protein amyloid self-assembly." Pierre-Gilles de Gennes Winter School 2010 – FEBS Advanced Lecture Course on Cytoskeleton, Contractility and Motility, February 2010
- C.F. Lee. "Protein amyloid formation: a theoretical physicists view." DPG Spring Meeting, March 2010
- C.F. Lee, C.P. Brangwynne, Z. Petrášek, J. Gharakhani, A.A. Hyman, and F. Jülicher. "Spatial organization of the cell cytoplasm: Protein gradients and liquid-liquid phase separation in the C. elegans embryo." DPG Spring meeting, March 2011.

- C.F. Lee, L. Jean, C. Lee, M. Shaw, and D.J. Vaux. "Interfacial effects on amyloid fibrilization." DPG Spring meeting, March 2011.

- C.F. Lee. "Perturbation analysis of a reduced model for collective motion: Effects of the initial condition." DPG Spring meeting, March 2011.

Articles completed and written at the mpipks

1. C.F. Lee (2010) Predicting rare events in chemical reactions: Application to skin cell proliferation. Physical Review E 82, 021103; E-print: arXiv:1005.4116.

2. C.F. Lee (2010) Fluctuation-induced collective motion: A single-particle density analysis. Physical Review E 81, 031125; E-print: arXiv:1001.2684.

3. C.F. Lee (2011) Singular perturbation analysis of a reduced model for collective motion: A renormalization group approach. Accepted in Physical Review E; E-print: arXiv:1102.0407.

4. L. Jean*, C.F. Lee* and D.J. Vaux [* = Joint first authors]. At equilibrium, hydrophobic-hydrophilic interfaces determine the thermodynamic properties of amyloid formation. Submitted.

5. C.F. Lee. Length distribution of self-assembled stiff and flexible polymers. Submitted.

Correlated Quantum Matter
(Dr. Emil Bergholtz)

I work on strongly correlated quantum matter using various analytical as well as numerical approaches. During my time at **mpipks**, I have so far published on three different topics; 1) Quantum information in condensed matter, in particular various entanglement measures as diagnostics of fractional quantum Hall (FQH) phases (Refs. 3,4). 2) Frustrated quantum magnetism, in particular work on the S=1/2 Heisenberg model on the three-dimensional hyperkagome lattice motivated by the exotic $Na_4Ir_3O_8$ compound (Ref. 2). 3) Limits of various FQH states and their relations to integrable models and to certain spin chains (Refs. 1,5-7).

Collaborations at the mpipks

- With Roderich Moessner and Andreas Läuchli, we have studied valence bond formation and discrete symmetry breaking on the three-dimensional hyperkagome lattice, motivated by the recent experiments on the exotic $Na_4Ir_3O_8$ compound. This material shows no sign of magnetic ordering down to the lowest temperatures, thus presenting a candidate for a quantum spin liquid. We have recently argued for a different scenario: using a series expansion around an arbitrary dimerized state we derived a valence bond crystal ground state with a 72 site unit cell that supports many, very low lying, excitations in the singlet sector. Low-energy spinful excitations (spinons and triplons) are effectively confined to various emergent lower-dimensional structures. If applicable to the recently studied sodium iridate compound, $Na_4Ir_3O_8$, this scenario has interesting observable implications, such as spatially anisotropic neutron scattering spectra and possibly multiple finite temperature signatures in the magnetic specific heat due to a multi-step breaking of discrete symmetries. Most saliently, here - as for several proposed states for analogous kagome and pyrochlore magnets - one might expect a clearly resolved Ising transition at relatively high temperature.

- With Andreas Läuchli and Masud Haque, we have provided new insights into the entanglement in FQH states by continuously varying the geometry, and thus the physical boundary between the system and the environment. For the von Neumann entropy, our method improved the control of the entanglement scaling significantly, and the precision extraction of the topological part, γ, was improved by about an order of magnitude (from an uncertainty of about 10-30% to about 1-3% in the simplest cases). For the entanglement spectrum (also with Juha Suorsa, Oslo), this allowed us to obtain a microscopic understanding of the entanglement levels by connecting to the thin-torus limit and also to study the interplay between two spatially separated edges.

External collaborations I currently work with several external groups. So far the following two cooperations have lead to publications:

- With Anders Karlhede and his group at Stockholm University, I work on fractional quantum Hall effects. During my time on PKS we, among other things, found a new solvable limit of the FQH system—on a thick and short cylinder—which is very similar to the Haldane-Shastry spin chain.
- With Masaaki Nakamura, Tokyo Institute of Technology, and Juha Suorsa, Oslo University, we have worked out relations between quantum spin chains and fractional quantum Hall states. In particular we have investigated the connection between the odd denominator rule for FQH states and integer versus half-integer spin chains.

Articles completed and written at the mpipks

1. "Effective spin chains for fractional quantum Hall states", E.J. Bergholtz, M. Nakamura and J. Suorsa, Physica E 43, 755 (2011).
2. "Symmetry Breaking on the Three-Dimensional Hyperkagome Lattice of $Na_4Ir_3O_8$", E.J. Bergholtz, A.M. Läuchli and R. Moessner, Phys. Rev. Lett. 105, 237202 (2010).
3. "Entanglement Scaling of Fractional Quantum Hall states through Geometric Deformations", A. Läuchli, E.J. Bergholtz and M. Haque, New J. Phys. 12, 075004 (2010).
4. "Disentangling Entanglement Spectra of Fractional Quantum Hall States on Torus Geometries", A.M. Läuchli, E.J. Bergholtz, J. Suorsa and M. Haque, Phys. Rev. Lett. 104, 156404 (2010).
5. Link between the hierarchy of fractional quantum Hall states and Haldane's conjecture for quantum spin chains,M. Nakamura, E.J. Bergholtz and J. Suorsa, Phys. Rev. B 81, 165102 (2010).
6. Spin chain description of rotating bosons at nu=1, E. Wikberg, E.J. Bergholtz and A. Karlhede, J. Stat. Mech. (2009) P07038.
7. Quantum Hall Circle, E.J. Bergholtz and A. Karlhede, J. Stat. Mech. (2009) P04015.

3.3.2 Junior Professorship

Unconventional superconductivity and magnetism in strongly correlated electronic systems
(Prof. Ilya Eremin)

The microscopic understanding of many-particle physics in correlated materials with underlying lattice structure is at the heart of current research efforts in solid state physics. This interest raised in the eighties with the discovery of materials with f-electrons, which behave as heavy fermion systems and further exploded with the discovery of cuprate and recently iron-based superconductors. Many unconventional superconductors are highly correlated and complex systems whose phase diagrams include magnetic, superconducting, and charge ordered phases in close proximity. Generally, I am interested in studying both analytically and numerically the possible mechanisms of the unconventional superconductivity and their fingerprints and consequences for the spin and the charge dynamics. Furthermore, I am also aiming to understand deeper the aspects of the co-existence and competition between unconventional superconductivity and magnetic and charge ordered phases. In April 2010 I became Associate Professor for Solid State Theory at the Ruhr-University in Bochum. The report covers the period of my stay at mpi**pks** till this date.

Projects at the mpipks Together with J.-P. Ismer (Ph. D. student at the mpi**pks** who is defending his thesis in May of 2011) I work on the understanding of the competition between density waves and unconventional superconductivity. Together with Peter Fulde and Alireza Akbari, I have also studied the properties of the rare-earth impurities in novel superconductors. For example, we have analyzed the bound state induced by the $4f$-impurity in the cuprate and iron-based superconductors. Together with Jun Chang we have investigated the Cooper-pair formation by anharmonic rattling modes in the β-pyrochlore superconductor KOs_2O_6. In collaboration with J. Knolle, and R. Moessner we have studied the spin wave excitations within itinerant scenario in the parent magnetic phase of iron-based superconductors (see also contribution on page 94). Our results were used by the neutron scattering experiments to elucidate the nature of the spin excitation in these compounds.

External collaborations With A. Chubukov from University of Wisconsin at Madison (USA) we have studied the selection of the magnetic order in the iron-based superconductors and together M. Korshunov and D. Maslov from the University of Florida the unusual behavior of the uniform susceptibility in these compounds. Together with Dirk Morr from UIC at Chicago we are working on the understanding of the evolution of the d-wave superconductivity in the presence of the magnetic and charge order. Another project in collaboration with the experimental groups of Prof. Büchner and D. Argyriou from IFW Dresden and HMI in Berlin applies to the study of unconventional superconductors with various spectroscopic techniques such as nuclear magnetic resonance or inelastic neutron scattering. Together with P. Thalmeier (MPI-CPfS) we are working on the understanding of physics of heavy-fermion compounds and superconductors with rattling phonons.

Further activities My duties as a junior-professor included not only scientific research which is done at the **mpipks** but also teaching at the Physics Department of the Technical University of Braunschweig. During the last two years I have given the course on Computational Physics I (Winter Term 2008/2009) for the Bachelor students. Together with Prof. Hans-Henning Klauß from TU Dresden I have organized the Internal Symposium of Division Low Temperature Physics of the German Physical Society Spring Meeting in 2008 on Superconductivity and Magnetism of iron-based superconductors.

Articles completed and written at the mpipks for the last two years

- Jun Chang, Ilya Eremin, and Peter Thalmeier, Superconductivity in beta-pyrochlore KOs_2O_6: treatment within strong-coupling Eliashberg theory, New Jour. Phys. 11, 055068 (2009), [Special issue on Superconductors with Exotic Symmetries]
- A. Chubukov, I. Eremin, and M.M. Korshunov, Raman response in a superconductor with extended s-wave symmetry: application to Fe-pnictides, Phys. Rev. B 79, 220501(R) (2009) (editor's choice) [selected for a Viewpoint in Physics 2, 46 (2009) article by Miles V. Klein]
- M. M. Korshunov, I. Eremin, D. V. Efremov, D. L. Maslov, A. V. Chubukov, Non-analytic spin susceptibility of a nested Fermi liquid: the case of Fe-based pnictides, Phys. Rev. Lett 102, 236403 (2009)
- A. Akbari, I. Eremin, P. Thalmeier, and P. Fulde, Theory of bound state of 4f-excitations and magnetic resonance in unconventional superconductors, Phys. Rev. B 80, 100504(R) (2009).
- K.-Y. Choi, P. Lemmens, I. Eremin, G. Zwicknagl, H. Berger, G. L. Sun, D. L. Sun, C. T. Lin, Self-energy effects and electron-phonon coupling in Fe-As superconductors, J. Phys. Cond. Matter 22, 115802 (2010)
- I. Eremin and A.V. Chubukov, Metallicity of the spin density wave state in iron-based superconductors, Phys. Rev. B 81, 024511 (2010).
- A. Akbari, I. Eremin, and P. Thalmeier, Magnetic impurity resonance states and symmetry of the superconducting order parameter in iron-based superconductors, Phys. Rev. B 81, 014524 (2010).
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- M. Nicklas, F. Steglich, J. Knolle, I. Eremin, R. Lackner, and E. Bauer, Pair-breaking by non-magnetic impurities in the non-centrosymmetric $CePt_3Si$, Phys. Rev. B 81, 180511(R) (2010).
- D. N. Argyriou, A. Hiess, A. Akbari, I. Eremin, M.M. Korshunov, Jin Hu, Bin Qian, Zhiqiang Mao, Yiming Qiu, Collin Broholm, and W. Bao, Incommensurate itinerant antiferromagnetic excitations and spin resonance in the $FeTe_{0.6}Se_{0.4}$ superconductor, Phys. Rev. B 81, 220503(R) (2010).
- J. Knolle, I. Eremin, A.V. Chubukov, and R. Moessner, Theory of itinerant magnetic excitations in the SDW phase of iron-based superconductors, Phys. Rev. B 81, 140506(R) (2010) [Editor's suggestion].

3.3.3 Gutzwiller-Fellowship

Diffusion or Absence of Diffusion in Infinite Arrays of Coupled Random Nonlinear Oscillators with Linear Anderson Localization?
(Prof. S. Aubry)

It is well-known that there is absence of diffusion in arrays of coupled random linear oscillators at strong enough disorder (Anderson localization). In that situation, the eigen spectrum of the linear dynamical equations is purely discrete and associated with a complete base of eigen states (Anderson modes) which are exponentially localized. Then any wave packet which is initially localized, is almost periodic in time since it decomposes as an absolutely convergent sum of those time periodic eigenmodes and consequently it remains localized forever without spreading.

When nonlinear terms are added to the Hamiltonian, the Anderson modes become coupled by higher order terms. This nonlinear coupling allows in principle energy transfer between the Anderson modes and it is thus non trivial to predict whether there is energy diffusion through the Anderson modes or not.

Many early works suggested on the basis of numerical simulations in such systems, that any initial wavepacket with finite energy should spread to zero amplitude. This spreading was characterized by the divergency as a function of time, of the second moment of the energy distribution of the wavepacket. It was found that this second moment was diverging as a power law of time, slower than standard diffusion (sub-diffusion). This numerical observation is explained with the assumption that most trajectories in an infinite nonlinear system are chaotic. Assuming this chaotic behavior is broad band, the Anderson modes far apart from the core of the wavepacket should be excited by the chaotic motion of the oscillator of the core. This effect should maintain energy spreading at all time if one assume that the chaos remains broad band forever.

Our investigations during my Gutzwiller fellowship at **mpipks** in 2009-2010 conclude that this explanation for energy spreading is not consistent with some exact analytical results (though we only have incomplete answers) and also with new numerical investigations. New questions arise and still remain opened. We essentially focused on the 1D random DNLS model which has been intensively studied earlier as a prototype model for this problem. It obeys the dynamical equation

$$i\dot{\psi}_n = (\epsilon_n + \chi|\psi_n|^2)\psi_n - C(\psi_{n+1} + \psi_{n-1})$$

where ψ_n is the complex coordinate at site n. ϵ_n are random uncorrelated onsite energies which for example are uniformly distributed in an interval $[-V, +V]$, C is the coupling constant between nearest neighbour sites and χ is the parameter of the onsite nonlinearity. Beside the energy, this model has a second invariant which is the total norm square $\sum_n |\psi_n|^2$. It is generally believed that energy spreading behaves similarly in other random nonlinear models with no extra invariant such as random nonlinear Klein-Gordon arrays.

We found numerically [**?**, JKA10]hat a finite norm wave-packet initially localized may generate two kinds of trajectories which both are obtained with a non vanishing probability. The first kind of wave-packets consists of trajectories which are recurrent in the sense of Harald Bohr. Those trajectories are almost periodic and thus cannot spread. Empirical analytical arguments suggest that KAM theory may still hold in infinite systems under two conditions which are (1) the linearized spectrum is purely discrete and (2) the considered solutions are square summable with a norm which is not too large. We check numerically that indeed in appropriate regions of the parameter space, many initial conditions can be found with finite probability which generate (non spreading) infinite dimension tori (almost periodic solutions) a fat Cantor set in (projected) phase space. Many are found in parameter domains where the Anderson localization length is rather short but this domain shrinks to zero measure very fast when the localization length diverges. Let us note that most early numerical simulations were done in domains with relatively long localization length where KAM tori survive only at very small amplitude. Otherwise, our finding is supported by few rigorous results but only on some specific models of infinite arrays of coupled nonlinear oscillators where KAM tori do exist with nonvanishing probability.

The second kind of trajectories look initially chaotic and often spread over long times. We first rigorously prove that initial chaos does not necessarily imply complete spreading for example when the norm of the wavepacket is too large. Otherwise, in some modified models, no spreading at all is proven to be possible despite the presence of initial chaos in contradiction with early beliefs. The nature of the asymptotic state is still unknown.

However, we attempt to present empirical arguments suggesting that if a trajectory starts with chaotic spreading, there will necessarily exist (generally large) critical spreading distances depending on the disorder realization where the trajectory will necessarily become sticking KAM tori. This effect could be viewed as "inverse Arnold Diffusion" since the trajectory approaches more and more KAM tori instead of leaving them. Since KAM tori become more and more rare as localization length increases, this effect could only manifest after longer and longer time so that it could be invisible at the available time scale in numerical simulation. After a certain timescale, the wave packet spreading should slow down more and more. This behavior should be associated with a self-organization of the chaotic behavior of the wavepacket becoming narrow band. In cases, where complete spreading is impossible and may be in all cases with initial chaos, the limit profile should be a trajectory with marginal chaos (with singular

continuous spectrum) at the edge of the KAM tori region. This limit state could nevertheless exhibit a long spatial tail and diverging second moment. This limit profile if any is not supposed to be unique as for an attractor in dissipative systems (since our system is Hamiltonian) but it should be highly sensitive to the initial conditions. These speculative ideas were built for consistency with the numerical data and the few exact analytical which are known, but further both more sophisticated analytical and numerical investigations are required to test them.

Several papers related to this problem were published in collaboration with invited visitors at mpi**pks**. In [1], Rolf Schilling and I investigate simplified non-linear infinite models where only a finite number of oscillators are nonlinear and the rest is linear. In that models, it was proven that limit states with singular continuous spectrum may exist. In another paper [2] Stefano Lepri, Rolf Schilling and I investigated a purely linear model with Anderson localization but where the localization length diverges for accoustic modes. Despite there is no wavepacket spreading, the wave packet develops long tails so that the second moment of the energy distribution diverges as a power law of time. Thus, the second moment divergency cannot be considered as a good criteria for energy spreading. In the next paper [3] Magnus Johansson, George Kopidakis and I present numerical evidence for the existence of non spreading wavepackets which may be considered as KAM tori in infinite dimensional systems. Finally, in the last paper [4] I summarize our results and set conjectures and unsolved questions.

[1] S. AUBRY and R. SCHILLING
Anomalous Thermostat and Intraband Discrete Breathers
Physica D238 2045 (2009)

[2] S. LEPRI, R. SCHILLING and S. AUBRY
Asymptotic Energy Profile of a Wave-Packet in Disordered Chains
PRE 82 056602 (2010)

[3] M. JOHANSSON, G. KOPIDAKIS and S. AUBRY
KAM tori in 1D Random DNLS Models?
EPL 91 50001 (2010)

[4] S. AUBRY
KAM tori and Absence of Diffusion of a Wave-packet in the 1D Random DNLS model. submitted to IJBC (2010) Special Issue edited by Prof. Gregoire Nicolis , Prof. Marko Robnik, Dr. Vassilis Rothos and Dr. Haris Skokos

3.3.4 Collaboration with Experimental Groups

A number of joint collaborations with experimental groups in Germany, Europe and the US has been partially supported by mpi**pks**.

- *Coupling of hair bundles enhances their amplification properties* with J. Barral, P. Martin, Institut Curie (Paris, France)
- *Stochastic adaptation in an auditory receptor cell* with K. Fisch and J. Benda, LMU München
- *Serial correlations in the drop-out statistics of an excitable laser under dichotomous driving* with J. T. Alsina and J. Garcia-Ojalvo, Universitat de Catalunya (Spain)
- *Local Motion analysis dependence of intracellular sub-diffusion on cytoskeleton components* with M. Otten and D. Heinrich, LMU München
- *Capturing of lost kinetochores by random angular movements of microtubules* with I. Tolić-Nørrelykke, MPI-CBG Dresden
- *Firing statistics of receptor cells under driving with stochastic oscillations* with A. Neiman and D. Russel, Ohio University Athens (USA)
- *Parasites and Food Webs* with K. Lafferty, United States Geographical Survey and UC Santa Barbara (USA)
- *Self-propelled particles* with I. Couzin, Princeton University (USA)
- *Molecular interferometry* with M. Arndt, University of Vienna (Austria)
- *Molecular interferometry* with H. Ulbricht, University of Southampton (UK)
- *Interface roughness in developing tissues* with C. Dahmann, MPI-CBG Dresden
- *Collective dynamics of motor molecules* with S. Diez, B CUBE and TU-Dresden
- *Role of pulling forces in cell division* with M. Dogterom, AMOLF Amsterdam (Netherlands)

- *Planar cell polaring in epithelia* with S. Eaton, MPI-CBG Dresden
- *Dynamics of morphogen signaling* with M. Gonzales-Gaitan, University of Geneva, (Switzerland)
- *Patterns in active fluids* with S. Grill, MPI-CBG, mpi**pks** Dresden
- *Dynamics of the ciliar beat* with J. Howard, MPI-CBG Dresden
- *Physic of cell division* with T. Hyman, MPI-CBG, mpi**pks** Dresden
- *Biophysics of mechanical-sensory hair cells* with P. Martin, Institut Curie, Paris (France)
- *Delayed coupling theory of vertebrate segmentation* with A. Oates, MPI-CBG Dresden
- *Biophysics of Cell locomotion* with J. Theriot, Stanford University, (USA)
- *Nuclear oscillation during meiosis* with I. Tolić-Nørrelykke, MPI-CBG Dresden
- *Dynamics of endosome networks* with M. Zerial, MPI-CBG Dresden
- *Filamentary self-compression of ultrashort laser pulses* with G. Steinmeyer, Max Born Institute Berlin
- *Multi-filament of ultrashort intense laser pulses in air.* with J. Kasparian, J.-P. Wolf, Universite de Geneve (Switzerland)
- *Multi-filament of ultrashort intense laser pulses in air* with U. Schramm, R. Sauerbrey, Helmholtz-Zentrum Dresden-Rossendorf
- *Terahertz generation by ionizing two-color femtosecond pulses in gases.* with K. Reimann, M. Woerner, T. Elsaesser, Max Born Institute Berlin
- *Ultracold Plasmas* with T. C. Killian, Rice University (USA)
- *Nonlinear Optics in Ultracold Gases* with C. S. Adams, Durham University (USA)
- *Rydberg Molecules* with T. Pfau, University of Stuttgart
- *Directional emission from Limacon-shaped microlasers* with T. Sasaki, T. Harayama, NTT Corporation, Kyoto, (Japan)
- *Whispering gallery modes in microdroplet lasers* with J. Haase, K. Leo, TU Dresden
- *Measurement of the Goos-Haenchen shift in microwave billiards* with J. Unterrhinninghofen, H.-J. Stoeckmann, Universität Marburg
- *Directional emission from Limacon cavities* with Q. Wang, F. Capasso, Harvard University (USA)
- *Farfield characteristics of triangular microlasers* with Q. Wang, F. Capasso, Harvard University (USA)
- *Angular emission characteristics of spiral microlasers* with M. Belkin, F. Capasso, Harvard University (USA)
- *Directional emission from microlasers* with H. Cao, Yale University (USA)
- *Insights into the dynamics and architecture of tension generating actomyosin networks* with O. Medalia, Universität Zürich (Switzerland)
- *The mechanics of zebrafish epiboly* with C.-P. Heisenberg, IST Austria
- *Regarding molecular aggregates in helium nano-droplets* with Prof. Stienkemeier (Freiburg)
- *Regarding photo ionization of fullerenes and fullerene negative ions* with Profs. Berrah (Kalamazou, USA)
- *Related to cluster experiments at the two FELs in Hamburg and Stanford* with T. Möller (Berlin)
- A close interaction via the *Max Planck Advanced Study group at the Center for Free Electron Laser Studies* has been established with Prof. Ullrich (Heidelberg)
- *Inelastic neutron scattering in novel superconductors* with D. Argyrious, Helmholtz-Zentrum Berlin
- *Magnetic materials with Coulomb phases* with A. Tennant, Helmholtz-Zentrum Berlin
- *Ultrasound studies on frustrated magnets* with S. Zherlitsyn and J. Wosnitza, High magnetic field laboratory, Helmholtz Zentrum Dresden-Rossendorf
- *NMR spectroscopy in iron-based superconductors* with B. Buechner, IFW Dresden

- *Non-centrosymmetric superconductors* with F. Steglich, MPI-CPfS
- *Raman spectroscopy in iron-based superconductors* with P. Lemmens, TU Braunschweig
- *Non-equilibrium behaviour in spin ice* with UNLP-Conicet La Plata–Santiago Grigera (Argentina)
- *Electron spin resonance, graphene* with F. Simon, Budapest University of Technology and Ecomonomics (Hungary)
- *Vortex configurations in trapped BECs* with V. Bagnato, Instituto de Fisica de Sao Carlos, USP (Brazil)
- *Experimental characterization of magnetic insulators* with H. Rosner, MPI-CPfS Dresden
- *Modeling and interpretation of inelastic neutron scattering experiments on low-dimensional quantum magnets* with C. Rüegg, London Center for Nanotechnology (UK)

3.3.5 Joint Workshop Program

Since 2008 mpi**pks** has been running a the new workshop program, *Trends in Complex Systems (TCS)*, together with the recently founded Institute for Cross-Disciplinary Physics and Complex Systems (IFISC) at Palma de Mallorca, Spain. There is a strong overlap in interdisciplinary and strategic research topics pursued at IFISC and mpi**pks**. In addition IFISC decided to establish a workshop program, using the experience of the successful workshop program implemented at mpi**pks**. Members of IFISC and mpi**pks** have been conducting joint research activities for several years already.

The joint program *Trends in Complex Systems (TCS)* consists of a series of IFISC-mpi**pks** workshops in Mallorca and Dresden. Each year one workshop is conducted in Dresden, and one in Mallorca. The funding is split in even parts. To ensure a smooth operation and mpi**pks** quality standards from the beginning, we have provided substantial transfer of experience in logistic management of the organization of workshops at mpi**pks** to the partner institute IFISC. In particular, the preparation of the workshops in Mallorca is done in parts at mpi**pks** and a staff member of the Visitors Program supports the organizational work during a workshop in Palma.

The first and second calls for proposals were very successful. We received a large number of workshop proposals of high quality. A referee board with international experts helped with the evaluation of the proposals. In 2009 we conducted the workshop *Synchronization and Multiscale Complex Dynamics in the Brain* in Dresden and the workshop *150 Years after Darwin: From Molecular Evolution to Language* in Palma. In 2010 the workshop *Living Organisms in Flows: From Small Scale Turbulence to Geophysical Flows* took place in Palma, and the workshop *Timing and Dynamics in Biological Systems* in Dresden. The success of the program was evident, and we can safely state that we reached all of the above goals.

3.3.6 Conferences, Workshops and Symposia

1. *Many-Body Systems far from Equilibrium: Fluctuations, Slow Dynamics and Long-Range Interactions*
   Seminar: February 16 - 27, 2009 — 75 participants
   Scientific coordinators: M. Henkel, D. Mukamel, M. Pleimling, G. Schütz
2. *Korrelationstage 2009*
   Workshop: March 02 - 06, 2009 — 170 participants
   Scientific coordinators: M. Grüninger, T. Kopp, H. Kroha
3. *Anderson Localization in Nonlinear and Many-Body Systems*
   Workshop: March 16 - 20, 2009 — 61 participants
   Scientific coordinators: B. Altshuler, S. Flach, A. Pikovsky
4. *Physical Biology Circle Meeting*
   Focus Workshop: April 01 - 03, 2009 — 93 participants
   Scientific coordinators: S. Grill, F. Jülicher

5. *Bloch Oscillations and Landau-Zener Tunneling: From Hot Electrons to Ultracold Atoms*
   Seminar and Workshop: April 14 - May 08, 2009 — 60 participants
   Scientific coordinators: E. Arimondo, Y. A. Kosevich, T. Pertsch

6. *Quantum Aggregates*
   Workshop: April 22 - 24, 2009 — 33 participants
   Scientific coordinators: J. Briggs

7. *DNA - Based Nanotechnology: Construction, Mechanics, and Electronics*
   Workshop: May 11 - 15, 2009 — 89 participants
   Scientific coordinators: G. Cuniberti, M. Mertig, H. Yan

8. *Enraging Perspectives - Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*
   Workshop: May 18 - 22, 2009 — 50 participants
   Scientific coordinators: W. Janke

9. *Quantum Fluid Clusters*
   Focus Workshop: May 25 - 27, 2009 — 55 participants
   Scientific coordinators: F. Stienkemeier, J. Tiggesbäumker

10. *Complex Dynamics in Large-Scale Interacting Brain Systems: Towards Physical Models of Sleep and Consciousness*
    Seminar and Workshop: June 08 - 25, 2009 — 63 participants
    Scientific coordinators: P. Achermann, E. Olbrich, T. Wennekers

11. *Topological Order: From Quantum Hall Systems to Magnetic Materials*
    Seminar and Workshop: June 29 - July 24, 2009 — 128 participants
    Scientific coordinators: R. Moessner, S. Trebst

12. *Dynamics and Statistics in Weather and Climate*
    Focus Workshop: July 29 - 31, 2009 — 61 participants
    Scientific coordinators: J. Bröcker, K. Fraedrich, H. Kantz

13. *Magnonics: From Fundamentals to Applications*
    Seminar and Workshop: August 02 - 29, 2009 — 86 participants
    Scientific coordinators: V. Kruglyak, D. Grundler, S. Demokritov

14. *Tunneling and Scattering in Complex Systems - From Single to Many Particle Physics*
    Seminar and Workshop: September 07 - 25, 2009 — 113 participants
    Scientific coordinators: A. Bäcker, M. Oberthaler, P. Schlagheck

15. *Key Experiments with X-ray Pulses from the Perspective of Theory*
    Focus Workshop: September 10 - 12, 2009 — 37 participants
    Scientific coordinators: J. M. Rost, I. Schlichting, L. Strüder, J. Ullrich

16. *Energy Dissipation in Nanocontacts and Molecular Bonds*
    Focus Workshop: September 28 - October 01, 2009 — 53 participants
    Scientific coordinators: R. Bennewitz, H. Hölscher, P. Reimann, A. Schirmeisen

17. *Delayed Complex Systems*
    Workshop: October 05 - 09, 2009 — 76 participants
    Scientific coordinators: W. Just, A. Pelster, M. Schanz, E. Schöll

18. *State-Dependent Delay Equations*
    Workshop: October 12 - 16, 2009 — 48 participants
    Scientific coordinators: J. Luca, Antony R. Humphries, J. Mallet-Paret

19. *Physical Principles of Protein Behavior in the Cell*
    Workshop: October 26 - 30, 2009 — 77 participants
    Scientific coordinators: M. Porto, H. Eduardo Roman, M. Vendruscolo

20. *TCS-PROGRAM: Synchronization and Multiscale Complex Dynamics in the Brain*
    Workshop: November 02 - 06, 2009 — 72 participants
    Scientific coordinators: J. Garcia Ojalvo, C. Mirasso, G. Pipa

21. *TCS-PROGRAM: 150 Years after Darwin: From Molecular Evolution to Language*
    Workshop: November 23 - 27, 2009 in Palma de Mallorca, Spain — 82 participants
    Scientific coordinators: J. A. Cuesta, S. C. Manrubia, A. J. McKane

22. *Atomic Physics 2009*
    Workshop: November 23 - 27, 2009 — 97 participants
    Scientific coordinators: U. Saalmann, F. Martin, J.-M. Rost

23. *Exploring Complex Dynamics in High-Dimensional Chaotic Systems: From Weather Forecasting to Oceanic Flows*
    Workshop: January 25 - 29, 2010 — 62 participants
    Scientific coordinators: J. M. Lopez , A. Politi, A. Pikovsky

24. *Quantum Gravity*
    Workshop: April 08 - 10, 2010 — 21 participants
    Scientific coordinators: B. Dittrich, R. Schützhold

25. *Perspectives in Highly Frustrated Magnetism*
    Workshop: April 19 - 23, 2010 — 86 participants
    Scientific coordinators: A. Keren, P. Lemmens, P. Mendels, F. Mila

26. *Self-Organization in Turbulent Plasmas and Fluids*
    Summer School and Workshop: May 03 - 14, 2010 — 130 participants
    Scientific coordinators: F. Jenko, R. Friedrich

27. *Optical Microcavities: Quantum Chaos in Open Systems Meets Optical Resonators*
    3rd Asian-German Workshop: May 17 - 21, 2010 — 53 participants
    Scientific coordinators: S. Shinohara, J.-W. Ryu, M. Hentschel

28. *Dual Nature of f-Electrons*
    Focus Workshop: May 25 - 28, 2010 — 53 participants
    Scientific coordinators: T. Durakiewicz, P. Fulde, G. Zwicknagl

29. *Particulate Matter: Does Dimensionality Matter?*
    Workshop: May 31 - June 04, 2010 — 62 participants
    Scientific coordinators: P. Charbonneau, K. Daniels, M. Schröter

30. *Interactions, Disorder, and Topology in Quantum Hall Systems*
    Workshop: June 07 - 11, 2010 — 87 participants
    Scientific coordinators: A. Mirlin, F. von Oppen

31. *TCS-PROGRAM: Living Organisms in Flows: From Small Scale Turbulence to Geophysical Flows*
    Workshop: June 07 - 11, 2010 in Palma de Mallorca, Spain
    Scientific coordinators: U. Feudel, R. E. Goldstein, E. Hernandez-Garcia,

32. *Quantum Information Concepts for Condensed Matter Problems*
    Seminar and Workshop: June 14 - 25, 2010 — 94 participants
    Scientific coordinators: I. Affleck, M. Haque, U. Schollwöck

33. *Few Body Dynamics in Atoms, Molecules and Planetary Systems*
    Focus Workshop: June 28 - July 01, 2010 — 48 participants
    Scientific coordinators: A. Buchleitner, F. Diacu, G. Tanner

34. *Correlated Phenomena in Low-Dimensional Systems*
    Seminar and Workshop: July 05 - 23, 2010 — 75 participants
    Scientific coordinators: J. S. Meyer, K. Shtengel, G. Refael

35. *Quo vadis Bose-Einstein condensation?*
    Summer school and Workshop: August 02 - 20, 2010 — 110 participants
    Scientific coordinators: M. Holthaus, A. Pelster

36. *Emergent Quantum States in Complex Correlated Matter*
    Workshop: August 23 - 27, 2010 — 72 participants
    Scientific coordinators: E. Bascones, A. Chubukov, I. Eremin

37. *Complexity in Periodically Structured Systems*
    Workshop: August 30 - September 3, 2010 — 40 participants
    Scientific coordinators: C. Denz, G.-L. Oppo

38. *Cold Rydberg Gases and Ultracold Plasmas*
    Seminar and Workshop: September 06 - 17, 2010 — 87 participants
    Scientific coordinators: C. S. Adams, T. Pohl, H. Sadeghpour

39. *Novel Simulation Approaches to Soft Matter Systems*
    Workshop: September 20 - 24, 2010 — 100 participants
    Scientific coordinators: J. Cerda, C. Holm, K. Kremer

40. *TCS-PROGRAM: Timing and Dynamics in Biological Systems*
    Workshop: September 27 - October 01, 2010 — 54 participants
    Scientific coordinators: F. Naef, A. Oates, J. Stelling

41. *The Dynamics of Nonlinear Stochastic Systems*
    Workshop: October 06 - 07, 2010 — 42 participants
    Scientific coordinators: I. Sokolov, U. Erdmann, B. Lindner

42. *Fluctuation-Induced Forces in Condensed Matter*
    Workshop: October 11 - 15, 2010 — 68 participants
    Scientific coordinators: S. Dietrich, A. Gambassi

43. *Spike-Frequency Adaption in Neural Systems*
    Focus Workshop: October 26 - 27, 2010 — 40 participants
    Scientific coordinators: B. Lindner, J. Benda

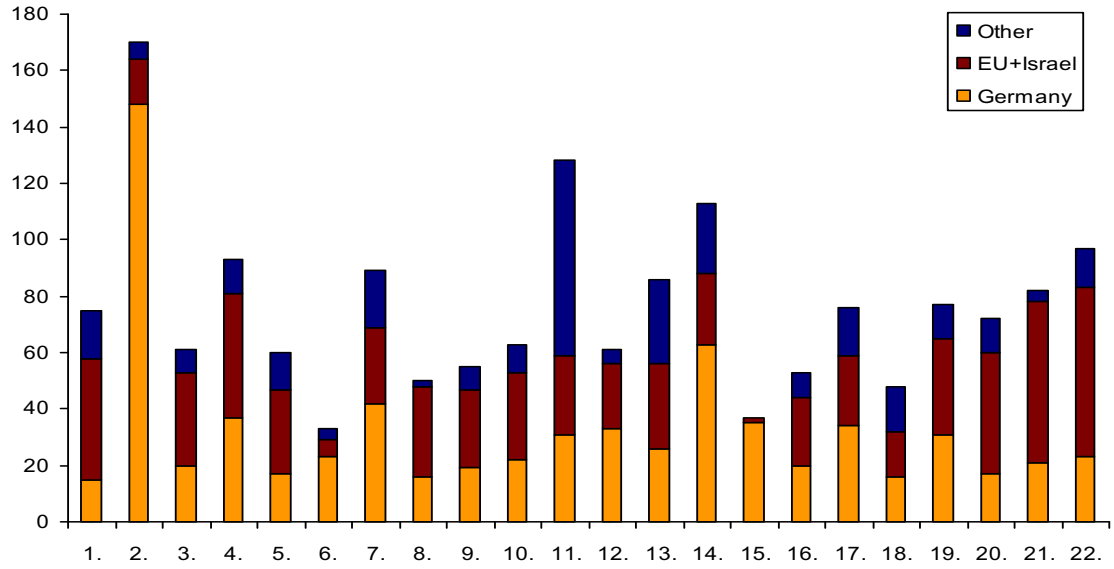
44. *Statistical Physics and Biology of Collective Motion*
    Workshop: November 08 - 12, 2010 — 72 participants
    Scientific coordinators: A. Deutsch, G. Theraulaz, T. Vicsek

45. *Molecules under X-ray Pulses*
    Focus Workshop: November 15 - 17, 2010 — 30 participants
    Scientific coordinators: S. Techert, J. Ullrich, J.-M. Rost

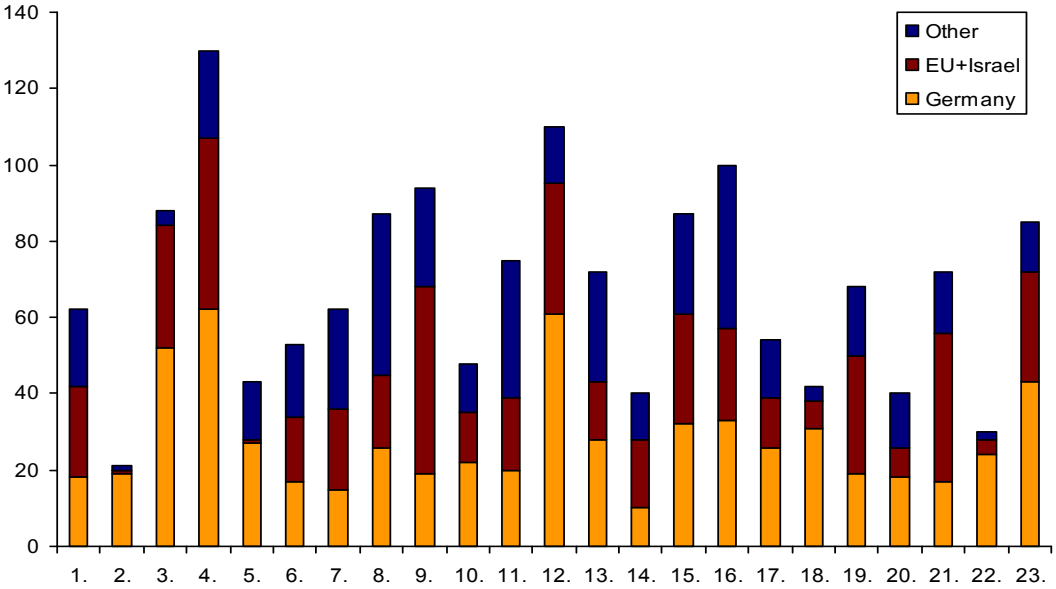
46. *Atomic Physics 2010*
    Workshop: November 22 - 26, 2010 — 85 participants
    Scientific coordinators: K. Hornberger, J.-M. Rost

3.3.7 Workshop Participation and Dissemination of Results

Statistics of Workshop participation



Number of Workshop/Seminar participants in the year 2009.



Number of Workshop/Seminar participants in the year 2010.

Dissemination of Workshop Results

As the topics of Workshops and Seminars at mpi**pks** are focusing on new and emerging fields of the physics of complex systems, scientific coordinators often consider the option of publication of proceedings, lecture notes or monographs related to the results of their event. The mpi**pks** supports such efforts in various ways. The following list summarizes the relevant publications:

- Workshop:
  Complex Dynamics in Large-Scale Interacting Brain Systems: Towards Physical Models of Sleep and Consciousness, June 2009
  Achermann, P., E. Olbrich and T. Wennekers: *The complexity of sleep*, Philosophical Transactions of the Royal Society A (Theme Issue June 2011) (in preparation)
- Workshop:
  Magnonics: From Fundamentals to Applications, August 2009
  V.V. Kruglyk, S.O. Demokritov and D. Grundler (Eds.): *Cluster Issue on Magnonics*, Journal of Physics D 43, Issue 26, 260301 265501 (2010)
- Workshop:
  Delayed Complex Systems, October 2009
  W. Just, A. Pelster, M. Schanz and E. Scholl (Eds.): *Delayed Complex Systems*, Philosophical Transactions of the Royal Society A 368, Theme Issue 303 - 513 (2010)
- Workshop:
  Physical Principles of Protein Behavior in the Cell, October 2009
  W. Porto, H.E. Roman and M. Vendruscolo: *Focus on physical principles of protein behavior in the cell*, Proteomics 10, Specific Issue 23, 4149 4334 (2010)
- Workshop:
  Perspectives in Highly Frustrated Magnetism, April 2010
  Deisenhofer, J. And P. Lemmens: Optical techniques for systems with competing interactions.
  In: *Introduction to frustrated magnetism.*, C. Lacroix, P. Mendels and F. Mila (Eds.) Berlin: Springer, 2011, S. 107 130. (Springer Series in Solid-State Sciences; 164)
- Workshop:
  Novel Simulation Approaches to Soft Matter Systems, September 2010 J.J. Cerda, C. Holm and K. Kremer (Eds.): *Novel Simulation Approaches of Macromolecular Theory and simulations.*, (in preparation)

3.3.8 Workshop Reports

Many-Body Systems far from Equilibrium: Fluctuations, Slow Dynamics and Long-Range Interactions, Seminar
Scientific coordinators: M. Henkel, D. Mukamel, M. Pleimling, G. Schütz

One of the aims of this seminar was to bring together people working on either slow dynamics or long-range interactions in order to permit a cross-fertilisation in studies of fluctuation effects. This choice seemed timely, in particular in view of recent recommendations for research directions of the American NSF and the DoE. It also became evident through the large number of applications. In spite of very generous aid from the mpi**pks**, we could only accept a little more than half of the total number of applicants.

Besides 20 longer lectures from our invited speakers, some 20 shorter talks gave especially younger colleagues the opportunity to present their work. It was satisfying to see that many different people participated through their questions and comments in these talks and further occasion for exchange was provided by the poster sessions (at the request of the participants, a third one was arranged). Still, the breaks between talks were sufficiently long for people to engage in long discussions, either to make progress in existing projects or to start new collaborations. We are happy that several experimentalists

participated which opened a particular window on the themes of this seminar, which in general are mainly theoretical.

All in all, we have been very happy and satisfied with the scientific success of the seminar and the perfect support provided by the **mpipks** for which we are extremely grateful.

Korrelationstage 2009, Workshop
Scientific coordinators: M. Grüninger, T. Kopp, H. Kroha

The Korrelationstage are a series of bi-annual conferences on strongly correlated electron physics, the style and topics of which have continuously been adapted to novel developments in the field and to the group of participating physicists. From a meeting of a few theoretical physicists in the late 80's, the Korrelationstage developed into a five-day conference with about 150 participants, roughly 30% of them being experimentalists. The Korrelationstage 2009 started with the welcome reception Sunday evening, March 1st, and in total 65 talks were presented (including the colloquium talk on Monday) until Friday noon. In order to stimulate focused discussions in the style of the small meetings of the early 1990s while keeping the conference open for a wide range of topics and participants, we modified the conference setup: Two focus topics were identified for the 2009 meeting, "heterostructures" and "nonequilibrium dynamics of strongly correlated systems", two timely and rapidly developing fields, with strong mutual stimulation between theory and experiment. For each focus topic, we invited two keynote speakers, Jochen Mannhart, Univ. Augsburg, and George Sawatzky, Univ. British Columbia (heterostructures) as well as Andrea Cavalleri, Univ. Hamburg, and Andrew Millis, Columbia University (nonequilibrium dynamics). Andrea Cavalleri gave the **mpipks** colloquium on Monday afternoon. Each of these special talks, to which we allotted twice the time (i.e., 40 minutes plus 10 minutes discussions), was excellent and, in fact, energized the Korrelationstage tremendously. We appreciate very much the support of the **mpipks** for this concept, in particular that the two speakers from the U.S. (Andrew Millis) and Canada (George Sawatzky) were funded. We consider the concept of keynote speakers introducing focus topics as extremely successful and recommend it strongly for future Korrelationstage.

One aim of the Korrelationstage is to give young scientists the opportunity to report on their work. About 20 talks were presented by first-time speakers, several of them advanced PhD students. They blended perfectly into the sessions with more experienced speakers without any reservation. The scientific level was high and the talks were mostly skillful.

The conference was open for all topics of strongly correlated systems, including sessions on low-dimensional systems, orbital phenomena, quantum phase transitions, high-T_c superconductivity, Kondo systems, metal-insulator transitions, magnetic order in Hubbard- and Heisenberg-type systems, theoretical methods for strongly correlated systems and condensates with ultracold atom gases. A special feature was the Thursday evening session on superconductivity in Fe pnictides, a novel field that had appeared in 2008. The session filled the lecture room despite the late hour.

Irrespective of the session, the scientific discussions were lively (this actually applied for all talks) and reflected the great interest and involvement of the participants in all topics which were presented. This was also valid for the poster sessions Monday and Tuesday evening. The conference Korrelationstage still represents a unique meeting for physicists working in the field of strongly correlated electrons, especially for the German community including international guests. It boosts the exchange of new ideas and is in particular a forum for young physicists who submitted applications in great numbers and contributed with very good or even excellent posters and talks.

Physical Biology Circle Meeting, Workshop
Scientific coordinators: S. Grill, F. Jülicher

The interface between Biology and Physics is an exciting and thriving field of research. On the one hand, many key questions in Biology will only find an answer through the thorough study of the underlying and relevant physical mechanism. On the other hand, the vast complexity of biological systems presents yet unsolved challenges to theoretical physicists that work in the areas of statistical physics, non-equilibrium thermodynamics and complex networks. The questions that need to be answered are plentiful, and answers require a detailed description of biological systems at cellular and sub-cellular scales. This meeting was part of an annual meeting of the European Associate Laboratory, in a collaborative effort between

the Institute Curie in Paris, the AMOLF in Amsterdam, EMBL in Heidelberg, and the Max Planck Institute for the Physics of Complex Systems in Dresden. November 2004 was the last time it took place in Dresden, and it has since taken place in Paris, Amsterdam and Heidelberg, followed by Dresden again this year. The main focus of this meeting was to bring together students, postdocs and PIs that apply modern experimental and theoretical approaches to solve problems in physical biology. Generally, a specific emphasis was put on topics that closely connect experimental and theoretical approaches. Topics discussed included cell motility, cell polarization, active polar gels and active membranes. Specifically, oral presentations covered the Min systems of subcellular organization, microtubule dynamics in vivo and reconstituted, meiotic nuclear oscillations in fission yeast, symmetry breaking in Caenorhabditis elegans, cleavage furrow stability, lipid sorting, polymersomes, and protein friction. A specific aim of this meeting was to allow graduate students to present their work at a rather early stage of their career, and all talks were given by graduate students. Talks displayed a remarkably high level of quality. Postdocs and other attendees presented their work at a poster session, which was a large emphasis of this meeting, with almost 60 presented posters. With over 90 participants fro all four institutions, this meeting was a large success. Many novel research topics were discussed, and a host of new collaborations between the respective participants were sparked. This meeting is of central influence to the growing field of physical biology, it sets the standard of how research should be done in this relatively novel field of research.

Bloch Oscillations and Landau-Zener Tunneling: From Hot Electrons to Ultracold Atoms,
Seminar and Workshop
Scientific coordinators: E. Arimondo, Y. A. Kosevich, T. Pertsch

Bloch oscillations and Landau-Zener tunneling are the fundamental properties of quantum dynamics of a particle in a periodic potential subject to an external static force. The wave-particle dualism leads to a completely counterintuitive behaviour of the Bloch-oscillating wave packet-particle. Since many years this behaviour attracted substantial interest in its deep theoretical understanding and clear experimental observation. The main purpose of this International Seminar and Workshop was to bring together leading experts in the study of Bloch oscillations and Landau-Zener tunneling in dierent systems and materials, such as semiconductor super lattices and devices for hot electrons, optical waveguide arrays, optical super lattices and photonic crystals for photonic wavepackets, ultrasonic super lattices and super lattices made of acoustic micro- and nanocavities for acoustic and phononic wave packets, optical lattices for ensembles of ultra cold atoms and Bose-Einstein condensates. The Seminar (April 14 - May 01, 2009) was devoted to lectures, research work and synergetic discussions. During the Seminar, several invited and contributed speakers (Bastard, Cataliotti, Holthaus, Ishkanyan, Jusserand, Khomeriki, Kolovsky, Krimer, Manevitch, Oberthaler, O'Dell, Renk, Ruo, Weitz) have given comprehensive lectures for young researchers, researchers from the **mpipks** and participants of our event from dierent fields of physics. Each week around 15 participants attended Seminar lectures. During the Workshop week (May 04 - 08, 2009), the invited and contributed talks were focused on the fundamental concepts, appealing physical analogies and interdisciplinary exchange of ideas, as well as on novel applications of Bloch oscillations and Landau-Zener tunneling in a broad spectrum of modern materials and actual systems. The total number of participants was more than 60 coming from all over the world. The participants represented an appropriate mixture of senior scientists and less experienced young researchers. The program provided opportunities to both groups to interact on various levels on the specific topics in the broad scope of the event. In particular the young researchers have been given the chance to interact and to present themselves during the poster sessions which have been organized along with the workshop program. In addition several talks have been given by the next generation scientist as well. The given presentations represented a balanced mixture of the different targeted fields of physics in which Bloch Oscillations and Landau-Zener Tunneling can be observed. For historical reasons semiconductor supper lattices had been in the focus of many scientists (Alekseev, Allen, Bastard, Beltram, Dignam, Domnguez-Adame, Fromhold, Hyart, Kosevich, Manevitch, Renk, Wacker), with presentations covering the development of this research since the pioneering work of Esaki and Tsu in early seventies and new approaches to the interpretation of complex experimental data including recent studies of ultrafast transient phenomena in ensembles of photo excited carriers. However it became clear that experimental studies of ultra cold atoms and Bose-Einstein condensates attract increasing interest with an impressive quality improvement of the experimental data (Biraben, Cirac, Daz, Fromhold, Gat, Holthaus, Kosevich, Kolovsky, Korsch, Morsch, Nagerl, Oberthaler, Salomon, Stringari, Weitz, Wimberger). In addition there have been presentations devoted to newly emerging fields, like photonic systems (Desyatnikov, Dignam, Dreisow, Kavokin,

Longhi, Malpuech, Peschel, Ruo) and photonic systems (Cirac, Jusserand, Kosevich). From the comments provided by many participants we can conclude the successful achievement of the goal of the conference, to provide a status of the interdisciplinary research field and to inspire future work which takes advantage of transferring and generalizing concepts among the different fields of physics. The meeting will facilitate further fruitful exchange of ideas between those fields. Owing to the success of the meeting, the organizers plan to publish selected lectures of the Workshop in a book. We thank the mpi**pks** for all the financial support to the Seminar and Workshop. Most importantly we would like to thank Claudia Poenisch and all the mpi**pks** staff for the excellent organization of the event. The very friendly atmosphere was an important part of the overall success of the conference.

Quantum Aggregates, Workshop
Scientific coordinators: J. Briggs

The meeting began on Wednesday 22 April and ran until Friday afternoon 24 April. There were 34 participants, 23 of whom spoke and 7 presented posters. Almost all participants stayed for the complete duration of the Workshop. The focus was on the structure, spectra and dynamical properties of quantum aggregates. From the enormous activity in this area, interest was concentrated on three rather separate fields, namely, molecular aggregates, aggregates of polaritons in quantum well cavities and aggregates of Rydberg-excited cold atoms. In the case of molecular aggregates there were two main themes; the study of the photosynthetic unit and the study of dye aggregates for use in organic solar cells. In the molecular and atom aggregate cases, the transport of electronic excitation over the aggregate was of particular importance. About 70the speakers were senior scientists who had participated in the Advanced Study Group sometime during the previous six months. Accordingly the group largely knew of each others work and this led to a lively discussion. In this respect the schedule of 30 minute talks followed by 15 minutes discussion time proved enormously successful and certainly to be recommended. Several talks were given by younger scientists, e.g. the two contributions on polaritons from London and Cambridge. Also successful were the oral poster talks presented as a prelude to the poster session itself. Two of these presentations, by doctoral students, were outstanding. The Workshop ended with a discussion session on Friday afternoon attended by around twenty participants. This had the aim of assessing the results of the Workshop and planning for the future. The major results of the Workshop emerged as:

1) the recognition that, despite the variety of topics covered, from the theoretical point of view, the systems are very similar so that the discipline Quantum Aggregates can be viewed as an established field cutting across solid state, atomic and molecular physics and chemistry.

2) the enormous advances in experimental precision (30% of talks were from experimentalists) represent a great challenge for the theory of such complex systems.

3) the general consensus was that the impetus gained from the ASG and Workshop should not be wasted and the benefits of bringing together workers from fields as diverse as photosynthesis and cold atoms should not be underestimated. Such meetings and opportunity to learn of advances in other fields are rare but can lead to surprisingly fruitful collaboration. Many participants expressed the desire to continue this activity and many options were discussed, e.g. a further mpi**pks** Workshop, a meeting funded by the Heraeus Foundation or VW Stiftung and, for the German participants, a DFG Schwerpunktprogramm. Certainly, the Workshop was a very appropriate way to end the activity of the Advanced Study Group.

Quantum Fluid Clusters, Focus Workshop
Scientific coordinators: F. Stienkemeier, J. Tiggesbäumker

The field of quantum fluid clusters is still dominated by work on helium nanodroplets which made up the main focus of this workshop. These offer a fascinating possibility to study quantum properties like e.g. superfluidity in finite size systems. A comprehensive theoretical understanding of such properties on the nanoscale as well as a detailed description of the interactions with dopant atoms and molecules and the dynamics of the systems are still missing. Work in this context is still in progress and the meeting succeeded in bringing together almost all experts in the field.

A couple of talks concentrated on the short–time dynamics from different points of view, i.e. XUV–excitations of pure droplets, ultrafast processes on the droplet surface as well as violent interactions in strong laser fields. Furthermore, for the first time the isolation of charge species in droplets was

introduced at the workshop. The presented results appear to be very promising in terms of spectroscopic studies; this direction will surely develop in the near future.

One of the main topics of the meeting was the theoretical description of the helium–impurity interaction leading to the formation of weakly bound and even exotic aggregates (*"The smallest droplet of acid"*, accepted as publication in Science 2009). Different approaches were controversially discussed between theorists applying i.e. density functional theory, path integral techniques as well as quantum Monto–Carlo simulations. Here, Manuel Barranco (University of Barcelona, Spain), Francesco Gianturco (University of Rome, Italy), Massimo Boninsegni (University of Alberta, Canada) and Robert Zillich (Universität Linz, Austria) presented new results. In terms of theoretical descriptions Joshua Jortner (Tel Aviv University, Israel) gave an excellent overview presentation. In order to communicate the results of the workshop to a broader audience, colleagues coming from nearby fields, e.g. E. Rabani (Tel Aviv, Israel) and R. Hinde (Knoxville, USA) have been invited. Furthermore, the conference brought up new topics and added promising future research areas:

1. Superfluidity of hydrogen clusters
2. Embedded clusters exposed to intense laser fields

Four out of the eleven sessions were devoted to these topics which have attracted considerable interest in recent times. Clearly evident from the conference, the field of quantum fluid clusters can give a major impact to this new directions in physics and chemistry. Concerning hydrogen clusters, Takamasa Momose (University of British Columbia, Canada), Peter Toennies (Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen) and Andrej Vilesov (University of Southern California, USA) highlighted recent activities. Young scientists were in particular encouraged to join the workshop. Roughly one quarter of the participants have been Diploma, Master and PHD students providing a rich and stimulating discussion during the poster session on Monday evening. Two oral contribution were given by PHD students. In conclusion, the focus workshop has proven, that the physics and chemistry of quantum fluid clusters is still relevant today and an active area of experimental as well as theoretical research. The organizers like to thank the Max–Planck–Institute for the grateful financial support and for helping us making this workshop possible.

Complex Dynamics in Large-Scale Interacting Brain Systems: Towards Physical Models of Sleep and Consciousness, Seminar and Workshop
Scientific coordinators: P. Achermann, E. Olbrich, T. Wennekers

The **workshop** was attended by 65 participants and brought together scientists working in multiple disciplines as diverse as experimental brain research, medicine, psychology, complex systems science, data analysis, and large-scale computational modeling of the nervous system. The main goal was to advance an integrated understanding of the complex dynamics of the brain that underly different brain states like sleep and consciousness. The 5-day workshop contained 21 invited and nine contributed talks. It featured world-leading experts in experimental sleep and cognition research (e.g., P. Maquet, V. Crunelli, S. Bressler), modelers (e.g., A. Destexhe, M. Bazhenov, P. Robinson, M. Wilson, S. Hill), theoreticians (e.g., J. Kurths, J. Jost), and data analysts (e.g., P.A. Valdes Sosa). A major topic was the physical origin of the slow oscillation, a most fundamental process characterizing sleep. It was covered by presentations of new experimental results (V. Crunelli, I. Ulbert) and different modelling approaches (J.-C. Claussen, M. Bazhenov, S. Hill). Sleep has further been suggested to be involved in memory consolidation for many years. Several talks addressed recent experiments investigating this hypothesis (J. Fell, R. Huber). Complexity physics provides a major novel direction in sleep research because the brain can be considered a complex network of cells and their connections. Presentations in this area explored network topologies of neural networks and their impact on network dynamics, especially synchronization phenomena (J. Kurths, J. Jost, C. Zhou). A further strand of research covered in the workshop was large-scale modeling of the brain as very detailed models of biological neural networks can now be simulated on high performance computers. This enables detailed studies of neurophysiological processes related to sleep control and sleep oscillations (D. Forger, P. Robinson, M. Bazhenov, S. Hill). One current challenge in the field of sleep research and neuroscience is the integration of different experimental approaches like macroscopic measurements such as EEG and fMRI with more microscopic data such as local field potentials or multi-unit recordings. To combine these techniques mathematical models based on statistical

inference can be used. These topics were addressed in the contributions of P.A. Valdes Sosa, I. Bojak and R.D. Pascual Marqui. As part of the workshop a public evening lecture "Why do we sleep?" was given by P. Achermann. The lecture was attended by approximately 200 visitors and was followed by a lively discussion. K. Friston, one of the leading theorists on cortical function, furthermore gave a colloquium talk entitled "Free-energy, perception and learning" to the members of the Max Planck Institute for the Physics of Complex Systems. A special discussion session during the workshop addressed problems regarding communication and epistemological barriers between the different disciplines. The workshop was a significant step to bridge such gaps and to initiate interactions between the different contributing disciplines. Young researchers (PhD students and postdoctoral fellows) presented their work in a poster session (19 posters) or as speaker in the main program (S. Postnova). Posters were at display during the entire workshop. A **seminar** complemented the workshop. This aimed at supporting immediate research work by the participants as well as setting up of new collaborations. The seminar lasted for 10 days and was attended by 13 participants, mainly young researchers. It included five tutorial lectures that provided introductions into complexity measures, state space models, sleep, neural assemblies and large scale simulation models. Three additional morning sessions targeted on open discussions with foci on challenges in time series analysis, a calculus of cognition, and the future of large-scale modeling. Beside these arranged talks and discussions, participants worked on collaborative projects of which some will continue in the future.

Topological Order: From Quantum Hall Systems to Magnetic Materials, Workshop
(Jointly with APCTP)
Scientific coordinators: R. Moessner, S. Trebst

The international seminar and workshop Topological Order: From quantum Hall systems to magnetic materials was devoted to a broad variety of physical systems that exhibit unconventionally ordered phases including frustrated magnets, quantum Hall systems, time-reversal symmetry breaking superconductors, ultracold atom systems, and topological insulators. It brought together theorists working on fundamental concepts of topological order, quantum phase transitions in constrained systems, spin liquid phases, and quantum information theory as well as experimentalists working on two-dimensional electron gases, quantum wells, and transitional metal compounds including Iridium oxides, spinels, and chiral magnets.

The three-week seminar program was structured around one or two daily talks, including two lectures devoted to pedagogical introductions in each week. The three weeks were not organized to have special focus topics, since one of the central objectives of the workshop was to bring together scientists from two seemingly disjoint communities, but with overlapping interests on the one hand scientists working on frustrated magnetism motivated primarily from a materials-science perspective and on the other hand scientists with a focus on topological phases and their harnessing for topological quantum computing with a particular emphasis on fractional quantum Hall based systems. Judging from the lively activity, vigorous discussions and overwhelmingly positive feedback throughout the program we believe that this concept has worked very well.

Nevertheless, some themes shaped the discussions of the individual seminar weeks more than others, mostly due to the varying roster of participants in each week. The first week greatly benefited from an introductory lecture of Alexei Kitaev (Caltech), one of the pioneers in the field of topological order and topological quantum computation. He reviewed fundamental aspects of topological order in microscopic models and then proceeded to an advanced mathematical description of the interplay of topological order and quantum critical behavior. Impressive progress in the theoretical description of quantum phase transitions in highly constrained systems was also reported by various speakers throughout the program including John Chalker (Oxford), Kai Schmidt (Dortmund), Claudio Castelnovo (Oxford), and Eun-Ah Kim (Cornell). Other topics of the seminar weeks included the exotic physics of highly frustrated magnets put forward in talks by Ribhu Kaul (Santa Barbara), Chris Henley (Cornell), Wolfram Brenig (Braunschweig), and Oleg Tchernyshyov (Johns Hopkins) as well as conceptual approaches to exotic spin liquid behavior discussed by T. Senthil (MIT). Quantum information approaches to topological order were highlighted in various talks including those by Frank Verstraete (Vienna) and Vincent Pasquier (CEA/IPhT).

A recurring theme of the seminar weeks was the conjectured non-Abelian statistics of anionic excitations in certain fractional quantum Hall states, especially the v=5/2 state. Several discussions evolved around possible experimental schemes to probe such a peculiar state of matter including quantum interferometers

put forward in talks by Ady Stern (Weizmann), Kirill Shtengel (UC Riverside), and Bernd Rosenow (MPI Stuttgart). Other aspects of non-Abelian quantum Hall states, including interaction effects, hierarchy constructions, and quasiparticle descriptions, were discussed in talks by Eddy Ardonne (Nordita), Andrei Bernevig (Princeton), Hans Hansson (Nordita), Gil Refael (Caltech), and Nicola Regnault (ENS Paris).

The culmination of the workshop was an international workshop held in the third week, which Xiao-Gang Wen (MIT) later described as the grand unification of topological order. The dense conference program not only covered the most recent theoretical developments, but also gained significant momentum from outstanding experimental talks. Alois Loidl (Augsburg) overviewed spinel compounds, Merav Dolev (Weizmann) reported on charge fractionalization in the v=5/2 FQH state, Christian Pfleiderer (TU Munich) discussed Skyrmion lattices in chiral metals and semi-conductors, Hidenori Takagi (University of Tokyo/RIKEN) reported on Ir oxides including the experimental observation of quantum spin liquid behavior in Na4Ir3O8 and experimental indications for a topological insulator in Na2IrO3. Satoru Nakatsuji discussed unconventional, spin nematic phases in NiGa2S4, and Laurens Molenkamp reported on the experimental observation of the quantum spin Hall effect in HgTe quantum well structures. These experimental talks were put into broader context by some impressive theoretical talks given by many of the world leaders in the field. A particular highlight was the colloquium of Michael Freedman (Microsoft, Station Q) on Topology, Physics, and Complexity: The birthing of the quantum computer, which gave an intriguing perspective on topological quantum computation.

The seminar and workshop was attended by more than 125 scientists including a large group of junior scientists who actively contributed in the discussions. The two poster sessions were largely shaped by the contributions of these junior attendees and were attended well past the originally scheduled discussion time.

This event was billed as a joint mpi**pks**-APCTP workshop, and it benefitted from the collaboration, as the APCTP was able to identify the most promising young scientists in its catchment area, thereby effectively enhancing the geographic reach to the benefit of all sides involved. As a result, the event assembled some of the most promising young researchers from Asia, Europe and North America, the three global hubs of condensed matter physics.

In summary, the event managed to attract an outstanding international roster of scientists at very different stages in their careers, ranging from doctoral students to a Fields medalist. The concept for a workshop on this budding field has been conceived in the summer of 2007, its topicality further increased over time, and it benefitted greatly from developments in the intervening two years: the program ended up providing a platform for a number of new and important developments in the rapidly evolving field of topological phases of matter.

Dynamics and Statistics of Weather and Climate, Focus Workshop
Scientific coordinators: J. Bröcker, K. Fraedrich, H. Kantz

Main focus: This short *focus workshop* dealt with the accuracy of predictions in weather and climate. Numerical weather predictions and climate simulations rely on detailed models of the Earth's atmosphere (and also ocean currents in the case of climate), which are initialized using observational data and subsequently integrated numerically. All aspects of this approach inevitably contain inaccuracies and errors. On this workshop, the different error sources and their consequences were discussed, along with possible ways to reduce these errors or at least to assess their magnitude. In general terms, erroneous representation of the underlying physics and the initial condition lead to wrong model dynamics and deviations between the statistics of prediction and reality.

Senior participants: The participants included leading experts working in the fields of weather forecasting, climate modelling, and predictability, such as M. Ghil, L.A. Smith, M. Latif, O. Talagrand, C. Penland, P.J. van Leeuwen, Kevin Judd, and Erich Becker

Young scientists: 10 out of the 30 talks of the workshop were presented by young scientists, typically senior PhD students or postdocs. The 20 posters were presented by younger participants. They had the chance to give a very brief overview of their poster (around 2 minutes) in a special session, which turned out to be very successful.

Scientific results: The statement that atmospheric models are only an approximation of reality, and that their dynamics are therefore different from nature, is not new. However, the talks of this conference gave a detailed and quantitative impression of model errors and forecast accuracy. In terms of atmospheric modelling, the audience was rather broad: Different time scales (weather and climate), different physical (sub-)systems (clouds, the atmosphere, and full climate models), different intentions (precise weather forecasts, long run climate projections), different methodologies (statistical prediction and downscaling schemes, ensemble optimization, data assimilation techniques). Therefore, this focus workshop stimulated the discussion between sub-communities. It reflected the state of the art and demonstrated which areas require strong and concerted efforts in the future. Several speakers expressed their concern regarding the validity and therefore the value of detailed global and regional climate predictions, as for example presented in the latest IPCC report and issued by local governments.
A number of topics emerged which, we believe, are of particular interest to the nonlinear dynamics community. Several new paradigms were suggested, such as covariant Lyapunov vectors, random attractors, and several new ideas for data assimilation. A deeper study and thorough assessment of these concepts could be an interesting subject of research for the nonlinear dynamics community, and several collaborations emerged during the workshop. Furthermore, the University of Hamburg presented their Portable University Model of the Atmosphere (PUMA). This model is well documented, simple compared to other atmospheric models, and possible to handle even for the non–expert, yet it is a realistic model of atmospheric motion. This renders PUMA a very interesting testbed for new concepts of nonlinear dynamics methods.

Magnonics: From Fundamentals to Applications, Seminar and Workshop
Scientific coordinators: V. Kruglyak, D. Grundler, S. Demokritov

The focus of the International Seminar and Workshop "Magnonics: From Fundamentals to Applications" held in Dresden from August 2nd to 29th, 2009, was on the newly emerging field of magnonics as highlighted by the title. The field encompasses current research efforts aiming at magnetic materials whose properties are tailored on the nanoscale and where spin waves (magnons) carry and process information. The efforts address the investigation of fundamental properties as well as the creation of novel magnetic field controlled devices. Magnonics is currently gaining momentum, attracting more and more researchers from various subfields of magnetism and materials research, as well as microwave engineering. So, the conference was very well timed and in fact was the first international conference of its kind. During the seminar it was announced that a symposium on magnonics was being initiated in the framework of the APS March Meeting 2010.
The event was very successful, having achieved its main aim of forming a community of magnonics researchers. Researchers from 19 countries and with a total number of 86 were attending the event. The seminar and workshop brought together, both, experts who exhibited world-wide leading positions in nanomagnetism and magnon research as well as young researchers just entering the field. The presentations covered the whole spectrum from fundamental magnonic properties to their application in the information technologies. The main scientific result of the conference in the broader sense was the emergence of magnonics as a sister-field in the family of functional nano-materials, also including electronics, photonics, phononics, plasmonics etc.
The round table discussions held in the course of the seminar, both, provided a further impetus for the search for new concepts addressing the practical realization of magnonic devices and helped to identify future challenges for magnonics. Of particular interest were talks of and discussions with such senior and well-known researchers as Professors Josef Barnas, Bob Camley, Gennadiy Melkov, Sergey Nikitov, Andrey Slavin, and Dan Stancil, who have contributed relevant works on magnon research since decades. The scientific "newcomers" to the field of magnonics, who are in some cases well established in related sub-fields of magnetism, presented excellent contributions. Bright talks were given by Andrii Chumak, Vladislav Demidov, and Alexey Kimel. The event was also very useful in terms of both establishing new collaborations and providing a forum for scientific discussions within existing ones. For example, in one case, a theoretical model successfully describing experimental data presented during the workshop was developed during the life time of the seminar!
The workshop has received a significant publicity, with several invitations to publish Proceedings and to prepare books received by its organizers and participants. After a careful consideration, it was decided to publish a cluster of review articles defining the scope of and the current state of the art in magnonics research in Journal of Physics D: Applied Physics (tentatively in April 2010). Finally, inspired by the

success of the event, it was decided to continue this meeting by transforming it into a conference series, with the next one tentatively held in Recife (Brazil) in 2011.

Tunneling and scattering in complex systems – from single to many particle physics,
Seminar and Workshop
Scientific coordinators: A. Bäcker, M. Oberthaler, P. Schlagheck

This conference was devoted to bringing together experts working on various aspects of tunneling in connection with open system dynamics such as scattering and decay. Being traditionally rooted in atomic and molecular physics, the topic of tunneling has proven its relevance in many other fields of physics, such as mesoscopic science and superconductivity, wave optics in microcavities, as well as ultracold quantum gases. Open issues arise here from the mathematical and conceptual point of view, especially concerning the semiclassical description of tunneling in terms of complex trajectories. They are, moreover, introduced by novel many-body experiments using Bose-Einstein condensates that consist of ultracold atoms.

In view of the diversity of communities that are involved in this topic, the organizers considered it useful to begin this conference with a one-week summer school devoted to the most relevant aspects of this topic. We were happy that we could gain Stephen Creagh (Nottingham) and Akira Shudo (Tokyo) as lecturers for that school, who gave excellent introductions into the mysteries and pitfalls of the complexified classical phase space, and who showed how those ones can help us to obtain a semiclassical understanding of tunneling. Martin Holthaus (Oldenburg) and Oliver Morsch (Pisa), on the other hand, taught us the basics of tunneling with ultracold bosonic quantum gases both from the theoretical and from the experimental point of view. Uzy Smilansky (Rehovot), finally, gave an easily accessible introduction into classical and quantum scattering in chaotic systems.

The didactical part of this meeting culminated on the first day of the main conference in the second week, when Eric Heller (Harvard) delivered an inspiring and motivating colloquium talk devoted to dynamical tunneling and the beauty of semiclassical physics. It was impressive to see how Eric Heller could relate various kinds of nonclassical phenomena, including those that one would most naturally associate with ordinary diffraction, with the notion of dynamical tunneling. On the same day, moreover, Steven Tomsovic (Pullman/WA) gave a very good introductory talk on chaos-assisted tunneling.

Apart from the colloquium talk, we had, in total, 30 oral contributions during this main conference, among them, 4 from atomic and molecular physics, 4 from mesoscopic science, 7 from ultracold quantum gases, 5 from electromagnetic and optical systems, and 9 from quantum chaos and semiclassics. It was an intriguing experience that quite a few speakers did not only focus on the understanding of tunneling and scattering in their respective context, but also pointed out the possible relevance and impact of these phenomena from the application-oriented point of view. This includes the influence of tunneling on the (uni-)directionality of light emitted from chaotic microcavities (e.g. talk by Jan Wiersig/Magdeburg), the usefulness of the semiclassical perspective in order to coherently control tunneling-induced reactions in molecules (talk by Srihari Keshavamurthy/Kanpur), the possibility to read individual quantum bits through tunneling across Josephson junctions (talk by Joachim Ankerhold/Ulm), as well as the impact of tunneling (or rather its inhibition) of K-shell vacancies on the creation of Bell states with diatomic molecules (talk by Reinhard Dörner/Frankfurt). During the lunch breaks and poster sessions, we could observe and participate at quite a few cross-disciplinary discussions, some of which might lead to novel theoretical approaches and experiments in the years to come.

The meeting ended with an informal workshop week where the participants of the conference had the occasion to continue their discussions. This week began with a three-days focus meeting devoted to nonlinear dynamics in complex scattering. Following the tradition of the annual "billiard workshops" that bring together the German quantum chaos community in (mostly) Marburg or Göttingen once per year since 2001, we reserved an entire afternoon session for contributed 30-minutes talks given by younger researchers, such as PhD students and young postdocs. We have to admit that this focus meeting turned out to be a bit less focused than originally anticipated, as some of the invited experts on scattering systems with intrinsic nonlinear dynamics (such as in nonlinear optics or Bose-Einstein condensates) decided to talk about different, more recent subjects of their research. The diversity of aspects discussed in this focus meeting, on the other hand, impressively revealed to us how seemingly different topics, such as localization, graphene, and microwave systems, are now about to become strongly connected to each other.

Altogether, we received very positive feedback from the participants, not only concerning the scientific aspects of the conference but also the perfect organization managed by our conference secretary Mandy Lochar. We should like to thank Mandy as well as the team of the **mpipks** visitors program for their continuous support without which this conference would not have been possible.

Key Experiments with X-ray Pulses from the Perspective of Theory, Focus Workshop
Scientific coordinators: J. M. Rost, I. Schlichting, L. Strüder, J. Ullrich

MOLX09 and MOLX10 have been organized with members of the Max Planck Advanced Study Group at the Center of Free Electron Lasers in Hamburg (MP-ASG@CFEL) as 2.5 days brainstorming meetings. The idea for the first meeting in 2009 was to generate new ideas from the theoretical side for innovative experiments with the new light sources. Topics had a focus on smaller systems under advanced X-ray light.

To spark discussions and act as a think tanks a special format of the meeting was chosen: Each speaker was asked to prepare slides for about 20 minutes while 60 minutes were reserved for his entire contributions - questions and interruptions were encouraged at any time. To further stimulate discussions, the number of participants was restricted to about 30, grouped in a half circle around the blackboard and the screen with only to rows. Participants ranged from PhD students to experienced researchers.

Most participants expressed enthusiastic support for this format and had the feeling they took home much more than from ordinary workshops. This success motivated a second meeting in the same format (this time also the posters were present in the same room throughout the workshop). However, the topic was quite different and far more challenging: What are the opportunities for short X-ray pulses to elucidate the dynamics of large molecules and assemblies in an environment, typically a solution?

Energy Dissipation in Nanocontacts and Molecular Bonds, Focus Workshop
Scientific coordinators: R. Bennewitz, H. Hölscher, P. Reimann, A. Schirmeisen

The workshop took place at the **mpipks** from Sept. 28 until Oct. 1, 2009, and was organized by Roland Bennewitz, Hendrik Hölscher, Peter Reimann, and André Schirmeisen. The main objective of this focus workshop is to bring together practitioners from several related fields, lately evolving into similar directions and thus calling for a forum to exchange those newly upcoming ideas on nanoscale dissipation. Particular emphasize has been put on friction force microscopy, non-contact atomic force microscopy, dynamic force spectroscopy, and related topics like cell rolling and adhesion, macroscopic friction and fracture, and irreversibility per se.

There were 32 invited talks, 14 poster contributions, and 3 participants without contribution. The workshop attracted participants from 3 continents and 14 different countries. Since several PhD-students and younger post-docs presented their results as talks and poster, we are convinced that there was a good balance between contributions by established senior researchers, younger post-docs and PhD-students.

A first highlight of the workshop was the colloquium talk by Robert W. Carpick (University of Pennsylvania), entitled "New insights into dissipative processes: Damping, adhesion, friction, and wear at the nanometer and atomic scale", showing that surfaces and interfaces become the primary regions where energy is dissipated, but that the essential underlying physics is still not satisfactorily understood in detail.

After the colloquium talk, a very vivid and inspiring poster session took place until late evening.

As a further highlight we mention the special final talk by Michael Urbakh (Tel Aviv University) on the subject "Temperature dependence of nanoscale friction". This talk summarized and exemplified in a very convincing manner the initial main idea of the conference, namely to bring together practitioners from different fields – in particular nanofriction and biophysics – lately evolving almost independently of each other into similar directions and thus calling for a timely forum to exchange those newly upcoming ideas.

The local organization was handled by Claudia Pönisch very smoothly and professionally. We like to thank her for the very enjoyable collaboration, the **mpipks** for providing infrastructure and financial support, and the SFB 613 for contributing supplementary traveling money.

Delayed Complex Systems, Workshop
Scientific coordinators: W. Just, A. Pelster, M. Schanz

A complex system normally involves interaction of subunits, and depending on the time scales the propagation speed of information may become relevant for the dynamics. Thus, dynamics with time delay is going to play a vital role in new emerging fields of science and technology, for instance, because the speed of modern data processing does not allow to neglect finite propagation times of signals any more. The workshop Delayed Complex Systems (DCS09) addressed a wide range of such topics, covering fundamental aspects and applications. We think this interdisciplinary workshop may stimulate future developments and will encourage new interactions between different lines of research within this rapidly expanding vibrant field of delayed complex systems. The workshop was very generously supported by the Max Planck Institute for the Physics of Complex Systems. We have received an enormous amount of positive feedback from the participants, and the workshop has been seen as an overall success. mpi**pks** is widely known for its excellent workshop and seminar program which is managed to the highest standards. The support by the local organisation committee, in particular by Ms. Roscina, was extraordinary, and the perfect organisation of the event was appreciated by all participants. We as scientific coordinators of the workshop are extremely grateful to mpi**pks** for having been given the opportunity to organise DCS09 at the Max Planck Institute.

The new era of complexity science faces two challenges, namely dealing with the nontrivial topology of interacting subunits, and the challenge caused by time delay with the associated dynamics taking place in infinite dimensional phase spaces. Within the last fifteen years the research activities have considerably increased as many new applications have emerged in different areas, such as electronic engineering, controlling chaos, laser physics, or neuroscience. In particular, there are striking analogies between lasers and neural systems in both of which delay effects are abundant. The dynamics of complex systems with time delay is thus one of the emerging fields in dynamical systems theory with a high impact on applications in science and engineering. The workshop addressed this issue on a very broad basis. The event covered both applications and experiments as well as mathematical foundations. The workshop had a particular focus on interdisciplinary science, bringing together researchers from different scientific disciplines to stimulate cross-fertilization of research. Key participants: The very generous support by mpi**pks** enabled us to invite more than 30 invited speakers, all world leading experts in their field, 22 of whom gave keynote review talks. Among these main contributions a few were highlighted by evening and opening lectures, and the mpi**pks** colloquium.

75 participants from 22 countries attended the workshop. Due to the generous support by mpi**pks** we could allocate substantial resources to support young researchers, i.e. PhD students and post-docs at an early stage of their career. It was very much appreciated that we could offer partial support for travel expenses, even for non-invited speakers. We gave priority to requests from young researchers from developing countries.

Selected plenary talks will be published by the end of this year as a theme issue on Delayed Complex Systems in the Philosophical Transactions of the Royal Society A. The theme issue will considerably contribute to the dissemination of the scientific results of the workshop. From a a wider cross-disciplinary perspective the workshop was quite successful in establishing links between different scientific communities, in particular with regards to fundamental aspects in mathematics, engineering and experimental laser physics, as well as neuroscience. This claim is supported by the outcome of the very fruitful round table discussion on future trends in in nonlinear dynamics with delay which was held at the workshop. Thus, academic beneficiaries are already visible by enhancing and stimulating research across different disciplines, in particular linking science with applications of technological relevance. In that respect the workshop may even have considerable socio-economic impact on a longer time scale, by knowledge transfer of modern developments in complex dynamical systems theory from science to technology.

State-Dependent Delay Equations, Workshop
Scientific coordinators: J. De Luca, A. R. Humphries, J. Mallet-Paret

This workshop surveyed recent advances and ongoing research across the field of Delay differential equations (DDEs), with particular emphasis on state dependent DDEs, neutral DDEs, mixed-type functional differential equations with both advanced and retarded arguments, and problems with a differential-algebraic structure, including the equation of motion of a charged particle in the action-at-a-distance electrodynamics. State dependent delay equations arise in many applications, but fall outside the scope

of the rapidly maturing theory of fixed delay equations, and give rise to challenging problems in both the mathematical analysis of the equations and the numerical computation and analysis of solutions. Although progress has been made in recent years on some model state-dependent problems, in particular monotone problems with positive or negative feedback, the behavior of more general and realistic systems remains poorly understood.

The workshop brought together researchers from different fields including physics, engineering, physiology and mathematics to exchange recent results, ideas, techniques and problems, and to discuss future directions in the field. Many of the participants were meeting each other for the first time, a clear sign that we were succeeding in the bringing practitioners from different fields together, as evidenced by direct feedback and the article at http://www.dynamicalsystems.org/ma/ma/display?item=315

Even the basic theory of state-dependent delays still raises many open questions, and the analysis and numerical analysis of these problems constituted the main themes of the workshop, and were the common point that united the participants from disparate fields. In his colloquium talk Hans-Otto Walther presented the mathematical framework for considering state-dependent delay equations as dynamical systems with semi-flows on an infinite-dimensional functional space, and the results and open problems of this approach.

Four talks, delivered by Gernot Bauer, Dirk Deckert and C.K. Raju and Savio Rodrigues, considered the equations of motion of charged particles in the action-at-a-distance electrodynamics, which are a neutral mixed-type implicitly state-dependent differential equation, and their formulation and numerical solution as (well-posed) initial value or boundary value problems. These were perhaps the most challenging equations considered during the workshop, but combinations of the different difficulties they pose (including neutrality, advanced and retarded arguments, implicit state-dependency and numerical solution) arose in other equations presented throughout the week.

Mike Mackey showed how delays arise in Bacterial operon dynamics, and other talks considered delays in microvascular blood flow, neural dynamics, epidemiology and population dynamics. State dependent equations (including implicitly state-dependent) were shown to arise naturally in a series of interesting engineering problems, including regenerative cutting and hybrid systems testing.

Analysis and numerical analysis were shown to work in consort in the talk of Alfredo Bellen concerning termination and regularization of solutions of state dependent neutral delay equations. Other numerical analysis talks tackled problems including computation of Lyapunov exponents, boundary value problems, spectral methods and delay dependent stability of numerical methods, the last of which resonated with the analysis talk of Ferenc Hartung considering linearized stability in state-dependent DDEs. Other analysis talks considered singular perturbed problems and slowly oscillating periodic solutions, computer assisted proofs, smoothness of manifolds and co-existence of periodic solutions. If delay problems are hard because of the infinite dimensionality, as are PDEs, partial differential delay equations are doubly hard and Wolfgang Ruess closed the meeting by presenting the theory and open problems of PDDEs.

A particular aim of the workshop was to give young scientists a forum to present their work, and interact with established researchers in the field, and of the 48 participants, 11 were graduate students, and another 11 postdoctoral researchers. These junior scientists participated fully in the workshop with 12 presenting posters in the poster session, and 9 giving talks. Some of them will likely be working in this field for a long time to come.

This was to the best of our knowledge the first workshop dedicated to state-dependent delay equations, and it brought together all manner of scientists that had not interacted before. Many interesting discussions ensued, a number of participants indicated that they are in the early stages of exploring completely new collaborations as a result of the workshop. No doubt the fruitions of these collaborations will be revealed at future SDDE workshops, but the first such workshop was at the mpi**pks** in Dresden, and it was a great success.

Physical principles of protein behavior in the cell, Workshop
Scientific coordinators: M. Porto, H. E. Roman, M. Vendruscolo

The workshop, which took place on 26-30 October 2009, was concerned with the problem of understanding the physical principles that govern the behavior of proteins in the cell. This theme is relevant since proteins are involved in essentially all of the biochemical reactions that take place in living organisms, including those required for the control of gene expression, metabolism, transport, and enzymatic

catalysis. The workshop was inspired by the realization that the mechanisms of protein regulation are being elucidated at an increasing pace, and many advances have been made in our understanding of how protein concentrations, localizations, and interactions are controlled within living cells. The introduction of novel experimental high-throughput techniques and of theoretical analysis methods have enabled the initial study of the networks of interacting molecules that underlie the functioning of the myriad biological pathways through which cells maintain homeostasis and promote development. Considering these advances we decided that it was timely to organize a meeting to discuss current achievements and future directions.

Our workshop had a distinctly interdisciplinary character and brought together researchers from the major areas relevant to understanding protein behavior in the cell, including protein expression, transport, localization, function, folding, misfolding, and aggregation. As a consequence, synergies between experimental, theoretical, computational, and statistical approaches were anticipated on two main fronts: to improve our understanding of the physico-chemical basis of protein behavior, and to suggest new methods for predicting and modulating it. Achieving these synergies will help provide an integrated view of the subject, and the workshop stimulated such developments by exploring the connections between different fields and by providing a suitable framework for exchanging ideas and methods. Our primary aim was to probe in depth the idea that further understanding of the physical principles that underlie protein behavior in the cell can greatly improve existing methods for characterizing and predicting structures, interactions, and functions of proteins, for modeling their evolution, and ultimately for suggesting new rational approaches for treating human diseases.

The workshop has been organized in topical sessions, 'Proteomics I and II' (R. Aebersold, K. Büssow, M.B. Mohan, P. Schwille, K. Lilley, M. Mann, and S. Brunak), 'Protein evolution' (E. Shakhnovich), 'Modeling cell behavior' (S. Grill, G.G. Tartaglia, and H. Bussemaker), 'Protein folding and misfolding I and II' (J. Frydman, S. Ventura, D. Müller, and A. Horovitz), 'Protein interaction' (P. Aloy, A. Plückthun, M. Schroeder, and J. Colinge), and 'Protein expression' (N. Luscombe, C.O. Wilke, R.N. Day, and E. Marcotte). Besides the contributions of the invited speakers, the workshop has also benefited from the very high level contributions by non-invited participants, both in the form of short oral presentations as well as in the poster sessions. The friendly and communicative atmosphere that developed from the very beginning favored the discussions, which was also facilitated by the fact that most talks contained references to the work of other participants.

One interesting additional outcome of the workshop has been to identify in a broad sense how physics can contribute to biology: (1) By developing new techniques. Standard methods such as X-ray crystallography and NMR spectroscopy have been developed in this way. More recently, and related to the theme of this meeting, mass spectroscopy and various types of imaging techniques. (2) By developing new statistical methods of data analysis. (3) By formulating models and theories to rationalize existing experimental observations and to propose new experiments.

Participants' reactions to our efforts to integrate the so far separated disciplines into a single workshop, and possibly into a common scientific community, have been unanimously enthusiastic. We plan to publish a selection of peer-reviewed papers in a special issue of an international journal.

The organizers wish to express their sincere gratitude to the **mpipks** for hosting and financing this workshop and for the very generous support.

TCS-Program: Synchronization and Multiscale Complex Dynamics in the Brain, Workshop
Scientific coordinators: J. G. Ojalvo, C. Mirasso, G. Pipa

The purpose of BSYNC09 was to bring together experimental neuroscientists working with different levels of description of brain activity, and physicists experienced in the study of multiscale processes, in order to bridge the gap currently existing between the theoretical and experimental approaches to the understanding of brain function. The result was a conference with an unusually diverse combination of invited speakers and participants, including highly recognized and well known scientists in clinical neurophysiology (Cornelis Stam, Jose Luis Cantero), experimental neural dynamics (Gilles Laurent, Wolf Singer, Maria V. Sanchez-Vives), psychiatry (Michael Breakspear), neuroimaging (Rainer Goebel, Fernando Maestu), complex network theory (Stefano Boccaletti, Mario Chavez, Victor Eguiluz), computational and theoretical neuroscience (Alessandro Villa, Klaus Obermeyer, Gordon Pipa, Fritz Sommer), nonlinear and stochastic physics (Lutz Schimansky-Geier, Benjamin Lindner, Arkady Pikovsky), neuronal

modeling (Hans Braun, Dmitry Postnov), and biomedical time series analysis (German Gomez-Herrero, Ernesto Pereda). Among the specic topics covered, some of the talks dealt with the application of complex-network approaches to characterize and understand the structural basis of brain dynamics and the resulting functional connectivity proles (M. Chavez, C. Stam, M. Valencia, A. Diaz-Guilera, V. Eguiluz, A. Arenas, S. Boccaletti). Another group of talks emphasized criticality and percolation as crucial characteristics of brain activity (M. Breakspear, W. Shew, J. Soriano). The existence of synchronization-based correlates of neurological disease was discussed by W. Singer, F. Maestu, O. Rosso, A. J. Pons, and F. Amor. The computational capabilities of the brain were analyzed from dierent perspectives in the talks of A. Villa, G. Pipa, F. Sommer, K. Obermeyer, J. Cabessa, and R. Vicente. The relevance of oscillatory activity in time and/or space for the correct operation of the brain was discussed by G. Laurent, T. Siapas, E. Niebur, M. Sanchez-Vives, and K. Takahashi. Theoretical studies of dierent aspects of synchronization in neuronal models were reported by L. Schimansky-Geier, H. Braun, A. Pikovsky, D. Postnov, and E. Ullner. The talks by G. Gomez-Herrero and E. Pereda provided an overview of techniques that allow us to determine correlation and causality in the functional activity of the brain. The importance of neuroimaging in monitoring the brain at the appropriate temporal and spatial scales was discussed by R. Goebel. The potential of anesthesia as a brain state adequate for the study of global brain activity was described by B. Scheller, while I. Fischer proposed a cross fertilization study between laser dynamics and neurons that would allow us to understand new mechanisms leading to particular synchronization mechanisms. A very stimulating collection of posters was also presented in the conference, and discussed during three dedicated sessions in the conference program. A wide variety of topics following the main themes described in the previous paragraph were presented in the posters. Additionally, a round table discussion was devoted to exchange opinions on the factors that most likely determine the collective activity of a healthy brain, the role of theoretical modeling in linking these factors with experimental data, and the importance of nonlinearity and noise in brain activity. In summary, the workshop BSYNC09 provided a setting in which experimentalists and theoreticians, and researchers at the neuronal and macroscopic scales of the brain, exchanged ideas, compared views and shared goals on what mechanisms underlie the normal coordinated function of the brain. Informal feedback from participants showed that they were very satised with the meeting, and were interested in repeating the experience again. Clearly the **mpipks** is an excellent setting for the exchange of interdisciplinary ideas, and we are very thankful for the support received from the institute.

TCS-Program: 150 years after Darwin: From molecular evolution to language, Workshop
Scientific coordinators: J. A. Cuesta, S. C. Manrubia, A. J. McKane

The theory of evolution has permeated our lives in many different ways. Beyond biology, many other disciplines use not only the metaphors of evolution and adaptation, but also formal mechanisms analogous to those proposed by Charles Darwin a hundred and fifty years ago. The publication of "On the origin of species" was commemorated in 2009, together with the anniversary of Darwiń s in 1809. The series Trends in Complex Systems provided an ideal scenario to bring together researchers from the variety of disciplines which now use the evolutionary paradigm. The main goal of the workshop was to review progress and different viewpoints, to learn from each other, and to initiate new transdisciplinary collaborations. During the five days of the workshop there were interesting presentations from many at the forefront of international research. The workshop had a conceptual time-line that spanned from the origin of life — and things that Darwin would have liked to know — as presented by Juli Peretó in the opening talk, to linguistic evolution and the origins of language, an issue discussed by Luc Steels in the closing talk of the conference. In between, sessions on the emergence of biological complexity and how evolution and adaptation can be mathematically formulated, on the role of games and cooperation, and on evolutionary economics, took place. There were especially noteworthy contributions discussing the patterns that underlie adaptive radiation (Sergey Gavrilets), the relevance of selection in genealogy (Bernard Derrida), and the intricacies of biological cheating and its feedback mechanisms (Peter Hammerstein). Moving to the interplay between evolution and human societies, challenging issues such as information transmission among humans (Bruce Edmonds), the co-evolution of genes and culture (Herbert Gintis), the motors of linguistic change (William Croft) and exciting proposals on the global world economy and climate change based on our use of energy (Gerald Silverberg) were elaborated on. It was especially welcome to see young researchers present clear and compelling summaries of work in their area. In this context we would mention the invited talk by Arne Traulsen, as well as many contributed talks, such as the one by Richard Blythe. The conference provided an inspiring environment

for invitees and the rest of the participants. Its success was largely due to the effort of all participants to communicate their research in ways that were both clear and attractive to their peers in other disciplines. Avoiding a too technical approach to issues in different fields gave us as a reward a broad picture of how universal evolutionary mechanisms are, and of how deeply they effect our understanding of the emergence of organization and complexity. Hopefully, the meeting represented a launching pad to develop unified views of evolution and adaptation, from inorganic chemistry to complex human behaviour.

Exploring Complex Dynamics in High-Dimensional Chaotic Systems, Workshop
Scientific coordinators: J. M. López, A. Politi, A. Pikovsky

The main focus of the Workshop was to study forecasting tools for high dimensional chaotic systems. There are a number of well-known approaches to tackle this problem in low dimensional systems, but making useful forecasts becomes tremendously difficult as the number of degrees of freedom increases. The Workshop analyzed two complementary approaches to predicting highly complex systems. On the one hand, the dynamical-system approach, that is based on concepts such as unstable and stable manifolds, Lyapunov vectors and exponents, chaotic attractors, etc are exploited to forecast the future. On the other hand, the optimization/control theory approach, which, starting from the knowledge of past time series, is based on the implementation of statistical tools like the ensemble Kalman filter, data assimilation, Bayesian estimations, etc. A common problem in either approach is how to deal with the fact that our observations do not coincide with the predicted trajectory and how to use the information from new observations to improve the performance of the prediction algorithm for the next time window. During the Workshop it has become clear that the unavoidable inaccuracies of the mathematical models (think of the ocean flow and weather model applications) limit the performance of any approach based solely on dynamical-system theory. At the same time, knowledge of the system dynamics (possibly in the presence of noise) is essential for the construction of ensembles of trajectories and thereby to make optimal predictions.

The most appreciated aspect of the Workshop has been the opportunity offered to each participant of fruitfully interacting with members of different communities: nonlinear dynamical systems, statistical mechanics, weather forecasts, and oceanic flows. Moreover, the whole range from fundamental theoretical problems through toy models up to particular applied implementations has been covered. As a result, profitable exchanges of ideas took place during the oral presentations at question time (more than for average Workshops), and during the two poster sessions. Quite remarkable was also the lively discussion during the Round Table, when the different methods adopted by the European and American forecasting centers were mutually compared. Finally, the friendly environment at the mpi**pks** Institute contributed to extend the discussions at all aspects, and to trigger new scientific collaborations.

Quantum Gravity, Workshop
Scientific coordinators: B. Dittrich, R. Schützhold

This focus workshop concentrated on the subject of quantum gravity. There are various approaches to quantum gravity. Due to severe difficulties, ranging from the operational to the conceptual, none of them has led so far to a completely satisfactory theory. These problems relate however to the same set of issues coming in different disguises in the different approaches. It is therefore important to bring the experts from different approaches together, to foster discussions and search for the best techniques among all the available approaches in order to make progress on these problems. The main aim of this workshops was therefore to bring quantum gravity researchers from different groups together, in particular from newly established ones in Germany. The speakers covered many groups, for instance Astrid Eichhorn (Jena), Christian Fleischhack (Paderborn), Dominico Guilini (Hannover), Samo Jordan (Utrecht), Claus Kiefer (Köln), Claus Lammerzahl (Bremen), Catherine Meusburger (Emmy Noether Group, Hamburg), Daniele Oriti (AEI, Potsdam), Frank Saueressig (Emmy Noether Group, Mainz), Martin Reuter (Mainz), and the the main current approaches to quantum gravity, among them loop quantum gravity, spin foams, group field theory, asymptotic safety, causal dynamical triangulations, quantum gravity phenomenology, cosmological imprints of quantum gravity and analogue models for quantum gravity. The workshop featured a number of overview talks typically delivered by the younger researches in each field, for instance on loop quantum gravity (Johannes Brunnemann), asymptotic safety (Frank Saueressig), cosmology (Gianluca Calcagni), group field theory (Daniele Oriti), causal dynamical triangulations (Samo Jordan) and analogue models (Lorenzo Sindoni). These were very much appreciated both by the younger and

more experienced researches as these were expressively aimed at people outside the community following the approach in question. In addition various more technical talks provided insights on subjects and problems common to a number of approaches. The workshop allowed for ample of discussion time, which was well used to clarify differences and common ground between the various extant approaches. Several participants expressed plans to organize future workshops of similar kind to foster further discussions and exchange of ideas. The atmosphere was very constructive and all the participants were extremely happy with the organization and infrastructure provided by the mpi**pks**. In particular the scientific coordinators wish to express their gratidue to Sofia Roscina for her excellent work in organizing this workshop.

Self-Organization in Turbulent Plasmas and Fluids, Summerschool and Workshop
Scientific coordinators: F. Jenko, R. Friedrich

The main goal of the TURB10 meeting which took place from May 3 through May 14, 2010 was to bring together leading scientists and young researchers from three neighboring fields, namely fluid turbulence, plasma turbulence, and dynamo theory. The meeting consisted of a one-week summer school - attended by 8 lecturers and about 70 participants from various countries - and a one-week international workshop with more than 80 participants. The latter focused on the topics of basic turbulence characteristics in plasmas and fluids (including the important question of universality), Lagrangian turbulence, structure formation and shear flows in turbulent systems, turbulence control, liquid metal and plasma dynamos, planetary dynamos, as well as turbulence in astrophysical systems. The talks are available on the internet at www.ipp.mpg.de/ mjpuesch/turb10

The quite unique scope of the meeting sparked a lot of interest internationally, so that it was overbooked by about a factor of two. Among the most prominent speakers were Profs. Bodenschatz, Brizard, Büchner, Carati, Christensen, Cowley, Eckhardt, Falkovich, Farge, Forest, Grauer, Hammett, Hansen, Hasinger, Jones, Krommes, Lathrop, Peinke, Pinton, Pumir, Rüdiger, Schlickeiser, Schneider, Schumacher, Shats, Stroth, Terry, Tilgner, Tsinober, Vassilicos, Wilkinson, and Zimbardo. At the same time, a large number of talented younger scientists presented very interesting oral and poster contributions. The participants came from a variety of different European and non-European countries including the US, Australia, Japan, Russia, Brasil, Argentina, and India.

According to the feedback of the participants, the meeting was very valuable for learning from and reaching out to the neighboring communities, and for establishing new contacts and connections. Putting one's own results into a broader perspective was conceived as helpful and important. Numerous cross-disciplinary topics were discussed, and common links discovered. People which had often been referring to each other's publications met personally for the first time. Also, a renewed sense of togetherness emerged from these two weeks which might well be the basis for further common activities and projects. Overall, the meeting may thus be judged as very successful.

Optical Microcavities: Quantum Chaos in Open Systems Meets Optical Resonators,
3rd Asian-German Workshop
Scientific coordinators: S. Shinohara, J.-W. Ryu, M. Hentschel

The focus of this workshop was on recent developments in the field of optical microcavities, with a special emphasis on their relation to other open quantum systems. The workshop brought together experimentalists and theoreticians, laser and mathematical physicists, researchers from Korea and Japan with European (mostly German) physicists, and, last not least, the various groups working on this subject in the Dresden research institutions. Whereas we had originally anticipated about 20-30 participants, the workshop was so well received that eventually up to 50 people gathered in the lecture hall. The rather long coffee breaks, poster sessions, and excursion were very well received and used for intensive discussions. The poster presenters, mainly PhD-students, appreciated the opportunity to introduce their work in five-minutes flash talks during a specially assigned session (that filled the gap caused by the absence of Henning Schomerus that resulted from volcano ash and flight cancellation). All talks were of high quality and the poster session was used for active and lively discussion not only by the younger participants.

The aims of the workshop were: (i) to share knowledge and foster further research collaboration on topical problems in optical microcavities, (ii) to review the most recent theoretical and experimental advances, (iii) to make the connection between real optical systems (where the openness arises from the dielectric nature of a cavity) and abstract open quantum mapping systems (where the opening is set by hand and therefore allows an easier control, understanding, and tailoring of the properties).

The main scientific results of the workshop were on the areas of

- Laser physics:
  - different levels of complexity in laser equations, origin of chaos
  - nonlinear dynamics and pattern formations in lasers
  - applications of laser chaos to communication and encryption
- Microscopic laser systems:
  - a variety of systems was introduced ranging from quantum dots to rolled-up microcavities
  - various possibilities of tuning of modes were explained
  - single-mode vs. multi-mode lasing
  - quest for directional emission from micro (i.e., non-Fabry-Perot) lasers - solution via
- Quantum chaos and microlasers:
  - universality of the far-field patterns associated with unstable manifolds of ray chaos
  - exceptional points: experimental detection and theoretical understanding
  - role of partial barriers in phase space for emission properties
  - deviations from geometric optics and wave-ray correspondence, including microresonators with negative index of refraction
- Connection between optical microcavities and general open quantum systems
  - understanding of tunneling rates in composite systems
  - scar functions approach to open quantum maps

The conference was characterized by a very open and cooperative atmosphere and intensive scientific exchange that resulted in the explicit wish to continue this series of meetings with the next meeting taking place in Korea in 2011. We consider the fruitful and intensive discussions among all participants as a sign of broadening one's horizons and the success of the workshop.

We would like to thank the APCTP, the DFG Research Group FG 760 and the DFG Emmy-Noether-Programme for generous support. We enjoyed and really appreciate the mpi**pks** hospitality and thank Claudia Pönisch for the local organization that despite a rather involved financial situation went absolutely smooth.

Dual Nature of f-Electrons, Focus Workshop
Scientific coordinators: T. Durakiewicz, P. Fulde, G. Zwicknagl

Workshops on the Dual Nature of f-electrons are organized by the same group biannually since 2006. The first event was organized in Santa Fe, NM, USA in 2006, next in 2008 at the same location. This year we moved to Dresden in order to attract the broader spectrum of European scientists. The number of speakers went up from 18 in 2006 and 17 in 2008 to 36 in the current edition. This number proves that Dresden was an excellent choice, with a guaranteed broad participation of scientists involved in f-electron research.The conference is traditionally focused on the issues of f-electron materials.

Just to list a few participants, we note the talk by Zachary Fisk on quantum criticality, a "blackboard presentation" by Gertrud Zwicknagl on the dual life of f-electrons and Gerry Lander's on neutron scattering in f-electron research. We also had a privilege to listen to Peter Riseborough, John Mydosh, Peter Oppeneer, Ladia Havela and Gabi Kotliar and several other excellent presentations. Dominant topics were: electronic structure and properties, superconductivity and magnetism, new materials, Kondo physics, competing ground states and quantum criticality. It is a tradition of the workshop to have a more or less even mix of theory and experiment, and to devote two afternoons to topical sessions and discussion panels. Students and postdocs presented three talks and several posters, and their presentation style and the message were very well accepted by the participants.

For this meeting, we decided to choose two specific areas for topical sessions and discussion panels: URu2Si2 and DMFT. The enigmatic hidden order state in URu2Si2 generates lot of interest in the community, with several novel results in both theory and experiment presented during the last two years. The six topical talks and a discussion panel were very well attended, and the discussion can be counted as one of the most heated debates in the field.

From the scientific point of view, out of over 30 or so theories attempting to describe the hidden order phase, two seem to be surfacing. One theory approaches the order parameter question from the point of view of the fluctuation induced lattice symmetry breaking, leading to well developed and strongly k-dependent gapping of the Fermi surface. In this approach, time-reversal symmetry is broken on a timescale comparable to the fluctuations time. The other, DMFT-based approach, describes the formation of multipolar order in the HO phase, which by itself does not invoke time-reversal symmetry breaking. As a result of this discussion it became clear that a careful new experiment confirming or excluding time-reversal symmetry breaking would help confirm one of the models.

The second panel of four talks and discussion session was devoted to the aspects of Dynamical Mean Field Theory (DMFT). The discussion showed that several approaches to DMFT from different groups are not always parallel, and important details like for example the treatment of RKKY interaction, require further clarification. Nevertheless, DMFT remains the rapidly growing approach to calculating many-body effects in f-electron systems. It has to be noted that the scientific coordinators are univocal in admiration for impeccable organization of the event provided by mpi**pks**. The institute is considerably helping the physics community. Mrs. Lantsch who was in charge for the workshop did an admirable job.

We would like to build on this success and we are contemplating the possibility of organizing the focused f-electron photoemission workshop in Dresden. There is a lot of new information coming up in ARPES and in calculations, and the field is evolving rapidly. It would be excellent to capture this energy and have most of the players in the field meet in one place for an exciting exchange of information. We can not think of a better place than MPI-Dresden to have this event, perhaps in the early Fall of 2012.

Particulate Matter: Does Dimensionality Matter?, Workshop
Scientific coordinators: P. Charbonneau, K. Daniels, M. Schröter

From May 30-June 4, more than 60 chemists, engineers, mathematicians, and physicists from 5 continents gathered for a workshop at the mpi**pks** to address the question "Particulate Matter: Does Dimensionality Matter?" The main focus of the conference was to better understand industrially-important materials, such as sand, glasses, colloids, foams, and emulsions by comparing their behavior – and that of related models – in 2, 3, and more dimensions. Looking at the world from a dimensional lens helped 19th century *Flatland* readers grasp the metaphorical role of the fourth dimension; higher dimensions can also help scientists shine new light on our relatively low-dimensional world. A flat layer of coins pushed together on a tabletop and a pile of oranges on a grocer's stand have both similarities and differences. They are both the densest possible packing of spheres in their respective dimensions, but the way in which they form, support stress, and rearrange, are different. Computers allow us to contrast similar systems in even higher dimensions. The scientific discussion was lively: not all participants agreed about the role of disorder and randomness, or even the importance of the number of dimensions. Yet, certain lines of agreement have started to appear, as well as key regimes in which to conduct future investigations. The original motivating scientific question was raised to a higher level than the organizers had anticipated. A new awareness of where to look for similarities and differences in dimensionality has arisen. For example, Corey O'Hern provided a provocative list of 16 dimension-independent properties of dense particulate matter. Friction, polydispersity, temperature, and particle shape are also important variables, but isolating the possible impact of dimensionality from these other factors is necessary if one hopes to make sense of the results. A particular emphasis on the dynamics and structure of disordered systems was noted. On the one hand, the role of dimensionality in theories of jamming and the glass transition led to animated discussions about the physical basis and range of validity of the many analytical approaches explored by various groups. The state of the question and the nature of the challenges ahead have become clearer as a result. On the other hand, the description of order and geometry in disordered systems using local parameters that are accessible in both simulations and experiments – and a need to understand how these different measures differ from each other – allowed the identification of parallel challenges in separate scientific communities. Several participating groups currently in a race to find the densest possible packing of tetrahedra were present. Record-holder Sharon Glotzer gave a lively presentation

of the history of the race. Various novel techniques that this packing problem has spawned were also presented, which opened a line of conversation on combining analytical tools with computational methods in higher dimensions. Connections of packing problems to disordered biological systems were enlightening to many in the community, and will probably yield new research directions. All postdocs and graduate students had posters and/or talks, and extensive lively discussions with senior participants during meals and breaks. Female graduate students and postdocs in particular were observed to network extensively with each other and with senior participants, which lays the groundwork for their future collaborations. Overall, the week-long meeting allowed the researchers to spend a focused period of time discussing these issues, allowing them develop ideas for future research directions, and to capture the momentum created by these often independent developments taking place around the world.

Quantum Information Concepts for Condensed Matter Problems, Seminar and Workshop
Scientific coordinators: I. Affleck, M. Haque, U. Schollwöck

The workshop and seminar was envisaged as an opportunity to explore emerging results at the interface of quantum information (Q.I.) theory and condensed matter physics, from a condensed matter point of view. It was intended that the programme would play a timely role in nucleating the emerging community focusing on this topic. The programme was very successful in fulfilling this goal. The event was perfectly timed for the wide dissemination of a number of significant results that have emerged very recently. The interest in the topic, and the number of condensed matter physicists using and studying Q.I.-inspired concepts, have only recently grown large enough to provide the critical mass necessary for such a programme. The two-week programme thus provided an interaction opportunity that was crucial at this stage of the development of the field. The topic has attracted some of the leading thinkers in condensed matter theory, and this was reflected in the concentration of prominent theorists among the participants. The workshop week also included a number of junior scientists working in Q.I. groups; the programme provided for this community a much-appreciated exposure to the condensed matter perspective. Format. There were 26 talks and a colloquium in the first (workshop) week, and 16 talks and a colloquium in the second (seminar) week. The unusually sparse workshop week provided excellent opportunities for discussion and collaboration, and the participants seemed to benefit immensely from this extra time. The first week had two after-dinner poster sessions. There were 45+ posters put up, and the accompanying vibrant discussions continued well beyond the scheduled time. The sessions were not organized by subtopic; instead different subtopics were mixed into each session. This seemed to work well as participants at each session got exposure to a variety of emerging themes. There were about 80 participants in the first week and about 25 participants in the second. Colloquia. Ian Affleck, one of the coordinators, was the speaker for the first week colloquium, which was a major highlight of the week. The colloquium was delivered to a packed auditorium and heavily attended, not only by the workshop attendees, mpi**pks** Report; Workshop & Seminar QICCMP10 members, and other mpi**pks** visitors at the time, but also by people from neighboring Dresden institutes. The talk focused on the phenomenon of the Kondo cloud and on entanglement measures used to characterize the Kondo cloud. The second week colloquium speaker was Paul Fendley, who gave an entertaining and informative talk on exact results on spin chains. Scientific highlights. Of the various aspects discussed at the workshop, we mention below only a few themes. One prominent direction was the connection of entanglement entropy in many-body states to more physical concepts such as noise or fluctuations. Fradkin, Levitov and Lehur gave reports on this line of work. A fascinating but poorly-understood aspect is the connection of the so-called entanglement spectrum with the spectrum or other properties of many-body systems. Läuchli, Poilblanc, Regnault, Pollmann, and Bray-Ali introduced some cross-section of recent developments on entanglement spectra. Several speakers (Eisert, Barthel, Corboz, Verstraete, Heidrich-Meisner) reported developments in computational techniques or their use, e.g., the development of tensor network algorithms to treat fermionic systems. Impurity models in condensed matter are widely viewed as having intricately entangled states. Several speakers reported the use of entanglement to characterize such states, or designs to use the entanglement in such systems (Laflorencie, Sodano, Sorensen, Bose). The organizers made some effort to have an experimental component to the workshop, although the topic is by its nature theory-oriented at this stage of its development. Weinfurter and Aeppli provided experimental highlights. There were also two reports from prominent condensed matter theorists (Joynt, Moessner) contributing in the other direction, i.e., applying condensed matter techniques to Q.I. problems, respectively the graph isomorphism problem and the quantum k-SAT problem. A number of speakers reported on continuing developments on entanglement/fidelity at quantum criticality or in particular condensed matter phases (Bonesteel, Misguich, Joel Moore, Refael, Schoutens, Kun Yang).

Summary. The workshop collected and attracted researchers approaching the interface of quantum information and condensed matter theory from a variety of perspectives, using a variety of techniques. The overall high quality of talks, the large attendance, and the positive feedback from participants, confirm that the programme was indeed successful in meeting its goals. The programme was conceived in mid-2008. In the beginning, there was some scepticism about whether the topic merited a two-week programme. However, the overwhelming interest in attending the programme (many applications had to be rejected) and the eventual participation of many leading researchers showed that a multi-week event was indeed necessary and useful. It is expected that the workshop and seminar will stimulate further growth of some of the topics highlighted during those two weeks.

Few Body Dynamics in Atoms, Molecules and Planetary Systems, Focus Workshop
Scientific coordinators: A. Buchleitner, F. Diacu, G. Tanner

Main Focus: Celestial mechanics and atomic physics share a common interest in studying the dynamics of few-body systems interacting via potentials. The methods and techniques used in the two research areas could not be more different, however. While the motions of planetary bodies is governed by -in general nonlinear ODE's with often complicated singularity structures, atomic and molecular systems are described by a linear PDE - Schroedinger's equation - and are solved by spectral methods, Green function expansions or complex rotation techniques etc. Recent advances in semiclassical techniques as well as steady experimental progress in short pulse laser and detector technology makes it necessary to consider the classical dynamics of charged particles in more detail. These efforts greatly benefit from techniques developed in nonlinear systems theory in general and in the context of gravitational few-body problems in particular. The focus of this workshop was to bring the two communities together and to discuss the state of the art in particular in the areas phase space structure of few-body planetary and atomic systems, dynamical aspects of the solar system and beyond, symbolic dynamics and chaos in few body systems, transition state theory, semiclassical treatment of few-body Coulomb systems and highly (multiply) excited states in atoms and molecules; experimental results and numerical techniques.

Summary of contributions by participants: The conference benefited in general greatly from the efforts of the speakers to make their topic of research available to a general audience. The talks by Robert Mackay on 2nd species orbits and Ernesto Perez-Chavez on relative equilibria in curved space gave fascinating insights in what can and can not be done in terms of rigorously proving the existence of dynamical features in few body planetary systems. Holger Dullin introduced us to a new geometric integrator for n-body problems and Florin Diacu gave an overview over singularity problems in the field in the colloquium talk. The transition to few-body Coulomb systems was provided by Andreas Knauf, Bruno Eckhard, Tobias Kramer and Agapi Emmanouilidou discussing electron-electron correlation effects in the classical dynamics of few and many body systems. Jaques Laskar worried us by demonstrating that the earth will collide with another planet at some point - it only has the choice to either do it with Mars or with Venus. Symbolic dynamics in 3-body problems was discussed by Mitsusada Sano and Kiyotaka Tanikawa and in a more general setting by Predrag Cvitanovic and modern transition state theory was explained to us by Holger Waalkens. Combining insight from classical dynamics with semiclassical techniques allows access to new quantum regimes for few electron atoms as demonstrated by Nark Nyul Choi and Joachim Burgdörfer. An overview over the state of the art of numerical and experimental techniques for analysing few-body quantum systems was given by Javier Madronero, Jose Luis Sanz-Vicario and Jan-Michael Rost as well as Lothar Schmidt, Hanns-Christoph Nägerl and Marcus Dahlstrom. Contributions by young scientists: Plenty of space was given to young scientists to present their work either in the form of posters (we had 16 poster contributions) or giving talks in the workshop itself. In fact, 5 talks were reserved for young scientist who are either still doing their PhD or are at an early post-doc stage. The newcomers had no problem to fill the allocated time of 45 min with interesting research ranging from applications of complex rotation methods (Celsus Bouri, Sören Roeren) to challenging dynamical features in 4D classical maps (Martin Richter) to chaos detection (Haris Skokos) and a new classication of equilibria in 3-body Coulomb problems (Florian Rupp).

Scientific results: The main benefit of this workshop was certainly that people got to know each other who would not have met otherwise. A hallmark of the workshop were the many discussions after talks and in the lunch and coffee breaks and there was a general interest to get to know more about each others problems and ideas. In particular, the planetary systems community showed great interest in the many open problems posed by considering few-body Coulomb systems and possible quantum implications.

Likewise, the results and deep insight in the dynamics of planetary systems impressed the 'quantum' community and the workshop may have helped that these techniques will cross disciplinary boundaries.

Correlated Phenomena in Low-Dimensional Systems, Seminar and Workshop
Scientific coordinators: J. S. Meyer, K. Shtengel, G. Refael

The LODI10 meeting hosted researchers in the field of strongly correlated low-dimensional quantum systems, broadly defined. Several focus area were represented: low-dimensional superconductivity, topological phases in two dimensions, phase transitions in cold atom systems, quantum magnetism, and dynamics of 1d systems. The variety of focus areas within the Low-Dimension header served to bring together key researchers (both theorists and experimentalists) in fields that are closely related, who traditionally attend more focused conferences and have few opportunities to interact. Several prominent researchers attended the meeting: Piet Brouwer (F.U. Berlin), Eugene Demler (Harvard U.), Konstantin Matveev (Argonne NL, USA), Alexander Mirlin (KIT Karlsruhe) and Felix von Oppen (F.U. Berlin), as well as Carlo Beenakker (Leiden U.) who gave the LODI10 colloquium, to name a few. The center of mass, so to speak, of our workshop consisted of a younger generation of participants: assistant and recently tenured professors such as B. Andrei Bernevig (Princeton), Victor Gurarie (CU Boulder), Israel Klich and Austen Lamacraft (U. Virginia), Karyn Le Hur (Yale), Olexei Motrunich (Caltech), and Anatoli Polkovnikov (Boston U.). We should also specifically mention a number of experimentalists, such as Alexey Bezryadin (UIUC), Marc Bockrath (UC Riverside), Michael Koehl (Cambridge), Jeanie Lau (UC Riverside), and Jens Martin (Harvard), who participated in our program and shared their recent experimental data. The workshop was also attended by four students and a large number of postdocs. Nearly all postdocs had an opportunity to present their work in a talk either during the seminar week (30 minutes), or during the workshop weeks (1 hour). Students and postdocs who did not give a talk instead presented a poster during two evenings in the seminar week. The meeting was characterized both by lively exchanges during the talks and question periods, as well as active informal discussions during breaks. We believe that several collaborations have been initiated, and more commonly, crucial information regarding new theoretical developments has been exchanged. Several completely new results have been presented: unique signatures of the entanglement spectrum of quantum Hall states (Bernevig), energy relaxation in Luttinger liquids (von Oppen, Rosenow), and exotic phase transition in 2d spinor condensates (Lamacraft). These are just a few examples of many talks presenting crucial progress in the field during the last two years. The young average age of the participants, the large number of prominent researchers that accepted our invitations, the relative breadth of topics discussed, as well as an excellent support infrastructure provided by the Max Planck Institute made the meeting an exciting venue.

Quo vadis Bose-Einstein condensation?, Summer School and Workshop
Scientific coordinators: M. Holthaus, A. Pelster

The conference Quo vadis Bose-Einstein condensation was designed to monitor the present state of ultra cold-atoms research 15 years after the groundbreaking first realizations of Bose-Einstein condensates from dilute atomic vapors, and to identify possible future lines of development. The event was structured into a two-weeks summer school primarily intended for Ph.D.-students and post docs working in this or a closely related area (August 2 - 13), and a subsequent workshop highlighting cutting-edge research (August 15 - 20). About 45 students and lecturers have participated in the summer school; about 115 researchers from 30 countries attended the workshop. The program of the summer school combined lecture series delivered by well-known senior scientists with others by younger ones who are presently at the verge of gaining international recognition. On the one hand, E. Zaremba (Kingston) and S. Stringari (Trento) gave extensive accounts of finite temperature effects in Bose-condensed gases and of the hydrodynamic theory of trapped quantum gases, respectively; on the other, lectures on semi classical techniques (O. Gat, Jerusalem), Quantum-Monte-Carlo methods (L. Pollet, Harvard), far-from-equilibrium effects (Th. Gasenzer, Heidelberg), the basics of quantum simulation (D. Weld, MIT), and on dipolar quantum gases (S. Ospelkaus, JILA/München) gave impressive evidence of the various new challenges arising from the high degree of control which can be exerted on ultra cold atoms in optical confinements. Additional lectures were given by the organizers on the Ginzburg-Landau theory for bosons in optical lattices, and on dynamical effects induced by external driving. Two seminars allowed the students to briefly introduce their own works. With three lectures per day the schedule of the school was somewhat dense, but still left ample time for discussions and exchange of opinions. The workshop program, consisting of 31 invited talks with a duration of 45 minutes each, an additional

mpi**pks** colloquium given by S. Ospelkaus on the subject of ultra cold polar molecules, and three poster sessions with more than 60 contributions, created a lively and fairly intense working atmosphere. Almost all of the invited speakers explicitly took up the quo vadis? theme, addressing future options and tasks. It became quite evident that there is not just one single dominant direction which the field is going to take, but rather there exist several strands which are likely to be explored simultaneously, stemming from recent results which were discussed in detail during the talks. Key topics included newly emerging possibilities for imaging single atoms in optical lattices, the exploration of nonstandard lattice geometries and of new trapping devices, the observation and explanation of dynamical effects involving solitons or deliberately perturbed condensates, and the specific behaviour of a unitary Fermi gas. With respect to the use of ultra cold atoms as quantum simulators, a major challenge now lies in the realization of even lower temperatures: The present record of 350 Picokelvin (held be W. Ketterles group at MIT) still is by a factor of 2 or 3 higher than the temperatures required for emulating, e.g., the XXZ-model with bosons in optical lattices. Each of the three evening poster sessions led to long and lively discussions among the participants. Last but not least, both the excursion to Meissen and the conference dinner provided welcome relaxation. The concept of this quo vadis meeting of bringing together leading experts from several subfields, and to include a significant fraction of Ph.D.-students, was quite well received; the benefits of strengthening the ties between the diverse directions of current cold-atoms research were emphasized several times. We are grateful to the Max Planck Institute for the Physics of Complex Systems for the generous support which has made this event possible.

Emergent Quantum States in Complex Correlated Matter, Focus Workshop
Scientific coordinators: E. Bascones, A. Chubukov, I. Eremin

The workshop took place at the mpi**pks** in Dresden from August 23 to August 27, 2010, and focused on a number of important open problems in the field of strongly correlated electronic systems. It brought together cutting edge researchers in the area of emergent quantum states in correlated electron systems. The scope of the workshop spanned a large number of topics including the physics of Fe-pnictides, cuprates, frustrated magnets, and topological insulators. In addition, the physics of the new states of matter such as nematic and/or metamagnetic phases, and the interplay between spin, charge, and orbital degree of freedom have also been addressed. During the workshop a number of phenomenological and microscopic theories of these systems have been discussed in informal but serious manner.

Over 75 participants from Europe, USA, Canada, and Japan took part in the meeting. The program included 40 oral presentations, both invited and contributed, as well as two poster sessions. The interchange of points of view between participants with distinct scientific interests gave rise to a highly stimulating atmosphere. During the workshop, a number of new and exciting results have been presented by, e.g., Louis Taillefer on "Fermi surface reconstruction and quantum criticality in cuprate superconductors", Subir Sachdev on the phase diagram of the high temperature superconductors, Kazuhiro Kuroki "Anion height as a key parameter in the superconductivity of pnictides and cuprates", Ashvin Vishwanath on "Topological insulators Correlation effects and topological field theories", Maurice Rice on "A kspace theory for the cuprate superconductors", Yong-Baek Kim on "Spin liquid and topological insulator in frustrated magnets". Many other, especially young, participants presented talks of high quality and showed new and interesting results. The talks, discussions, and posters at EQUAM 10 demonstrated that the field of correlated electrons is developing rapidly and has great prospects.

Two main results of the Workshop are (i) a focused exchange of ideas on the recent experimental and theoretical developments in the field of high-temperature superconductivity and the origin of non-Fermi-liquid physics in strongly correlated electron systems, and (ii) an involvement of young scientists in the discussion which has stimulated new research collaborations.

We would like to thank mpi**pks** for its hospitality and excellent infrastructure provided to the participants of the workshop. We also would like to thank the team of secretaries and, in particular, Mandy Lochar for their kind assistance and support of this meeting.

Complexity in Periodically Structured Systems, Workshop
Scientific coordinators: C. Denz, G.-L. Oppo

Aims of the workshop: Spontaneous generation of periodic and aperiodic structures in spatially extended nonlinear systems has been a centerpiece of research in complex systems for a long time. Nowadays,

however, technology and sophisticate experiments are capable to generate periodic structures over a wide range of spatial scales. The interaction of nonlinear media with the background structure leads to the formation of super-structures, localization of energy and controllable disorder. The purpose and focus of this workshop is to bring together theory, simulation and experiments of complex systems with periodic background structures. The workshop aims to bridge the gap between atomic and BEC scientists on one side and photonics researchers on the other.

Achievements: The blend of speakers and topics has allowed for a cross-fertilization between BEC with optical lattices and spatially modulated photonic devices. Although the experiments are (naturally) quite different, the theoretical and simulation approaches have many similarities and allow for insights and investigations of common complexity features. Among the highlights of the discussed topics are: localization, gap and discrete solitons, nano-photonic structures, ultracold gases, intracavity photonic crystals, optical realizations of Dirac equations, slow light, waveguide arrays, classical and quantum transport, defect modes, surface waves, random systems, Rabi oscillations, strongly correlated bosons, vortices, compactons, nanowires, and gap-waves.

Invited Speakers & Presenters): F. Abdullaev (Uzbekistan), R. Boyd (USA), C. Conti (Italy), C. Denz (Germany), C. Fort (Italy), D. Gomila (Spain), M. Johansson (Sweden), Y. Kivshar (Australia), V. Konotop (Portugal), Y. Kosevich (Russia), R. Livi (Italy), S. Longhi (Italy), B. Malomed (Israel), M. Molina (Chile), M. Oberthaler (Germany), K. Sengstock (Germany), D. Skryabin (UK), M. Stepic (Serbia), A. Sukhorukov (Australia), B. Theralle (Germany), W. Vos (Netherlands), and M. Weitz (Germany).

Format: The workshop has combined a number of innovative methods to foster deep insight into the field, vivid exchange of active topics of research, addressing of important questions and discussions of future aspects. Apart from the lectures of the distinguished invited speakers that have stimulated a substantial amount of discussion, we organized a round table introduced by experts, special discussion sessions to address special issues of importance, and two poster sessions. A session on research perspectives was based on short presentations of all invited speakers with material about future research directions. The roundtable and the perspective session were broadcasted via video-conferencing with major Centers for Complexity and Nonlinear Science (IFISC Mallorca (Spain), CeNoS Mnster, (Germany), INLN Nice (France) and ICSS Strathclyde (UK)). A highlight of stimulating discussion was the review of last day discussion of half an hour in the morning of the next lecture day. It revealed to be very important to discuss open questions from the day before, and resulted in a strong commitment of all participants to this discussion in the morning.

Participants and young researchers: The Workshop was attended by 40 participants from 14 different countries and around 20 attendants through video-conferencing. Poster sessions have been enhanced by short presentations to introduce the material of the posters. Discussion then continued at the specific posters including leading scientists. All young researchers in the PhD and early PostDoc phase have presented their work with outstanding quality for the content and presentation. The discussion sessions have been very successful leading to possible future international collaborations in specific research topics.

Further activities: A publication of the presentations of the workshop as a multiauthor book at Wiley has been suggested to the participants, and is on the way of being prepared.

Cold Rydberg Gases and Ultracold Plasmas, Seminar and Workshop
Scientific coordinators: C. S. Adams, T. Pohl, H. Sadeghpour

The CRYP10-Workshop was part of a joint Tandem-Workshop program between the **mpipks** and the Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP, Cambridge, USA), intended to complement and expand the scope of a preceding Rydberg Physics workshop held at ITAMP in 2009. This timing and backto- back format proved to be very successful and remarkably demonstrated the rapid progress in the field. The workshop brought together 89 scientist from 15 different countries, among them a large number of world-leading experts on cold Rydberg atom physics. The first week featured 38 invited talks given by a balanced mix of senior researchers as well as younger scientists. The program has covered the full spectrum of topical research in the field. Two sessions on Quantum Information presented theoretical schemes for applications of cold Rydberg atoms in quantum information science and reported on recent experimental breakthroughs in realizing first quantum phase gates with Rydberg atoms. This was complemented with a session on Rydberg Atom Traps, constituting one major prerequisite for future work on such applications. New developments towards Rydberg-interaction based

approaches to nonlinear quantum optics were presented in the Rydberg Optics session. Three sessions devoted to the physics of Ultracold Plasmas provided an experimental and theoretical discussion of collective phenomena arising from the electron as well as ion dynamics, the formation of a novel type of ultracold plasmas from cold molecular beams and the recombination of Rydberg atoms in magnetized plasmas, being of outmost importance for the production of antihydrogen atoms. Two sessions on Single Atom Control and Rydberg Spectroscopy gave an account of the impressive degree of control over internal and motional states, currently achievable. A wide range of questions concerning the dynamics of cold Rydberg gases, from few-body effects to many-body problems, has been addressed in three sessions on Rydberg Molecules and Many-body Dynamics. Over the past few years research on cold Rydberg systems has become increasingly diverse. The described workshop program fully reflected this interdisciplinarity, and aimed at merging these different aspects to possibly work out new ideas and directions for future research. Judging from the entirely positive feedback, this objective has been met successfully. Subsequently, a one-week Focus Workshop was devoted to tutorial talks as well as discussions among a smaller group of researchers, intended to explore common interests and follow up on outstanding topics that arose during the first week. The first four days featured two 90min introductory talks by senior researchers followed by presentations from postdocs and PhD students. The number of participants was deliberately held to a limited number, in order to provide a more informal environment. Indicated by the lively discussions during all talks, this concept was very well received by the younger scientists, as it gave the sometimes rare opportunity to clarify questions in greater detail. In addition to the last day, which was kept free, the relaxed schedule provided plenty of time for additional round table discussions and specific project work. Indeed, several collaborations between the participating groups were initiated during the second week, attesting to the general success of the Focus Workshop as well.

Novel Simulation Approaches to Soft Matter Systems, Workshop
Scientific coordinators: J. Gerda, C. Holm, K. Kremer

We would like to thank the mpi**pks** for giving us the possibility of organizing the NSASM workshop in September 2010 by providing the funding and a really professional organization and logistics for the event. In our opinion the workshop managed to fulfill all the objectives we have proposed: (a) International speakers of renowned prestige have shared their knowledge and experience on different topics in the area of simulation in Soft-Matter: adaptive resolution schemes, multiscaling approaches, coarse graining strategies for various soft matter systems, various techniques for mesoscale hydrodynamics, rare events, new sampling schemes, inverse Monte Carlo problems, among others, with a broad world-wide audience that includes graduated Ph.D. students, post docs and professors. This meeting has definitely strengthened the ties between groups over the world in the common objective of obtaining more efficient algorithms for Soft Matter simulations. At the same time people are now more aware of the advantages and caveats of the different cutting- edge methods. (b) From a pedagogical point of view, the different round tables with the speakers and the ample time allowed for discussions during the workshop has allowed to the most younger ones to be able to ask and interact with top-experienced researches without been ashamed, getting in this way the maximum benefit of the workshop because they have not just had a passive role but a very active one. (c) In what refers to helping to the diffusion of the scientific results and discussions done and presented during the workshop, we have organized the following procedures: c.1 - We have asked the speakers, and poster authors to send us their presented works so they are available at the workshop home-page for everyone interested in the field. Participants have answered very positively to this request, and we have managed to collect a large part of the contributions to the workshop. c.2 - An special issue (not just a simple proceedings) with the most remarkable works will be soon published in the Macromolecular Theory & Simulations journal (Wiley-VCH). We hope that these actions will help to spread and strengthen the outcomes of the workshop. Finally we would like to remark that several participants have communicated their opinion about this event. We were very pleased that all of them found the workshop very useful for them and we have got many requests from the participants to renew in a two or three-year period this sort of workshop. Once again we would like to thank the mpi**pks** for the superb opportunity that they have provided to the Soft-Matter community enabling us to meet and work together.

TCS-Program: Timing and Dynamics in Biological Systems, Workshop
Scientific coordinators: F. Naef, A. Oates, J. Stelling

Biological rhythms attracted theorists long before the molecular era of modern biology, and important contributions came from theoretical or geometrical reasoning. However, how complex and stochastic dynamics of underlying molecular and cellular processes translates into temporally ordered macroscopic behaviour is still poorly understood. The coupling of biological oscillators provides an additional layer of rich phenomenology. This workshop aimed to bring theorists and experimentalists together to learn about new conceptual and technical developments, to foster a common language, and to build bridges between experimental data on timing and theoretical explanations and methods. The workshop tried to identify principles of timing that are general biological strategies, regardless of the model system or the absolute timescale. Plenary lectures were given by three important participants spanning the experimental theoretical spectrum. Michael Hastings is an experimental biologist working on the circadian clock and presented the outstanding technical advances he and his colleagues have made in recording the dynamics of the system and probing the underlying genetics. Jean-Pierre Eckmann is a leading theorist in networks, presented his work on information flow in biological networks including for models of self-organizing neurons in culture. Joe Howard is a biophysicist whose lab uses theory and experiment to understand coupled mechanical oscillators such as molecular motors in cell behaviors such as flagella beating. Other prominent participants included John Tyson, whose work on the dynamical analysis of the cell cycle is pioneering; this time he present an insightful analysis of the stochastic molecular events during the yeast cell-cycle. There were a number of younger researchers whose presentations were stimulating and sparked discussions, notably the presentations of Ronny Straube, Luis Morelli, Ernesto Nicola, Achim Kramer. The poster sessions were particularly well attended by all of the participants, and this gave the younger researchers an extended time for discussion with the more experienced. We asked those participants who presented a short talk selected from the abstracts to also present a poster, and this contributed to the critical mass for discussion at the sessions. The general scientific outcome is perhaps best estimated by the exchange of information between experimentalists and theorists. Experimentalists were introduced to theoretical concepts and practicalities of modelling. Several reported that they intended to seriously engage in modelling their systems. Theorists were exposed to new biological systems and phenomena. One example of this was the presentation of newly discovered short period embryonic oscillators in neural and somitic tissue. It was felt that timing was an unusual topic for a conference, but one that merited serious further consideration in its own right.

The Dynamics of Nonlinear Stochastic Systems, Workshop
Scientific coordinators: I. Sokolov, U. Erdmann, B. Lindner

The Workshop brought together experts working on applications of stochastic processes in various fields ranging from neurobiology and cellular biophysics to classical statistical physics. We were happy to welcome internationally renown researchers such as Vadim S. Anishchenko, Hans-Albert Braun, Werner Ebeling, Jordi Garcia Ojalvo, Peter Hänggi, Jürgen Kurths, Jerzy Luczka , Alexander Neiman, Arkady Pikovsky, Francesc Sagués, Lutz Schimansky-Geier, Eckehard Schöll, and Peter Talkner. The meeting was devoted to Prof. Lutz Schimansky-Geier on the occasion of his 60th birthday. In a keynote lecture, Peter Hänggi gave an entertaining review of Prof. Schimansky-Geier's work and highlighted, in particular, his contributions to the study of noise-induced phenomena in bistable and excitable systems, of pattern formation, of active Brownian motion, and of synchronization in stochastic nonlinear systems. Several talks at this workshop dealt with the nonlinear stochastic dynamics of various biological systems. Jordi Garcia Ojalvo presented experimental and theoretical studies of noise-driven excitability in simple genetic circuits. The dynamics of intracellular calcium was discussed by Martin Falcke; response properties of simple model neurons (talk by Jan Freund) and of mechano-sensitive haircells (presented by Alexander Neiman) were further highlights. A number of speakers devoted their talks to a deeper discussion of noise-induced phenomena such as noise-induced transport in periodic structures (Jerzy Łuczka) or coherence resonance in systems with type I or type II excitability and delayed feedback (Eckehard Schöll). Somewhat related to the latter problem, Vadim Anishchenko discussed the more general theoretical problem of how the notion of self-sustained oscillations can be generalized in a stochastic setting. A more applied but likewise fascinating problem was addressed by Francesc Sagués; he presented both experimental and theoretical results on transport and diffusion of paramagnetic colloids, which are driven and controlled by magnetic fields. Arkady Pikovsky showed results on the stability of solitons on disordered nonlinear lattices, and Jürgen Kurths discussed novel approaches on network-analysis of

climate data. Finally, Peter Talkner demonstrated an interesting extension of the common first-passage calculus to nonstationary situations with time-dependent transition rates. In summary, the workshop gave a stimulating state-of-the-art review of various applications involving the dynamics of nonlinear stochastic systems.

Fluctuation-Induced Forces in Condensed Matter, Workshop
Scientific coordinators: S. Dietrich, A. Gambassi

Fluctuation-induced effective forces emerge whenever a fluctuating medium is perturbed by the presence of immersed objects. Examples of such forces can be found in rather different contexts ranging from physics and physical chemistry to biology. The main focus of the workshop was to explore and discuss analogies and differences among these various manifestations, with particular emphasis on unifying theoretical and experimental approaches. Bridging the gap among different communities interested in such forces and exploring possible applications were among the main motivations of the meeting. In order to achieve this goal the workshop gathered leading theoreticians (25) and experimentalists (12) who delivered talks on various topics as well as a number (9) of invited senior or junior scientists and several applicants (20). A comprehensive overview of the multifaceted nature of fluctuation-induced forces was presented in the Workshop Colloquium by Mehran Kardar, a renowned and leading contributor to the field. The topics which the experimental and theoretical talks dealt with include van-der-Waals and Casimir forces, the related phenomenon of wetting, solvation and critical Casimir forces, forces induced by fluctuations of interfaces or within fluctuating membranes, effective forces in confined equilibrium and non-equilibrium systems, depletion interactions in colloidal suspensions and their role in biological systems, dynamics of fluctuation-induced forces and their applications in soft matter systems, forces induced by charge fluctuations and related phenomena etc. Important issues such as the geometry-dependence of such forces and the non-trivial associated many body effects, as well as the emergence of universal asymptotic behaviors have also been discussed in the light of recent advances in theoretical and experimental techniques, some of which were reported during the workshop. Virtues and limitations of the various analytical, numerical, and experimental approaches for studying such forces in different contexts were also discussed in detail. There was a vigorous response of the scientific community for being part of this workshop. On site, the participation in the workshop was very active and enthusiastic, as demonstrated by the lively and collegial discussions which followed each talk or during the poster session as well as in the free time. The meeting provided also an occasion for establishing personal contacts in view of future collaborations and for strengthening existing ones. It was very pleasing to see a sizable group of young scientists taking part in the workshop. A lasting impact of this meeting is expected to be that the rather diverse sub disciplines of this research area develop a common language and a mutual understanding of the common basis of their research. In addition, the workshop showed that the intensive theoretical efforts attract now an increasing number of sophisticated and powerful experimental studies. This points towards very promising future developments.

Spike-Frequency Adaption in Neural Systems, Focus Workshop
Scientific coordinators: B. Lindner, J. Benda

The Workshop brought together experts working on the various aspects of spike-frequency adaptation (SFA). Among the participants were internationally renowned researchers, as, for example, Fabrizio Gabbiani, Simon Laughlin, David McAlpine, Alexander Neiman, and Klaus Obermayer. The program consisted of eight sessions each being devoted to a specific topic of adaptation, including specific sensory modalities (auditory, visual, and electrosensory systems), effects of particular adaptation properties (sub-vs. suprathreshold currents, stochastic adaptation, multiple adaptation time scales). Two lively poster sessions and one flash-talk session fostered the active involvement of younger researchers (PhD students and Postdocs) into the workshop program. Computational advantages and drawbacks of SFA in the multi-staged mammalian auditory system were addressed by David McAlpine. Kai Hildebrandt and Martin Nawrot discussed similar issues in comparably simple invertebrate systems - the auditory system of the grasshopper and the insect olfactory pathway. These talks illustrated the complex demands on adaptation processes in sensory systems. The talk by Maurice Chacron addressed experimentally the severe differences in the effect of sub- and suprathreshold adaptation currents on the information transfer of a neuron in the electrosensory line lobe of the weakly electric fish. Feedback and adaptation in the latter neurons were also the topic of John Lewis, who related their performance to behavioral

aspects (two-point discrimination task). Alexander Neiman presented experimental and modeling results from the passive electrosensory system of the paddle fish and discussed the contributions of adaptation and epithelial oscillations on the spike statistics of receptor neurons. Adaptation currents do not exist in isolation but may interact with each other yielding adaptation that can extend over many different time scales. This point was highlighted in the talks by Renaud Jolivet (discussing, in particular, adaptation induced by Na,K pump), Brian Lundstrom (introducing fractional differentiation as a mathematical description of adaptation with multiple time scales), and Richard Naud (presenting methods to extract adaptation models from data). The theoretical analysis of neural systems is far from trivial, especially in a stochastic setting in which the various neural noise sources are taken into account. How to deal with these kinds of models analytically or with efficient numerical schemes was discussed in the talks by Giancarlo La Camera, Eilif Muller, William Nesse, Magnus Richardson and Tilo Schwalger. In agreement with some of these theoretical results, Karin Fisch presented first experimental evidence for the stochasticity of an adaptation current due to the noise of the finite number of ion channels which mediate such a current. Fascinatingly diverse were the topics related to adaptation in the visual system. Fabrizio Gabbiani gave insights on the working of looming sensitive neurons in locust, which is subject to SFA. Rafael Kurtz showed experimental results supporting a positive role of SFA in feature extraction from natural stimuli (optic flow for a moving blow fly). The importance of SFA for plasticity of orientation maps in the visual cortex was addressed by Klaus Obermayer. In the same system, Lars Schwabe discussed theoretically the impact of SFA on contextual effect in strongly connected networks. In the beautiful final presentation of the workshop given by Simon Laughlin some of the undue simplifications regarding the role of adaptation were reviewed and a number of remaining questions were posed triggering a lively concluding discussion. In summary, the workshop on Spike-Frequency Adaptation in Neural Systems provided a broad review of this modern and dynamic research topic in neuroscience. Experimentalists got a comprehensive overview to the exhaustic theoretical studies of SFA in single neurons, whereas theoreticians learned that the investigation of functional aspects of SFA in sensory systems is still in its infancy and is heavily in need of guiding theories. Thus, the workshop triggered some unexpected insights, potentially resulting in new exciting research projects and collaborations.

Statistical Physics and Biology of Collective Motion, Workshop
Scientific coordinators: A. Deutsch, G. Thraulaz, T. Vicsek

Main focus: Research on collective motion had arrived at a stage where it deserved its own dedicated meeting, the first of its kind. It can be assumed that there must be a number of unifying principles connecting the spectacular manifestations of "moving together" in living systems, being one of the most relevant manifestations of collective behavior in nature, and that the corresponding big picture is likely to emerge from a meeting like the COLMOT workshop in Dresden. One important goal of the workshop was, which has indeed been achieved that the meeting was attended by the best theoreticians, experimentalists and modelers, physicists, biologists, and mathematicians working on the subject. In particular, I. Couzin, R. Goldstein, H. Chat, C Marchetti, S. Ramaswamy and D. Sumpter are worldwide acknowledged leading specialists in their field. Beyond new theoretical insights fascinating examples of collective motion were presented at the workshop including systems ranging from cultures of migrating tissue cells to ant colonies and flocks of birds.

Invited speakers: Ezequiel Albano (Universidad Nacional de La Plata, Argentina), Markus Bär (Physikalisch-Technische Bundesanstalt, Germany), Eshel Ben-Jacob (Tel Aviv University, Israel), Hugues Chat (CEA Saclay, France), Iain Couzin (Princeton University, USA), Andras Czirok (University of Kansas, USA & Eötvös University, Hungary), Jacques Gautrais (Universite Paul Sabatier, France), Irene Giardina (Universit Roma 'La Sapienza', Italy), Raymond E. Goldstein (University of Cambridge, UK), Carl-Philip Heisenberg (Max-Planck-Institut für Molekulare Zellbiologie und Genetik, Germany), Charlotte K. Hemelrijk (Rijksuniversiteit Groningen, The Netherlands), M. Cristina Marchetti (Syracuse University, USA), Mitsugu Matsushita (Chuo University, Japan), Fernando Peruani (Max-Planck-Institut für Physik komplexer Systeme, Germany), Sriram Ramaswamy (Indian Institute of Science, India), Lutz Schimansky-Geier (Humboldt-Universität zu Berlin, Germany), Christian Schmeiser (Universität Wien, Austria), David J.T. Sumpter (Uppsala University, Sweden)

Summary of contributions: The conference benefited significantly from the clear efforts of the speakers to make their topic of research understandable to the highly interdisciplinary audience. The majority of the invited speakers had a mathematical/physical background but keynote speakers included also biologists

(e.g. Carl-Philip Heisenberg, Charlotte K. Hemelrijk). Theoretical topics focused on "Evolution of collective behavior" (Ian Couzin), "The order of the flocking transition" (Sriram Ramaswamy), "Derivation and stability of hydrodynamic equations for self-propelled particles" (Eric Bertin), "Fluctuations in self-propelled particles" (L. Schimansky-Geier), "Collective decision making" (Larissa Conradt), "Collective behavior in large groups" (Francesco Ginelli), "Modelling active fluids" (M. Cristina Marchetti), "Structural properties of networks formed upon swarming" (Ezequiel Albano), "Minimal models for collective motion" (Hugues Chate), "Clustering, spatial patterns and information spreading in self-propelled particle systems" (Fernando Peruani). Biological examples of collective behavior covered bacteria (Markus Br, Mitsugu Matsushita, Masayasu Mimura), cell cultures (Andras Czirok, Inbal Hecht, Carl-Philip Heisenberg), bird flocks (Kunal Bhattacharya, Charlotte K. Hemelrijk, Irena Giardina), fish swarms (Jacques Gautrais, David Sumpter), ants (Andrea Perna), and locusts (Jan Haskovec).

The workshop featured a distinguished colloquium talk by Raymond E. Goldstein on "Microfluidics of cytoplasmic streaming" and a very interesting movie session (Collective Minds: The Intelligence of Swarms, ARTE, 2009 with contributions by Guy Theraulaz).

Contributions by young scientists: Plenty of space was given to young scientists to present their work either in the form of posters (we had 33 poster contributions) or giving talks in the workshop itself. In fact, 15 talks were reserved for young scientist who are either still doing their PhD or are at an early post-doc stage. The newcomers had no problem to fill the allocated time of 45 min with striking research ranging from theoretical problems as "The phase diagram of migrating cells" (Christophe Deroulers) and "Onset of collective motion due to escape and pursuit" (Pawel Romanczuk) to practical/biological considerations "From passive to active navigation: how a cell can find its way" (Inbal Hecht). The "newcomers" had a lot of chances to interact and they indeed did with the leaders of the field.

Scientific results: The main benefit of this workshop was certainly to discuss the latest scientific results and, furthermore, that people with different physical/mathematical and biological origins got to know each other who would not have met otherwise. Intense discussions after the talks and in the lunch and coffee breaks were a workshop hallmark and there was a general interest to get to know more about each others problems and ideas. A great opportunity to strengthen interactions was provided by the workshop dinner and the workshop excursion including a guided tour through the old town of Dresden with a life demonstration of the famous Silbermann organ at the Cathedral by cathedral organist Thomas Lennartz. In general, presentations of new theoretical results and recently gained deep insight into striking biological examples of collective behavior impressed the 'collective behaviour' community and the organizers are already a workshop follow-up within the next two years. Furthermore, a special issue on "Statistical Physics and Biology of Collective Motion: from Cells to Organisms" is under preparation. This will contain a selection of the Colmot workshop presentations. In conclusion, the COLMOT Workshop has the potential of launching a new field of activity and a series of related conferences.

Molecules under X-ray Pulses, Focus Workshop
Scientific coordinators: S. Techert, J. Ullrich, J.-M. Rost

MOLX09 and MOLX10 have been organized with members of the Max Planck Advanced Study Group at the Center of Free Electron Lasers in Hamburg (MP-ASG@CFEL) as 2.5 days brainstorming meetings. The idea for the first meeting in 2009 was to generate new ideas from the theoretical side for innovative experiments with the new light sources. Topics had a focus on smaller systems under advanced X-ray light.

To spark discussions and act as a think tanks a special format of the meeting was chosen: Each speaker was asked to prepare slides for about 20 minutes while 60 minutes were reserved for his entire contributions - questions and interruptions were encouraged at any time. To further stimulate discussions, the number of participants was restricted to about 30, grouped in a half circle around the blackboard and the screen with only to rows. Participants ranged from PhD students to experienced researchers.

Most participants expressed enthusiastic support for this format and had the feeling they took home much more than from ordinary workshops. This success motivated a second meeting in the same format (this time also the posters were present in the same room throughout the workshop). However, the topic was quite different and far more challenging: What are the opportunities for short X-ray pulses to elucidate the dynamics of large molecules and assemblies in an environment, typically a solution?

Atomic Physics 2010, Workshop
Scientific coordinators: K. Hornberger, J.-M. Rost

This year's atomic physics conference brought together experimentalists and theorists from various areas in atomic and molecular physics. While the first half of the meeting was devoted to timely topics of general interest, the second half focused on the quantum dynamics of molecular motion. We had more than 80 participants from mainly European countries, as well as a few visitors from overseas. The program consisted of 42 invited talks, each one with 15 minutes of allocated discussion time. On Tuesday and Thursday we had poster sessions where more than 40 posters were presented. The ensuing discussions continued well into the late evening.

The meeting started out on Monday with a variety of topics of current interest, thus highlighting the breadth of present day atomic and molecular physics. We heard talks on ultra-cold atoms in optical lattices, on evidence for electronic entanglement in the decay products of dimers, and on energy transfer on quantum aggregates to name a few. The institute-wide colloquium talk was presented by Reinhard Drner, who explained how two loosely bound atoms can be ionized with a single photon in the COLTRIMS experiment pioneered by their group. The topic of photo-ionization was taken up on Tuesday, with presentations on a ultra-fast ionization processes in systems ranging from helium nano-droplets and poly-atomic molecules to metal clusters. The general program was rounded out on Wednesday with talks on optimally controlled phase gates in optical lattices and time resolved spectroscopy amongst others.

The second half of the meeting began on Wednesday, focusing on the quantum dynamics of molecular motion. The presentations covered recent breakthroughs in manipulating the motion and the orientation of molecules, ranging from dimers to large biochemical species. Such tasks are required e.g. for studying state-resolved reactions and for demonstrating molecular entanglement, as a number of talks pointed out. The meeting brought experts from the fields of decelerating and trapping molecules in contact with specialists on molecular cooling and alignment, and with researchers working on the interferometry of molecular matter waves and on molecular collision and reaction studies. It became clear that these different communities share an interest in controlling molecular quantum dynamics, and the ensuing discussions led to an exchange of ideas between the various fields.

3.4 Externally Funded Research and Relations to Industry

3.4.1 DFG Projects

Individual Projects

- *Directed Transport within Hamiltonian Dynamics: From Theory to Cold Atoms Experiments*, *Dr. S. Flach*
- *Molecule Interferometry and Metrology*, *Dr. K. Hornberger*
- *Quantum Chaos in Optical Microcavities*, *Dr. M. Hentschel*

3.4.2 EU Funding

- European Research Network *European Network in Systems Biology*, *Prof. Dr. F. Jülicher*
- ESF-Research Networking *Arrays of quantum dots and Josephson junctions*, *Dr. S. Flach*
- ESF-Research Networking *Highly Frustrated Magnetism*, *Prof. R. Moessner*
- EU-FP7 *Systems Biology of Mitosis*, *Prof. F. Jülicher*
- EU-FP7 *Topological effects in matter with strong spin-orbit coupling*, *Prof. R. Moessner*
- EU *COST Action CM0702: Chemistry with Ultrashort Pulses and Free-Electron Lasers: Looking for Control Strategies Through Exact Computations*, *Dr. U. Saalmann*
- EU *Marie Curie Actions - Networks for Initial Training: COHERENCE Cooperativity in Highly Excited Rydberg Ensembles - Control and Entanglement*, *Dr. T. Pohl*
- EU *Marie Curie Actions - Networks for Initial Training: CORINF Correlated Multielectron Dynamics in Intense Light Fields*, *Prof. J.-M. Rost*

3.4.3 Additional External Funding

- VW-Stiftung,*Neutronal Control of Flight in Drosophila*, *M. Zapotocky*
- DAAD, *Dynamics of Molecules and Clusters* , *Prof. J.-M. Rost*
- VW, *Electron spin resonance of kondo ions in heavy fermion compounds: theory and experiment*, *Prof. I. Eremin*
- HFSP Fellowship, *Physical Characterization of cortical dynamics in establishment of polarity in the C. elegans zygote*, *Prof. F. Jülicher, Dr. J. Bois*
- VW-Stiftung *Towards molecular engines: cooperative coupling of molecular motors in engineered environments*, *Prof. F. Jülicher*

3.4.4 Scholarships

- *Justin Bois*, HFSP
- *Vardan Apinyan*, Klaus-Tschira-Stiftung
- *Jan Hayda*, Klaus-Tschira-Stiftung
- *Ondrej Marsalek*, Klaus-Tschira-Stiftung
- *Dorotta Kormonika*, Klaus-Tschira-Stiftung
- *Przemyslaw Swatek*, Klaus-Tschira-Stiftung
- *Jana Paterova*, Klaus-Tschira-Stiftung
- *Eva Pluharova*, Klaus-Tschira-Stiftung
- *Lukas Sistik*, Klaus-Tschira-Stiftung
- *Frank Uhlig*, Klaus-Tschira-Stiftung
- *Johannes Knolle*, Studienstiftung
- *Nenad Pavin*, VW Stiftung
- *Ernesto Nicola*, VW Stiftung
- *Elena Shchekinova*, VW Stiftung
- *Debashish Chaudhuri*, VW Stiftung

3.4.5 External Cofunding of Workshops and Seminars

2009

- International Focus Workshop (50% of budget)
  Physical Biology Circle Meeting
- Seminar and Workshop (9% of budget)
  Topological Order: From Quantum Hall Systems to Magnetic Materials
- Focus Workshop (29% of budget)
  Dynamics and Statistics in Weather and Climate
- International Workshop (17% of budget)
  Atomic Physics

2010

- International Workshop (53% of budget)
  Perspectives in Highly Frustrated Magnetism
- 3rd Asian-German Workshop (100% of budget)
  Optical Microactivities: Quantum Chaos in Open Systems Meets Optical Resonators

- Workshop (21% of budget)
  Particulate Matter: Does Dimensionality Matter?
- Workshop (12% of budget)
  Fluctuation-Induced Forces in Condensed Matter
- International Workshop (19% of budget)
  Complexity in Periodically Structured Systems

3.4.6 Patents and Licenses

- *Prof. Holger Kantz, Dr. Mario Ragwitz*
  Verfahren und Vorrichtung zur Vorhersage von Strömungsparametern turbulenter Medien, since 2002

3.5 Teaching and Education

3.5.1 Lectures at Universities

Wintersemester 08/09

Stochastic processes Prof. Dr. H. Kantz, TU Dresden

Sommersemester 09

Biophysik Dr. S. Grill, Universität Leipzig
Bifurcations and phase transitions Dr. T. Gross, TU Dresden
Biophysik III Theoretical Physics Prof. Dr. F. Jülicher, Dr. S. Grill, TU Dresden
Waveguide Theory Dr. S. Skupin, Universität Jena

Wintersemester 09/10

Atmospärische Vorhersagbarkeit Dr. J. Broecker, Universität Innsbruck
Fundamentals of Modern Optics Dr. S. Skupin, Universität Jena
Nonlinear Dynamics Prof. Dr. H. Kantz, TU Dresden

Sommersemester 10

Biophysik III Theoretical Physics Prof. Dr. F. Jülicher, Dr. S. Grill, TU Dresden
Group Theory for Physicists Dr. S. Kirchner, TU Dresden
Waveguide Theory Dr. S. Skupin, Universität Jena
Zeitabhängige Dichtefunktional-Theorie Dr. U. Saalmann, TU Dresden

Wintersemester 10/11

Dynamics and modelling of the atmosphere Prof. Dr. H. Kantz, Dr. J. Broecker, TU Dresden
Fundamentals of Modern Optics Dr. S. Skupin, Universität Jena
Symmetrien in der Physik Dr. S. Kirchner, TU Ilmenau
Theoretische Festkörperphysik Dr. S. Kirchner, TU Ilmenau

3.5.2 Degrees

Habilitations

- *Lindner, B.: Stochastic processes in biophysics.* Dresden, 2010

Dissertations

- *Ates, C.: Anregungsdynamik ultrakalter Rydberggase.* Dresden, 2009
- *Farhadifar, R.: Dynamics of the Cell Packing and Polar Order in Developing Epithelia.* Dresden, 2009
- *Fischer-Friedrich, E.: Pattern formation by the Min system of Escherichia coli.* Saarbrücken, 2009
- *Friedrich, B. M.: Chemotaxis of sperm cells.* Dresden, 2009
- *Laubrich, T.: Statistical analysis and stochastic modelling of atmospheric boundary layer wind.* Wuppertal, 2009
- *Niemann, M.: From Anomalous Deterministic Diffusion to the Continuous-Time Random Walk.* Wuppertal, 2009
- *Croy, A.: Zeitaufgelöster Elektronentransport in Quantendotsystemen.* Dresden, 2010
- *Dierkes, K.: Nonlinear amplification by active sensory hair bundles.* Dresden, 2010
- *Gnodtke, C.: Dynamik endlicher Vielteilchen-Systeme in intensiven Röntgenlaserpulsen.* Dresden, 2010
- *Handt, J.: Ab-Initio molecular dynamics studies of laser- and collision-induced processes in multi-electron diatomics, organic molecules and fullerenes.* Dresden, 2010
- *Le, D.-A.: Electrons in 5f systems.* Dresden, 2010
- *Mayer, M.: Mechanics of the C. elegans cell cortex.* Dresden, 2010
- *O'Brien, A.: Charge degrees of freedom on the kakome lattics.* Dresden, 2010
- *Sudan, J.: Uncovering the Physics of Frustrated Quantum Magnets using the Correlation Density Matrix Approach.* Lausanne, 2010
- *Willans, A.: Disorder in an exactly solvable quantum spin liquid.* Oxford, 2010

Diploma

- *Herde, D.: Analysis and modeling of highway traffic flow.* Dresden, 2009
- *Kämpgen, A.: Cooperation and the adverse reaction to social ties.* Würzburg, 2009
- *Khuc Trong, P.: Establishment of PAR Protein Polarity during Asymmetric Cell Divisions in Caenorhabditis Elegans.* Kaiserslautern 2009
- *Latzel, P.: Chemotactic Signaling in Sperm Cells.* Dresden, 2009
- *Meisel, C.: Self-organized criticality in adaptive neural networks.* Freiburg, 2009
- *Merkel, M.: Synaptic Short-Term Plasticity and Information Transmission.* Dresden, 2009
- *Zimmer, E.: Analyzing endocytosis using generalized modeling.* Dresden, 2009
- *Droste, F.: Analyzing self-organized critical dynamics on adaptive networks by moment expansions.* Berlin, 2010
- *Knolle, J.: Spin Density Waves in Iron Arsenide Superconductors .* Dresden, 2010
- *Kotik, D.: Ultrakalte Quantengase unter dem Einfluss raumzeitlich lokalisierter Störungen.* Dresden, 2010
- *Seiinger, M.: Opinion dynamics in social networks.* Würzburg, 2010

3.5.3 Appointments and Awards

Appointments

- *Dr. V. Averbukh* accepted the offer for a faculty position at the Imperial College London
- *Dr. B. Dora* accepted the offer for a staff position at the Department of Physics, Budapest University of Technology and Economics, Hungary
- *Prof. I. Eremin* accepted the offer for a Professorship at the Ruhr University Bochum
- *Prof. K. Hornberger* accepted the offer for a Professorship at the University of Duisburg
- *Prof. H. Kantz* accepted the offer for a Honorary Professorship at the University of Dresden
- *Prof. S. Kirchner* accepted the offer for a Adjunct Assistant Professorship at the Rice University (Houston, USA)
- *Prof. A. Läuchli* accepted the offer for a Professorship at the University Innsbruck
- *Prof. B. Lindner* accepted the offer for a Professorship at the Humboldt University Berlin

Awards

- *Fulde, P.:* Ehrenmitgliedschaft am Helmholtz-Zentrum Dresden-Rossendorf 2009
- *Fulde, P.:* Tsungming Tu Award - National Science Councils, Taiwan 2009
- *Grill, S.:* Arches Award 2009 (BMBF, Minerva Stiftung)
- *Fulde, P.:* Marian-Smoluchowski-Emil-Warburg-Preis (DPG) 2010
- *Grill, S.:* EMBO Young Investigator Award 2010
- *Pohl, T.:* Gustav Hertz Prize of the German Physical Society 2010
- *Grill, S.:* Paul Ehrlich- und Ludwig Darmstaedter-Nachwuchspreis 2011
- *Hentschel, M.:* Hertha-Sponer-Preis (DPG) 2011

3.6 Public Relations

3.6.1 Long Night of Sciences

On June 19, 2009 and June 18, 2010 the institute participated in the *Long Night of Sciences* jointly with the Technische Universität Dresden and many other research institutes in Dresden. We opened the doors for everyone interested in visiting our institute from 6pm to 12pm. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, a physics show, a physics quiz, a science cinema, poster presentations and a lot of different presentations of their work. The resonance was very good with about 2500 visitors counted at each event.

3.6.2 Science in the City Hall

Public lecture by Prof. Dr. Rüdiger Wehner (Universität Zürich), approx. 300 visitors

The **mpipks**, the Technische Universität Dresden and the City of Dresden are running a series of public lectures called *Wissenschaft im Rathaus*. The following lectures were delivered during the period 2009-2010:

- 23. April 2009, Prof. Dr. Keppler, *Vulkaneruptionen: Ursachen, Vorhersagen und Auswirkungen*, about 300 participants
- 16. September 2009, Prof. Dr. Schüth, *Elemente eines neuen Energiesystems - Antworten aus der Wissenschaft*, about 280 participants
- 27. Oktober 2009, Prof. Dr. Wikelski, *Vogelzug: Wie fliegt die Gans über den Mount Everest*, about 350 participants
- 14. April 2010, Prof. Dr. Herrmann, *Vom Winde verweht: Entstehung und Bewegung von Dünen*, about 250 participants
- 27. Oktober 2010, Prof. Dr. Helbing, *Was die soziale Welt zusammenhält.*, about 320 participants

3.6.3 mpipks School Contact Program

Public lecture with Prof. Beate Paulus (FU Berlin) for Junior Doctors

mpi**pks** offers lecturing at high schools on a permanent basis. High school teachers receive updated lists of available lecture topics offered. About fifteen lectures are given annually.

Our Institute participates in the program Junior Doctor with numerous events for students from 3rd class onwards. We provide each school year about 6 lectures for pupils in this context. The program Junior Doctor is a part of the joint project Netzwerk "Dresden - Stadt der Wissenschaft" of the scientific community of Dresden.

3.6.4 Dresden-Journalist in Residence Program

The mpi**pks** has obtained extra funding for a journalist-in-residence program for three years which started in 2008. Together with the other two Max Planck Institutes in Dresden we award a three-month *Journalist in Residence* fellowship to a science-oriented free-lance journalist each year. Representatives from all institutes and the Editor in Chief of *Dresdner Neueste Nachrichten* meet to select the fellow among the applicants. Successful fellows get detailed insights into of the scientific research and every-day life at the institutes, can form first-hand opinions on the particulars of the scientific life, and conduct independent investigations which help to achieve the long-term goals of the fellow.

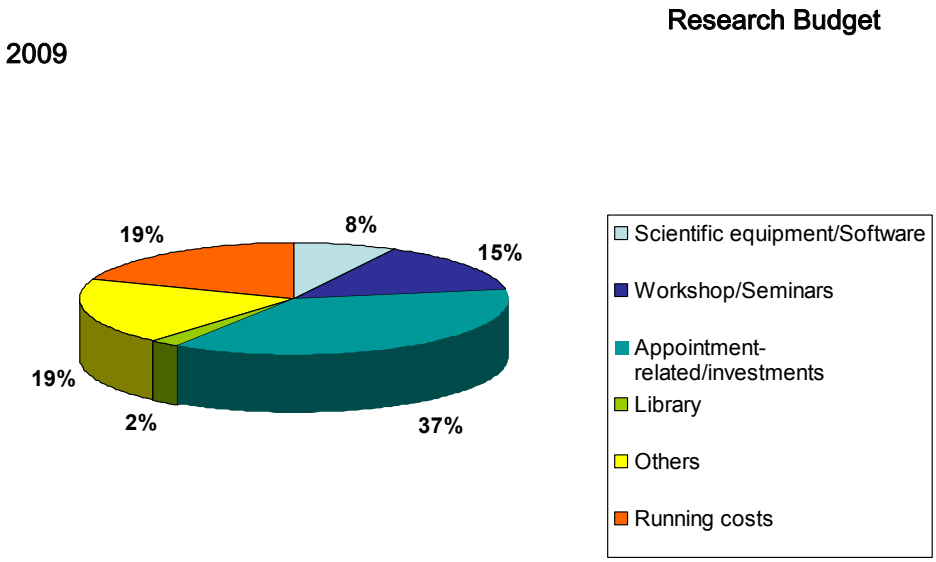
In return scientists at the institutes have a chance to interact closely and over an extended period with a journalist. They learn how their work can be communicated to the public and how to interact with journalists in the first place.

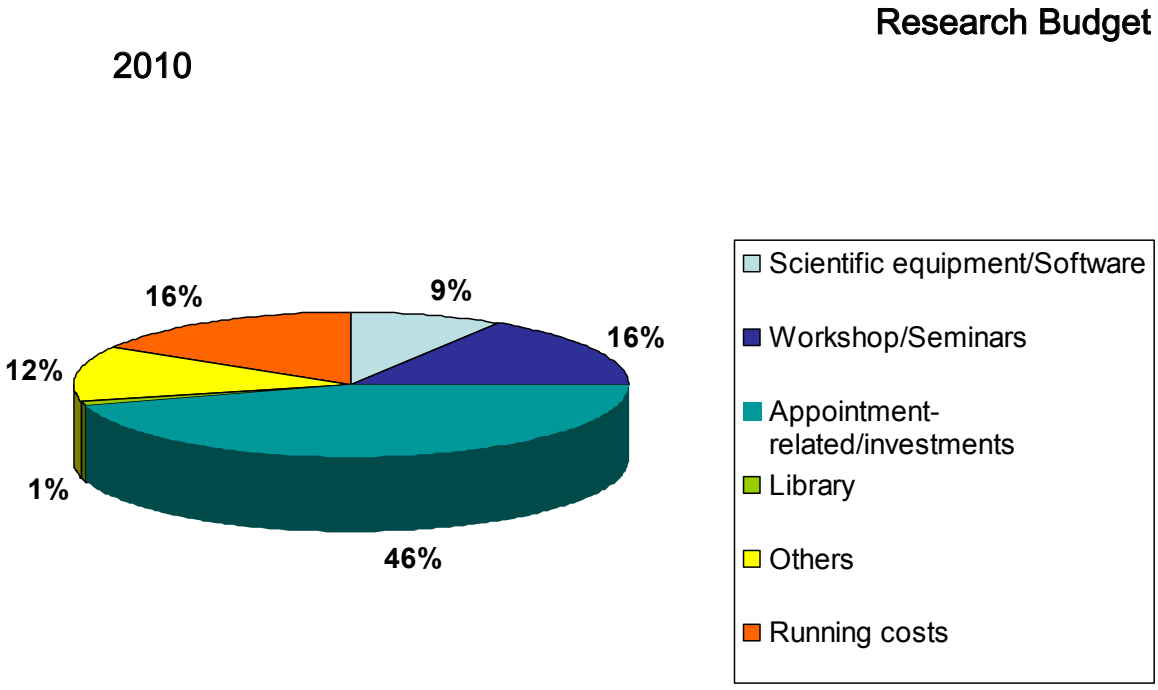
The *Dresden-Journalist in Residence* fellow 2009 was Mr. *M. Anhäuser*. He is a print journalist with ambitions towards new forms of publication, e.g., in the internet. Some of his studies resulted in online publications about the work in experimental laboratories, getting into the details of smart materials, and about the general agenda of public support for science.

Mrs. Sabine Sütterlin, a free lance science journalist, was the *Dresden-Journalist in Residence* fellow 2010. She focused on a science blog which report on different stages of her field studies in the three Max Planck Institutes in Dresden, where researchers explore complex systems, molecular processes in cells and solid state materials. Furthermore, she organized in cooperation with the TU Dresden a Science Slam with over 400 guests. Some of her science blogs can be found on http://www.scienceblogs.de/komplett-komplex/ .

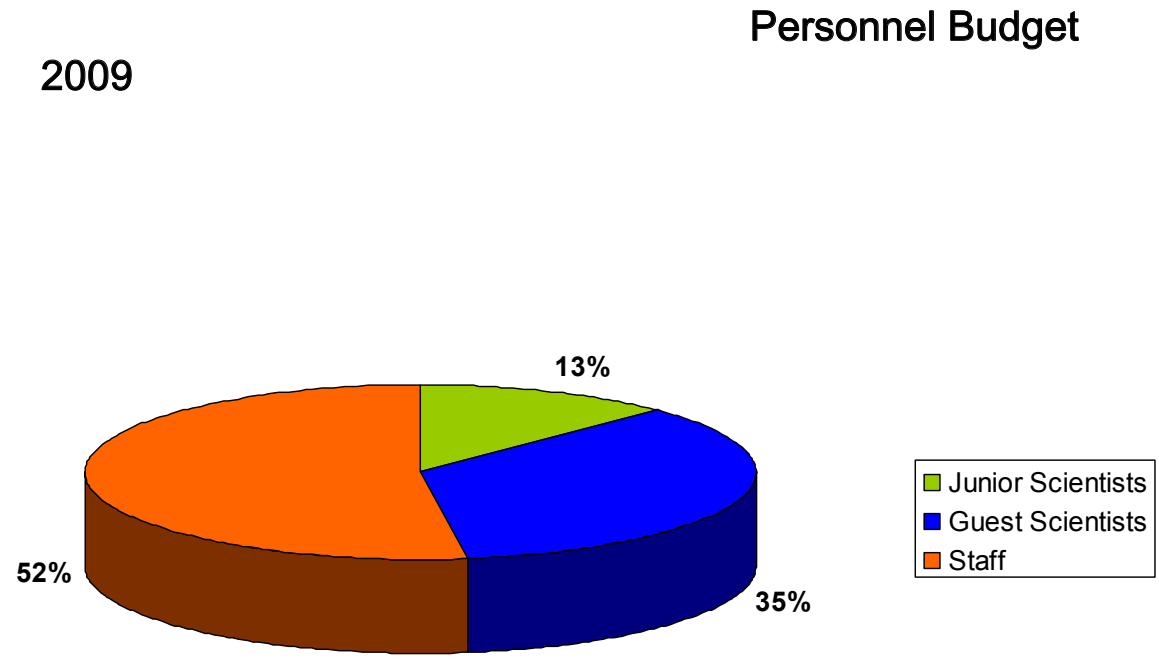
3.7 Budget of the Institute

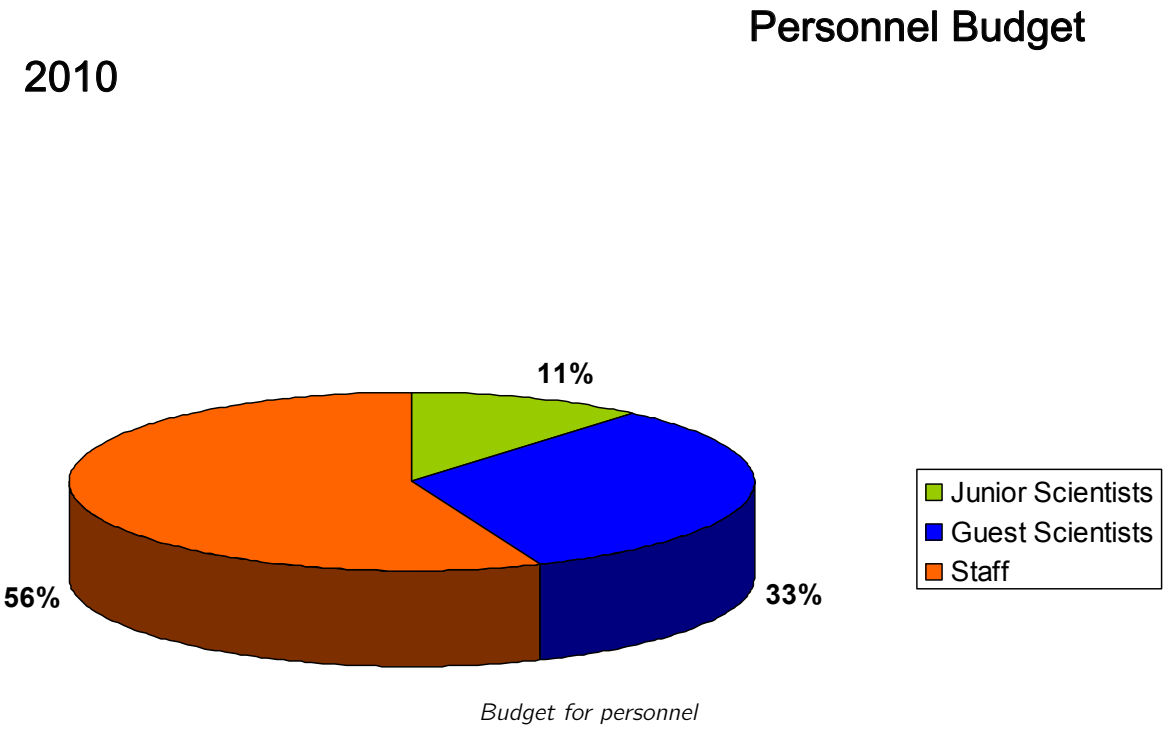
The following figures break the budget down according to costs for research and personnel, respectively for the two years 2009 and 2010.





Research budget during the past two years





Budget for personnel

3.8 Equipment and Premises

3.8.1 Computer Facilities

Computing facilities

Many of our scientists are doing extensive numerical calculations, this is why the main focus of our computer equipment in our institute is on the computational throughput, whereas the request for graphics is rather moderate on average. This implies that most offices are equipped with X-Terminals (Thin Clients) and only about one third of our scientists use workstations. Currently the institute hosts approximately 320 servers with a total of 3000 CPU cores on site and, new since 2010, a compute cluster located in Garching with an additional amount of 1500 CPU cores.

Our computers offer from one to 128 CPU cores and a maximum of 1 Terabyte of main memory and upto fifty Terabytes of local disk space. We use both Gigabit and Fast Ethernet as a local area network interconnect. By the end of 2010 about 95 % of the computing power available was based on Linux systems and 5 % on systems running HP-UX on Intel IA64 CPUs. In order to maximize the computational throughput in our computing cluster, we run a network queuing system which achieves an overall average utilization of more than 90 % of the available CPU time. Besides the Unix cluster there are about 20 PC's in our institute, running a Windows operating system, mainly for office applications. We also offer about 50 laptops for our scientists in order to provide them the possibility to continue their work while they are abroad. Furthermore we are running a Windows Terminalserver in our network in order to offer access to a Windows environment from every desktop. For numerical and analytical calculations there are various software packages available for our scientists. During the last years we noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C or Fortran.

For our short-term guests who participate in seminars and workshops we run a separate small cluster. We offer those guests the possibility to connect their own laptops to our network or use X-Terminals to access that cluster. The separation was introduced for both greater convenience and higher security.

We are connected to the Internet using a bandwidth of 100 MBit/s. Redundancy is achieved by automatic failover to the neighboring institute's internet connection (and vice versa for their connection) in case of problems with our primary Internet connection.

The computer department is run by five employees with their respective main tasks being Unix and networks, web and Windows, hardware and general user support. In addition to those five people we employ one trainee and one student of the Berufsakademie Dresden. Smaller to medium programming tasks are done by our staff and two students who are working part-time in the computer department. Large programming tasks have to be given to external companies.

Future

Linux will continue to be the main operating system for our number crunchers in the near future, at present running mainly on Intel Xeon based hardware. Other operating systems like HP UX will only play a minor role for some specialized applications. We expect that the near future will see graphics processing units (GPU) being used to some extent by our scientists, since they allow for considerable speedups for some of the codes used at our institute. Due to the fact that the number of cores per CPU is steadily increasing we expect that the total number of systems at our institute will only change moderately in the near future.

History

Since about 2002, we have developed a Linux based PC cluster that delivers several times the cpu performance of the previously used servers. The new extension building which was finished late 2005 added several new offices and also an excellent new server room for our computers. In 2007 we decided to complement our linux environment by computers based on Intel's IA64 (Itanium) architecture in order to support some applications that perform particularly well on this platform.

In 2010 a large parallel cluster was bought which is installed at the RZG in Garching and is run by the staff there. The following table shows the development of the computer resources on site at our institute in Dresden over time. The numbers do not include our parallel cluster located in Garching.

year	computers	main memory (GB)	disk space (TB)
1996	33	13	0.5
1998	66	60	2.0
2000	95	310	8
2002	162	590	22
2004	327	2600	90
2006	345	5500	190
2008	360	15000	510
2010	400	22000	560

3.8.2 Library

The library of the mpi**pks** has several tasks. Most evidently, it provides a large stock of scientific books and journals for the use of all members of mpi**pks**. For these it is accessible 24 hours per day and provides scientists with media and scientific information in many forms. Scientists from outside the institute can also use the library resources during regular office hours.

Currently, our library stock consists of about 4800 monographs, about 16.000 bound journal volumes and 55 scientific journal subscriptions in print and online, which can be found in the online catalogue.

The automatic check out system permits institute employees to borrow books at any time. A modern Bookeye machine and Xerox machine allows printing, scanning and copying.

Via the library homepage, our users have access to about 30.000 online journals and 40.000 e-books, as well as numerous literature and factual databases, online encyclopedias, dictionaries, the Virtual Max Planck library, the e-Doc Server, international catalogues etc.

As an additional service, the librarian has access to online document delivery systems. Books or references which are not available in the library or online can be obtained quickly, usually within 24-48 hours, through a simple web-based order form and manual processing by the librarian.

Finally, the library is also responsible for reporting the publication activities of mpi**pks**, e.g., for the yearbook of the Max Planck Society or the scientific report. Also the demands of Open Access are related to this activities: The old MPG data base e-Doc and the new data base PubMan which are institutional repositories with a wide variety of services are fed with mpi**pks** publications meta data by the librarian.

A library steering committee of scientists representing the departments and research groups of the mpi**pks** makes sure that the needs of scientists are optimally served by the library. In quarterly meetings decisions such as new journal subscriptions are made.

At present our library consists of two separate sections: the main library where one can find books and the newest journal issues and old journal volumes with 8 reading desks, and the reading room in the second floor. Copies of the most important books and journals for each group are available there for easy access. This room invites for discussions and is very well accepted.

Our library, as well as most others, is in a transition phase where the classical services continue to be indispensable while new media and new services attain increased relevance. It is foreseeable that print issues of journals might be fully replaced by online access in a few years, where the online access is guaranteed by the centralized MPDL. Instead, the library will be more and more involved in the dissemination of publications created by mpi**pks** members through Open Access and an institutional repository.

3.8.3 Guest Houses

To accommodate the large number of short and long term visitors, the Max Planck Institute for the Physics of Complex Systems provides three guest houses with different apartment types for up to 75

guests in total.

Panorama of the Guest Houses

Guest house 1 has 20 single and 5 double rooms (with two separate bedrooms). All of them have a bathroom, a terrace or a balcony, and are equipped with telephones. Our guests use two fully equipped communal kitchens and one meeting room, with a small library and a TV set.

Guest house 2 offers ten one-bedroom apartments with kitchen, for up to two persons, and three large two-bedroom apartments with a living room, bathroom and kitchen for up to three persons (e.g. families). One of these apartments is suited for handicapped persons. All apartments have a balcony or a terrace, and are equipped with TV connection ports and telephones. In the basement of guest house 2, two washing machines and a tumble dryer are available. They are accessible from all three guest houses.

Guest house 3 allows to accommodate guests in five large two-bedroom apartments with similar equipment as the ones in guest house 2. They are situated on the second floor. On the first floor, two similar apartments have been converted into offices and are used by short term guest scientists.

The guest house rooms and apartments are regularly cleaned and towels and bed linen exchanged. Cots and TV sets can be rented free of charge. In almost all apartments of the guest houses, WLAN is available.

Aditionally, the institute provides a special apartment for scientists with children. It can be used by institute members and workshop participants under certain conditions and upon consultation with the visitors program. Also child daycare can be arranged for workshop participants.

3.9 Committees

3.9.1 Scientific Advisory Board

According to the rules of the Max Planck Society the **mpipks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and chances for success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the biennial research report and prepares, usually every two years, a report for the President of the Max Planck Society on the research of the institute. Currently the Scientific Advisory Board has the following members:

Gugliandolo, L.
Professor Dr.

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et Hautes Energies
Université Pierre et Marie Curie - Paris VI
Toue 24, 5éme etage
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Frey, E.
Professor Dr.

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Valenti, M.-R.
Professor Dr.

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3.9.2 Board of Trustees

In accord with the rules of the Max Planck Society the mpi**pks** has formed a Board of Trustees. The board members discuss and consult the proposed budget, the annual report, and the budget of the last year of mpi**pks** together with the directors. The Board of Trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. The Board of Trustees had the following members during the period of this report (current membership is until December 31, 2012):

Birgel, D.

Chefredakteur
Dresdner Neueste Nachrichten
Hauptstraße 21, 01097 Dresden

Eschelbacher, H. C.
Dr.-Ing.

Ministerialdirigent a. D.
Hauptstraße 124, 53604 Bad Honnef

Kretschmer, M.
Dipl.-Ing., MdB

Mitglied des Deutschen Bundestages
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Dresdener Straße 6, 02826 Görlitz

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Rektor der
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Schmidt, F. Dr.-Ing.	Staatssekretär a.D. Birkenstraße 18, 01328 Dresden
Freifrau von Schorlemer, S. Dr.	Sächsische Staatsministerin für Wissenschaft und Kunst Wigardstraße 17, 01097 Dresden
Schroer, Ch. Professor, Dr.	Prodekan der Fachrichtung Physik Institut für Strukturphysik Technische Universität Dresden 01062 Dresden
Tschira, K. Dr. h.c.	Geschäftsführender Gesellschafter Klaus Tschira Stiftung gGmbH Schloss Wolfsbrunnenweg 33, 69118 Heidelberg
Weber, S.	Vorsitzender des Vorstandes Sächsische Aufbaubank Pirnaische Straße 9, 01069 Dresden

3.10 Members of the mpipks

(as of December 2010)

1. mpi**pks positions** — **43**
   - Scientific personnel — 17
     - *Scientific members* — *3*
     - *Research staff (including four junior research groups)* — *14*
   - Technical staff — 6
   - Administration and infrastructure staff — 20

2. **Externally funded research staff** — **3**

3. **PhD students** — **68**
   - PhD students with internal supervision — 50
     - *German PhD students* — *31*
     - *Foreign PhD students* — *19*
   - PhD students with external supervision[a] — 18
     - *PhD students with external funding* — *8*
     - *IMPRS PhD students with external supervision* — *10*

4. **Guest scientists** — **67**
   - German guest scientists — 18
   - Foreign guest scientists — 49

[a] Including 14 IMPRS members

The research positions are generally limited in time. Only *Prof. H. Kantz*, head of the group "Time Series Analysis" is employed on a permanent position. Furthermore, *Priv. Doz. Dr. S. Flach*, head of the Visitors and Workshop Program, is a permanent staff member of the scientific service.

Chapter 4

Publications

4.1 Light-Matter Interaction

2009

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4.2 Ultracold Matter

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